

ELECTRONIC SUPPLEMENTARY INFORMATION FOR

Oxidation of 4-substituted TEMPO derivatives reveals modifications at the 1- and 4-positions

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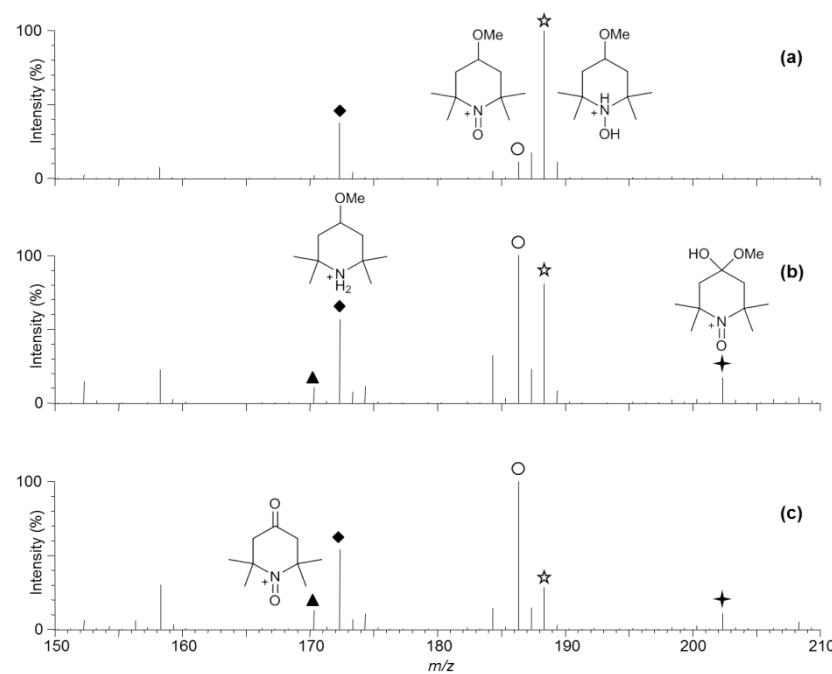


Figure S1: ESI-MS spectra of 4-methoxy-TEMPO **3** (in 4:1 CH₃CN:H₂O) at various stages of irradiation in the presence of TiO₂. Oxidation products TEMPONE **5**, piperidine **3H**, and the intermediate 4,4-didubstituted species are highlighted. (a) Pre-irradiation; (b) during irradiation; (c) post-irradiation.

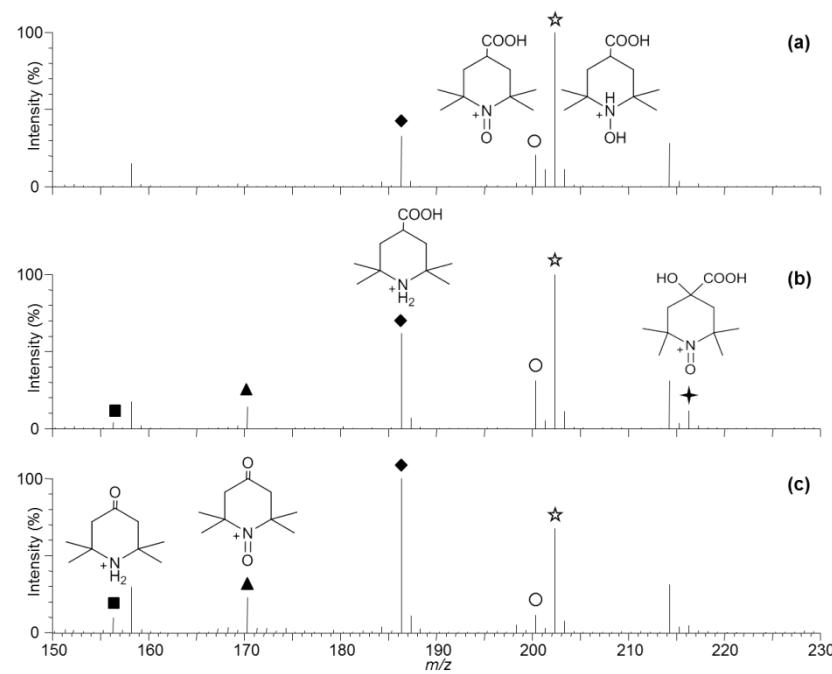


Figure S2: ESI-MS spectra of 4-carboxy-TEMPO **4** (in 4:1 CH₃CN:H₂O) at various stages of irradiation in the presence of TiO₂. Oxidation products TEMPONE **5**, piperidines **4H** and **5H**, and the intermediate 4,4-didubstituted species are highlighted. (a) Pre-irradiation; (b) during irradiation; (c) post-irradiation.

It is noted that not all TEMPONE related ions generated by ESI of pure TEMPONE (Table 2, main text) are observed in these spectra. This is not surprising given that the relative abundance of the different oxidation states will be influenced by the solution composition, which is different in each instance. What is unequivocal however is that the CID spectra of m/z 170 arising from oxidation of **3** and **4** are identical to the same ion obtained from ESI of pure TEMPONE.

Table S1 – Calculated thermodynamic parameters of C–H bond homolysis in selected HALS in gas phase and in water solution at 298.15 K and 333.15 K.

Bond	$\Delta S_{gas}^{298.15}$ J mol ⁻¹ K ⁻¹	$\Delta H_{gas}^{298.15}$ kJ mol ⁻¹	$\Delta G_{gas}^{298.15}$ kJ mol ⁻¹	$\Delta G_{gas}^{333.15}$ kJ mol ⁻¹	$\Delta G_{solv}^{298.15}$ kJ mol ⁻¹
(1-H ⁴)·	124.236	412.443	375.402	376.230	393.076
(1-H ³)·	129.017	412.144	373.677	374.515	392.607
(1-CH ₂ H)·	120.902	422.488	386.441	387.260	405.203
(2-H ⁴)·	120.843	392.117	356.087	356.772	375.226
(2-H ³)·	129.764	414.047	375.357	376.160	396.463
(2-CH ₂ H)·	121.563	427.539	391.295	392.156	410.015
(3-H ⁴)·	117.854	396.176	361.038	361.726	381.767
(3-H ³)·	124.712	414.936	377.753	378.593	398.858
(3-CH ₂ H)·	120.845	422.034	386.004	386.819	404.390
(4-H ⁴)·	115.724	378.009	343.506	344.204	365.448
(4-H ³)·	125.765	415.467	377.970	378.820	398.072
(4-CH ₂ H)·	122.126	427.737	391.325	392.193	410.213
(5-H ³)·	118.523	377.886	342.548	343.265	361.018
(5-CH ₂ H)·	123.961	427.978	391.019	391.892	410.326

Table S2 – Calculated kinetic and thermodynamic parameters of hydrogen abstraction by HO[•] from **1–5** in gas phase and in water solution at 298.15 K.

	Reaction Scheme	$\Delta S_{gas}^{\ddagger}$ J mol ⁻¹ K ⁻¹	$\Delta H_{gas}^{\ddagger}$ kJ mol ⁻¹	$\Delta G_{gas}^{\ddagger}$ kJ mol ⁻¹	$\Delta G_{solv}^{\ddagger}$ kJ mol ⁻¹	ΔS_{gas} , J mol ⁻¹ K ⁻¹	ΔH_{gas} , kJ mol ⁻¹	ΔG_{gas} , kJ mol ⁻¹	ΔG_{solv} , kJ mol ⁻¹
1.4		-131.894	-0.947	37.367	42.994	20.137	45.716	-87.212	-84.200
1.3		-124.997	-2.560	33.597	41.938	24.917	45.417	-88.937	-84.669
1.2		-140.373	-10.975	24.934	31.426	16.803	55.761	-76.173	-72.073
2.4 ^a		-134.819	66.567	105.499	103.264	15.674	32.585	-106.173	-109.186
2.3		-138.934	-9.798	30.702	36.203	25.261	54.496	-87.121	-88.167

2.2		-140.483	-9.869	25.963	24.131	17.060	67.988	-71.184	-74.614
3.4		-128.838	0.370	38.465	43.050	15.420	46.228	-102.403	-103.826
3.3		-130.106	-10.243	25.040	29.716	21.412	65.178	-85.239	-86.285
4.4		-140.871	-5.699	35.321	37.770	12.505	32.052	-119.692	-119.902
4.3		-140.335	-13.947	23.921	27.457	21.639	69.716	-84.753	-86.803
5.3		-134.735	-7.196	27.364	32.037	14.121	17.604	-120.043	-123.725

^a For reaction 2.4, standard transition state optimisations for H⁴ abstraction lead to geometries in which the attacking •OH instead interacts with the covalently bound 4-OH substituent. A series of constrained optimisations were performed. While the final “transition structure” contains a single imaginary frequency consistent with H⁴ abstraction, we expect that the resulting structure is not fully optimised and the reported barrier is thus likely to be significantly overestimated.

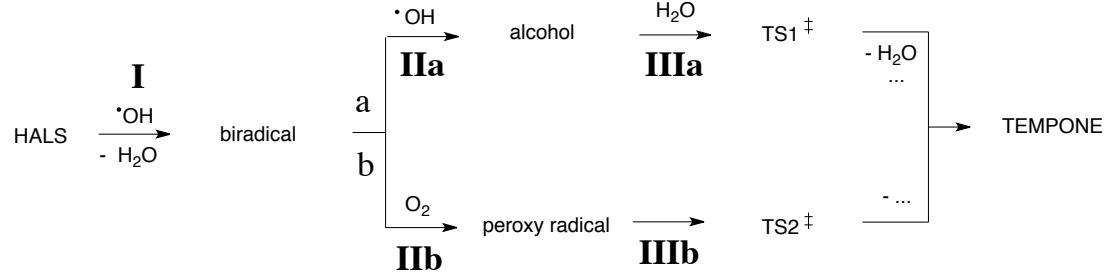
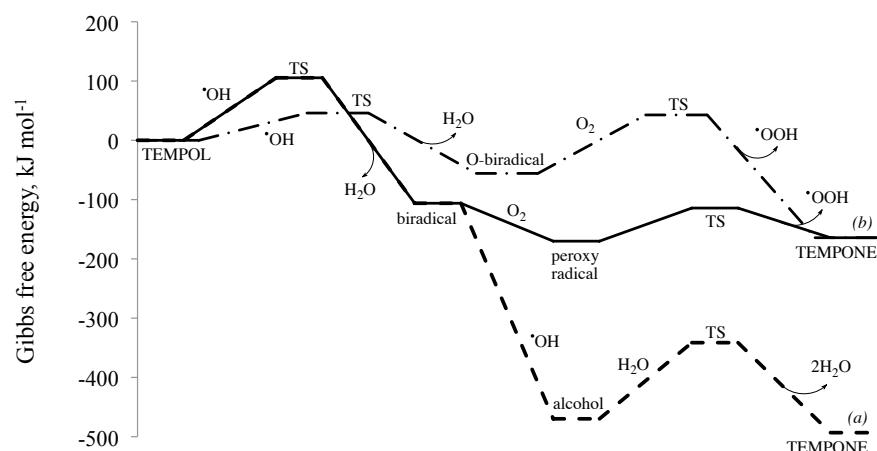


Table S3 – Calculated kinetic and thermodynamic parameters of reactions I–IIIb for selected HALS in gas phase and in water solution at 298.15 K.

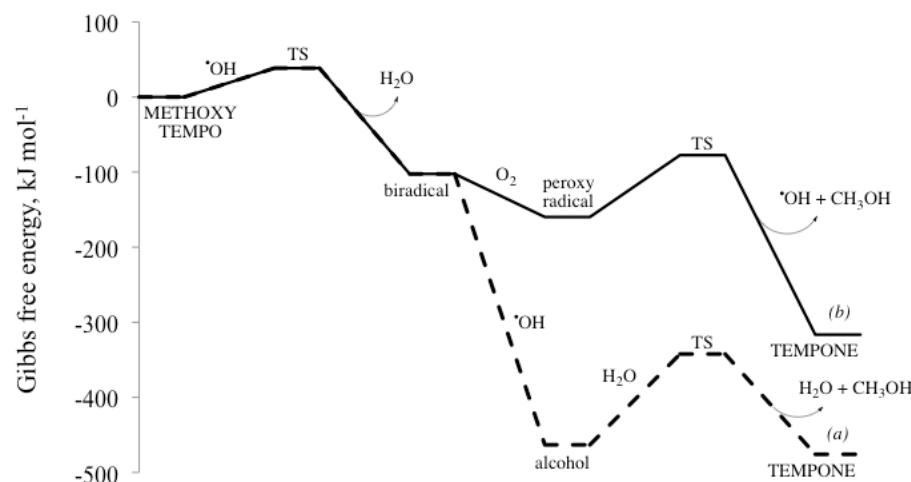
	$\Delta S_{gas}^{\ddagger}$ J mol ⁻¹ K ⁻¹	$\Delta H_{gas}^{\ddagger}$ kJ mol ⁻¹	$\Delta G_{gas}^{\ddagger}$ kJ mol ⁻¹	$\Delta G_{solv}^{\ddagger}$ kJ mol ⁻¹	ΔS_{gas} , J mol ⁻¹ K ⁻¹	ΔH_{gas} , kJ mol ⁻¹	ΔG_{gas} , kJ mol ⁻¹	ΔG_{solv} , kJ mol ⁻¹
TEMPOL 2								
I	-	-	-	-	15.674	-101.500	-106.173	-109.186
IIa	-	-	-	-	-170.412	-414.476	-363.667	-368.874
IIIa	-155.954	91.181	128.468	135.492	173.679	28.418	-23.364	-19.037
IIb	-	-	-	-	-171.107	-114.977	-63.962	-71.302
IIIb	1.312	58.049	55.868	60.458	187.644	61.769	5.823	-2.945
Alternative pathway to TEMPONE 5 exclusive to TEMPOL 2 via alkoxy radical (Scheme 5)								
1	-132.527	9.381	46.031	54.885	10.072	-52.806	-55.809	-54.972
2	-137.701	79.959	98.642	99.728	22.138	-101.902	-108.503	-128.460
4-methoxy-TEMPO 3								
I	-	-	-	-	15.420	-97.806	-102.403	-103.826
IIa	-	-	-	-	-172.873	-412.360	-360.818	-368.367
IIIa	-157.043	83.516	120.944	129.212	191.522	44.441	-12.661	-13.229
IIb	-	-	-	-	-172.519	-108.845	-57.408	-69.769
IIIb	-22.058	90.215	82.427	83.312	323.911	-60.094	-156.668	-166.315
4-carboxy-TEMPO 4								
I	-	-	-	-	12.505	-115.964	-119.692	-119.902
IIa	-	-	-	-	-161.494	-363.936	-315.787	-320.533
IIIa	-142.570	252.197	281.953	292.510	180.502	64.732	10.915	10.975
IIb	-	-	-	-	-171.275	-55.530	-4.464	-16.783
IIIb	-17.010	80.704	76.935	82.399	307.727	-151.882	-243.631	-234.725

Figure S3: Normalised energy profiles for H⁴ abstraction and subsequent TEMPONE formation *via* addition of either O₂ or HO· to (a) TEMPOL **2** (including alternative pathway *via* alkoxy biradical) (b) 4-methoxy-TEMPO **3** (c) 4-carboxy-TEMPO **4**.

a)



b)



c)

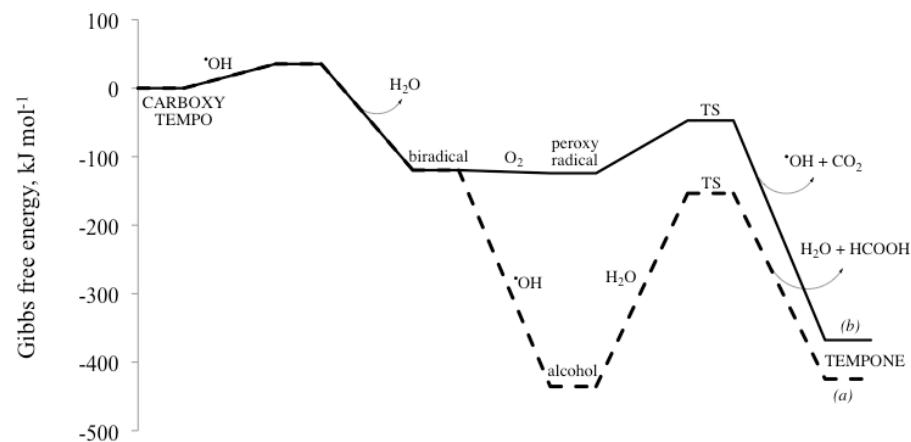


Table S4 – Contributions to the gas and solution-phase free energies of species at 298.15 K.

Species	E_{gas}^0 (Hartrees)	T_c (Hartrees)	ZPVE (Hartrees)	S_{gas} (J mol K ⁻¹)	G_{gas} (Hartrees)	ΔG_{solv} (water) (kJ mol ⁻¹)
$\cdot\text{H}$	-0.50012	0.00236	0	114.606	-0.51078	10.21
1	-483.12855	0.01292	0.25839	436.214	-482.90677	-2.55
(1-H⁴)·	-482.45776	0.01328	0.24368	445.844	-482.25143	-3.01
(1-H³)·	-482.45795	0.01336	0.24368	450.624	-482.25209	-1.76
(1-CH₂H)·	-482.45393	0.01312	0.24384	442.510	-482.24722	-1.92
2	-558.27898	0.01416	0.26240	459.829	-558.05464	-10.13
(2-H⁴)·	-557.61689	0.01423	0.24893	466.066	-557.40666	-9.12
(2-H³)·	-557.60787	0.01451	0.24798	474.987	-557.39932	-7.15
(2-CH₂H)·	-557.60229	0.01444	0.24761	466.785	-557.39325	-9.54
3	-597.52536	0.01570	0.29016	494.397	-597.27565	-1.34
(3-H⁴)·	-596.86200	0.01570	0.27704	497.644	-596.62577	1.26
(3-H³)·	-596.85373	0.01606	0.27555	504.503	-596.61941	1.63
(3-CH₂H)·	-596.85092	0.01588	0.27562	500.636	-596.61626	-1.09
4	-671.51277	0.01592	0.27278	506.930	-671.28164	-9.87
(4-H⁴)·	-670.85626	0.01588	0.25963	508.047	-670.63844	-6.07
(4-H³)·	-670.84088	0.01631	0.25809	518.089	-670.62532	-7.91
(4-CH₂H)·	-670.83595	0.01622	0.25793	514.450	-670.62023	-9.12

5	-557.06618	0.01376	0.23912	457.755	-556.86528	-5.98
(5 -H ³)·	-556.40947	0.01379	0.22565	461.671	-556.22245	-5.65
(5 -CH ₂ H)·	-556.38919	0.01409	0.22415	467.109	-556.20399	-4.81
·OH	-75.66288	0.00330	0.00814	178.292	-75.67168	-7.36
H ₂ O	-76.36340	0.00378	0.02076	188.850	-76.36031	-11.38
TS(1 -H ⁴)·	-558.78836	0.01505	0.26421	482.663	-558.56391	-3.85
TS(1 -H ³)·	-558.78897	0.01526	0.26400	489.560	-558.56530	-1.13
TS(1 -CH ₂ H)·	-558.79211	0.01463	0.26457	474.184	-558.56676	-2.51
TS(2 -H ⁴)·	-633.91226	0.01622	0.26747	503.756	-633.68578	-11.80
TS(2 -H ³)·	-633.94284	0.01595	0.26923	499.641	-633.71440	-4.06
TS(2 -CH ₂ H)·	-633.94209	0.01590	0.26850	498.092	-633.71425	-11.55
TS(3 -H ⁴)·	-673.18575	0.01792	0.29702	543.103	-672.93248	3.81
TS(3 -H ³)·	-673.18870	0.01786	0.29599	541.835	-672.93638	4.02
TS(4 -H ⁴)·	-747.17458	0.01792	0.27897	544.428	-746.93952	-6.86
TS(4 -H ³)·	-747.17751	0.01777	0.27890	544.964	-746.94272	-5.65
TS(5 -H ³)·	-632.72803	0.01577	0.24475	501.665	-632.52448	-0.46
Biradical (2)	-557.61691	0.01421	0.24898	465.399	-557.40657	-9.12
Alcohol (2)	-633.44458	0.01501	0.26655	473.279	-633.21677	-13.77
TSa-(2)	-709.76879	0.01653	0.28510	506.175	-709.52464	-10.08
O ₂	-150.18748	0.00331	0.00371	205.057	-150.20375	3.60

Peroxyl radical (2)	-707.85175	0.01594	0.25783	499.348	-707.63469	-4.94
TSb-(2)	-707.82394	0.01582	0.25225	500.660	-707.61273	-0.33
TS(2-H ^{OH})·	-633.93567	0.01609	0.26922	506.048	-633.70782	-0.67
(2-H ^{OH})·	-557.59750	0.01391	0.24842	459.798	-557.38739	-5.27
TS (2-H ^{OH} + O ₂)·	-707.75057	0.01691	0.24848	527.153	-707.54505	7.61
HOO·	-150.75868	0.00380	0.01376	228.884	-150.76711	-15.65
Biradical (3)	-596.86200	0.01573	0.27694	498.511	-596.62594	1.26
Alcohol (3)	-672.68877	0.01652	0.29442	503.929	-672.43506	-5.73
TSa-(3)	-749.01607	0.01812	0.31306	535.736	-748.74573	-0.71
CH ₃ OH	-115.60228	0.00424	0.05048	237.344	-115.57452	-8.24
Peroxyl radical (3)	-747.09451	0.01755	0.28570	531.048	-746.85156	0.42
TSb-(3)	-747.05375	0.01647	0.28038	508.991	-746.81470	1.38
CH ₂ O	-114.37950	0.00381	0.02632	218.560	-114.37419	0.63
Biradical (4)	-670.85629	0.01591	0.25955	508.954	-670.63862	-6.07
Alcohol (4)	-746.66451	0.01695	0.27668	525.752	-746.43058	-10.25
TSa-(4)	-822.92580	0.01938	0.29273	572.032	-822.67865	-3.01
HCOOH	-189.57025	0.00410	0.03326	248.146	-189.56107	-12.13
Peroxyl radical (4)	-821.06829	0.01784	0.26801	542.736	-820.84408	-6.86
TSb-(4)	-821.03152	0.01712	0.26270	525.726	-820.81141	-1.17
CO ₂	-188.39048	0.00359	0.01137	214.063	-188.39983	-0.46

APPENDIX 1: Geometries of the species in this study

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3-LYP/6-31G(d) level.

•H

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(1 - H⁴) •

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6,-0.2761612\\PG=CS [SG(C1H1N1O1),X(C8H16)]\\@

(1 - H³) •

1\1\GINC-V1252\FOpt\UB3LYP\Gen\C9H17N1O1(3)\DMM574\17-Nov-2010\0\\#B3LYP/gen 6D OPT IOP(2/17=4) Freq=noramman maxdisk=268435456\\tempo3rad.freq\\0,3\c,-0.0353188841,0.0529783725,-0.0633649752\n,0.1166192673,0.2737230833,1.4114865239\c,1.3792678433,0.0401323366,2.1906253544\c,2.2939783617,-0.9120623953,1.4787759492\c,2.2571116551,-1.1058744235,0.001708685\c,0.8046802378,-1.1652919681,-0.4906972183\o,-0.7339554136,1.0645326589,1.9601261179\c,0.9649124141,-0.5402512901,3.5603962441\c,2.079214445,1.4109439578,2.4112760114\c,0.3860259649,1.3370505036,-0.8086085107\c,-1.5217450103,-0.2300403806,-0.3340833204\h,2.7854860687,-2.0270054973,-0.2740499135\h,0.4653626413,-1.5058230973,3.4332517422\h,1.8519977096,-0.6883597884,4.1857454567\h,0.2811918159,0.1452431999,4.0660085107\h,2.9431783625,1.2878787128,3.0730161201\h,2.4314563307,1.8360795709,1.4661589243\h,1.3735654512,2.1097012458,2.8697683483\h,-0.1721721659,2.1889180872,-0.4095306302\h,1.4548078112,1.5472805319,-0.7015734746\h,0.1656087098,1.2444982021,-1.8783311932\h,-2.139267874,0.6182038581,-0.0343876804\h,-1.6692441993,-0.420724774,-1.4029165025\h,-1.8554058517,-1.1110765118,0.2242449536\h,0.334573644,-2.0724581615,-0.0905686851\h,0.7709252741,-1.2418574298,-1.5845325341\h,3.1321787132,-1.29390332,2.0562759494\h,2.792778967,-0.292958441,-0.5236064159\\Version=EM64L-G09RevA.02\\State=3-A'\\HF=-483.0541429\\S2=2.007857\\S2-1=0.\\SA=2.00038\\RMSD=9.940e-09\\RMSF=4.673e-06\\Dipole=0.8327709,-0.4989699,-0.5797424\\Quadrupole=-1.0297196,-0.5011343,1.5308539,1.2747555,2.4943082,-0.7775798\\PG=C01 [X(C9H17N1O1)]\\@

(1 - CH₂H) •

1\1\GINC-V1260\FOpt\UB3LYP\Gen\C9H17N1O1(3)\DMM574\17-Nov-2010\0\\#B3LYP/gen 6D OPT IOP(2/17=4) Freq=noramman maxdisk=268435456\\tempoCH3rad.freq\\0,3\c,-0.0415184498,-0.0355940161,-0.0196230424\n,-0.0447975859,

-0.0802129137,1.4834865197\c,1.2139658363,0.0207219845,2.2991255402\c,
2.3388996212,-0.8033036628,1.6363730769\c,2.4839196091,-0.5104313449,0
.1428588878\c,1.1648993917,-0.8283697703,-0.5652388347\o,-1.1150296164
,0.3476598322,2.0524518072\c,0.8953484376,-0.5709449579,3.6947491339\c
,1.6014746803,1.4669786293,2.4544054123\c,-0.0068409594,1.4385023657,-
0.4742015022\c,-1.3469495134,-0.6900126839,-0.4968157554\h,3.29099784,
-1.1186118719,-0.28357032\h,0.5771188458,-1.6155891406,3.5981794934\h,
1.7926687369,-0.5337921476,4.3210982963\h,0.0958798052,-0.0075876057,4
.176631566\h,2.6096110471,1.7222612101,2.7688741566\h,0.8204720567,2.2
106295425,2.5715622315\h,-0.8412284092,1.9810423796,-0.0202396808\h,0.
9229173724,1.9369559891,-0.1836895824\h,-0.1028208524,1.4976593889,-1.
5644979977\h,-2.2143679138,-0.141920243,-0.1250561078\h,-1.3731578672,
-0.699992767,-1.5921975272\h,-1.4152767884,-1.7232998496,-0.1400627706
\h,0.9587394134,-1.9019771062,-0.4542381018\h,1.240936908,-0.634099439
4,-1.6421966004\h,3.2738360153,-0.599443884,2.172575756\h,2.1213394127
,-1.8710637557,1.7742605279\h,2.7657937281,0.5389102809,-0.0101990832\
\Version=EM64L-G09RevA.02\State=3-A\HF=-483.0477151\S2=2.007618\S2-1=0
.S2A=2.000035\RMSD=4.515e-09\RMSF=2.508e-06\Dipole=0.9838431,-0.19471
83,-0.4538484\Quadrupole=-2.0304821,0.8062471,1.224235,0.3043843,2.912
048,-0.0275124\PG=C01 [X(C9H17N1O1)]\\@

2 (TEMPOL)

1\1\GINC-V1259\FOpt\UB3LYP\Gen\C9H18N1O2(2)\GXG501\22-Feb-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram an maxdisk=268
435456\\hals2.freq\\0,2\c,-0.0233830139,0.0228338986,-0.0106375593\N,-
0.0046684766,0.0035575777,1.4920519475\c,1.2414449718,-0.0059518382,2.
3321945282\c,2.3521937443,-0.8068683983,1.6237683593\c,2.4972317306,-0
.4908074713,0.1352520151\c,1.1700606479,-0.7799654728,-0.5658696309\o,
-1.0583680502,0.4632436653,2.066551095\c,0.8831736108,-0.6875060354,3.
663249394\c,1.6784232812,1.4488760936,2.6089641608\c,-0.0000542273,1.4
870798219,-0.5000242843\c,-1.3396900967,-0.6369073239,-0.454075801\o,3
.5753446138,-1.2132621498,-0.4556821552\h,0.512795185,-1.703488869,3.4
898973533\h,1.7740649918,-0.7466136842,4.2980738739\h,0.1079867095,-0.
1254576595,4.1871404853\h,2.482132072,1.4634135932,3.3536235219\h,2.04
57523279,1.9539868211,1.710535273\h,0.8286095542,2.0149634598,3.000455
5235\h,-0.7877781612,2.05174953,0.0064781152\h,0.9577434246,1.97874946
89,-0.3047624454\h,-0.1814619189,1.5240559056,-1.5800245898\h,-2.19718
92511,-0.0730010255,-0.0826171319\h,-1.3822232937,-0.6747329611,-1.548
1249247\h,-1.4084082698,-1.659770479,-0.0687439693\h,0.9589430737,-1.8
548172532,-0.4567009016\h,1.2649756323,-0.5817330598,-1.6395249345\h,3
.3038425471,-0.628123378,2.1370443302\h,2.134052546,-1.8815611298,1.71
99243846\h,2.7762689835,0.55909675,-0.0024799629\h,3.3771413621,-2.159
3848077,-0.3600670608\\Version=EM64L-G09RevB.01\State=2-A\HF=-558.9282
04\S2=0.753685\S2-1=0.\S2A=0.750009\RMSD=5.863e-09\RMSF=5.810e-06\Dipo
le=0.4159051,-0.4249074,-0.2296087\Quadrupole=-6.3099342,4.9422642,1.3

6767,0.3964875,5.8601096,-0.2096737\PG=C01 [X(C9H18N1O2)]\\@

(2 - H⁴) •

\1\GINC-V1254\FOpt\UB3LYP\Gen\C9H17N1O2(3)\DMM574\17-Nov-2010\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\tempol4rad.f
req\\0,3\c,-0.0274540316,-0.1514490342,0.0232021902\c,-0.0082202468,-0
.0558295926,1.5644792605\n,1.4124649037,-0.0467850721,2.0626964885\c,2
.5621781987,0.6306629901,1.3683869566\c,2.4045144366,0.4972210561,-0.1
629319866\c,0.9962186677,0.7276955615,-0.6103295503\c,-0.7257468596,1.
2222274866,2.044792679\c,-0.6905881887,-1.2909316786,2.1716215987\o,1.
5529028242,-0.1976405823,3.3314062689\c,3.8470223663,-0.0784844257,1.8
229033472\c,2.6109516604,2.1143263666,1.7871977953\o,0.7563365101,0.97
85879009,-1.9440320103\h,3.8032623055,-1.1473881327,1.5890338813\h,4.7
090519552,0.3551629596,1.3035353516\h,3.9875809358,0.0309723357,2.8994
400955\h,3.555801333,2.564537509,1.4607470499\h,1.7922266207,2.6859252
344,1.3404409987\h,2.5471014227,2.1919046706,2.8761114385\h,-0.5523386
273,1.3642040342,3.1153036488\h,-0.3769682842,2.1069844809,1.504433875
4\h,-1.804617804,1.1293644019,1.87550507\h,-0.7168420846,-1.2217744185
,3.2603388707\h,-1.7158164446,-1.3649617739,1.7923264416\h,-0.15333043
34,-2.2048984627,1.8973833452\h,0.1519593054,-1.2027141255,-0.27397564
87\h,-1.0297257928,0.105058253,-0.3386247627\h,3.0991743539,1.20358058
21,-0.6406788112\h,2.7319073624,-0.514952569,-0.4713698967\h,1.5165891
898,1.4568879549,-2.3120795526\\Version=EM64L-G09RevA.02\State=3-A\HF=
-558.2732046\S2=2.006683\S2-1=0.\S2A=2.000027\RMSD=4.752e-09\RMSF=9.79
8e-06\Di pole=0.350829,0.4228255,-1.0000688\Quadrupole=2.9123963,0.8955
856,-3.8079819,1.9884957,-4.5671952,0.0162077\PG=C01 [X(C9H17N1O2)]\\@

(2 - H³) •

\1\GINC-V1259\FOpt\UB3LYP\Gen\C9H17N1O2(3)\DMM574\17-Nov-2010\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\tempol3rad.f
req\\0,3\c,0.0422162415,-0.1099264678,0.0143545051\c,-0.0123141073,0.0
175934725,1.5465220359\n,1.3867396694,0.0689841987,2.0790660317\c,2.52
07108237,0.7899058223,1.4137471274\c,2.2434504831,1.0377137225,-0.0394
46036\c,0.8933031474,0.9680200818,-0.6686809724\c,-0.7757075334,1.2798
783463,2.0011983687\c,-0.6866908122,-1.2291819865,2.1399181666\o,1.541
0758347,-0.1739367044,3.3304572099\c,3.7778995078,-0.0968114603,1.5738
036505\c,2.7561791698,2.1345369545,2.1567124363\o,0.978064514,0.754344
536,-2.0801768807\h,3.6433959476,-1.0535106486,1.0594079069\h,4.649746
1955,0.4088648253,1.1455711135\h,3.9602602547,-0.2907805151,2.63348107
44\h,3.6470166623,2.6314790609,1.7587085187\h,1.904705625,2.8113487823
,2.0366679169\h,2.9013044364,1.936716057,3.2222905113\h,-0.723283839,1
.3624629744,3.0908760076\h,-0.362443761,2.196390491,1.5686713294\h,-1.
8290021102,1.2132567947,1.7060600462\h,-0.7313311475,-1.1649828086,3.2
282623513\h,-1.7041550316,-1.3170564395,1.7437176256\h,-0.1308342632,-
2.1341021118,1.8733000539\h,0.4656417626,-1.0913170692,-0.2419193715\h

, -0.9750638694, -0.0827852657, -0.3913155498\H, 3.0425612749, 1.4992282331
, -0.6158429411\H, 0.3765753476, 1.9384692135, -0.5918473147\H, 1.516843006
9, -0.0439028503, -2.2091145998\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-
558.26265\\S2=2.007744\\S2-1=0.\\S2A=2.000037\\RMSD=8.779e-09\\RMSF=1.773e-
05\\Dipole=0.0557761, 0.0391714, -0.4696616\\Quadrupole=4.8973592, 2.323301
2, -7.2206604, 0.7477421, -2.9639069, 4.5861726\\PG=C01 [X(C9H17N1O2)]\\@

(2 - CH₂H) •

1\1\GINC-V1260\FOpt\UB3LYP\Gen\C9H17N1O2(3)\DMM574\17-Nov-2010\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\tempolCH3rad
.freq\\0,3\c, -0.025360937, 0.0239529152, 0.0093016076\c, -0.0249734226, 0.
0397085269, 1.5554176544\N, 1.3854924666, 0.0345419561, 2.0813455783\c, 2.5
51913476, 0.6964925598, 1.4037614609\c, 2.3844728554, 0.6298220773, -0.1276
766649\c, 0.9817568814, 0.9867712185, -0.6199959807\c, -0.7564032195, 1.296
974628, 2.1056916342\c, -0.7044895308, -1.1910978446, 2.0757376651\o, 1.504
6954255, -0.1498476377, 3.3463484162\c, 3.8129516099, -0.0793492097, 1.8191
268205\c, 2.6668130754, 2.1545445274, 1.8989577692\o, 0.9018037636, 0.97484
82377, -2.0431541345\H, 3.7330593999, -1.1316860421, 1.5268010586\H, 4.6901
778236, 0.352834307, 1.3252385611\H, 3.9535863471, -0.0339443657, 2.9005765
182\H, 3.6049082114, 2.5962199552, 1.5447771115\H, 1.8453725047, 2.78369551
67, 1.5430859791\H, 2.6641166347, 2.1687290113, 2.992357876\H, -0.642761871
3, 1.3293689718, 3.1920098101\H, -0.3584664134, 2.225634445, 1.6819159628\H
, -1.8229314284, 1.2430610675, 1.8634234866\H, -0.3959761734, -1.617375887,
3.0210620838\H, -1.6283449884, -1.5178004601, 1.6095723885\H, 0.2165074089
, -0.9928940055, -0.3328299894\H, -1.0358703049, 0.2514387211, -0.348419377
2\H, 3.1219720486, 1.291882827, -0.5951892901\H, 2.6107082864, -0.392342115
1, -0.4675687365\H, 0.7376018931, 2.0193777945, -0.3495928967\H, 1.11265377
13, 0.0736135813, -2.3379810808\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-
558.2537765\\S2=2.007671\\S2-1=0.\\S2A=2.000035\\RMSD=5.641e-09\\RMSF=7.252
e-06\\Dipole=0.0168364, -0.0643093, -0.639501\\Quadrupole=4.3651038, 1.5345
357, -5.8996395, 1.0836102, -1.7725962, 5.554148\\PG=C01 [X(C9H17N1O2)]\\@

3 (4-methoxyTEMPO)

1\1\GINC-V1328\FOpt\UB3LYP\Gen\C10H20N1O2(2)\GXG501\22-Feb-2011\0\\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram maxdisk=26
8435456\\hals3.freq\\0,2\c, -0.0213518243, -0.0031239874, 0.0333863736\N,
-0.1036190519, 0.0982346236, 1.5300777105\c, 1.0630247468, -0.0606170969, 2
.46256913\c, 2.0634585938, -1.0865612816, 1.8936013099\c, 2.3581575426, -0.
9016244089, 0.4022249959\c, 1.0521835334, -1.0303967981, -0.3734888143\o, -
1.0944203922, 0.7758962282, 1.9890760904\c, 0.5047820949, -0.5768319952, 3.
7994249417\c, 1.7215685874, 1.3181193234, 2.6873339111\c, 0.2737712184, 1.3
952563813, -0.5515000664\c, -1.3973927824, -0.477581592, -0.463111597\o, 3.
2312040727, -1.9098742847, -0.0987285578\H, -0.0161754009, -1.5295532888, 3
.6579206946\H, 1.3266321885, -0.7329577858, 4.5069167002\H, -0.2003866946,
0.1401788361, 4.223809057\H, 2.4665000152, 1.2523098924, 3.4884864983\H, 2.

2251681253,1.6924025331,1.7907489348\H,0.9563565765,2.0422221752,2.980
5035443\H,-0.4429369441,2.1163363607,-0.1487363744\H,1.2840038886,1.74
28915665,-0.3141946849\H,0.1742044685,1.3737810447,-1.6425534395\H,-2.
1721712587,0.2435169796,-0.1964261165\H,-1.3758233875,-0.5945513773,-1
.5521475523\H,-1.6568550571,-1.4430670446,-0.0163171719\H,0.6717573484
, -2.0468517122,-0.210303239\H,1.248328178,-0.9335340518,-1.4471810158\
H,2.9823937613,-1.0280542501,2.4887304914\H,1.6642516751,-2.1008939186
,2.0217562049\H,2.8154438441,0.0848023948,0.2211384038\C,4.5955010956,
-1.7200469376,0.2169807758\H,5.1500934228,-2.5128125507,-0.2921512284\
H,4.9622235477,-0.7440580764,-0.139978142\H,4.7969443065,-1.7917639357
,1.2962665769\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-598.2354829\\S2=0
.753692\\S2-1=0.\\S2A=0.750009\\RMSD=3.637e-09\\RMSF=4.761e-06\\Dipole=1.07
65252,-0.0708124,-0.1766004\\Quadrupole=-0.1316041,-1.307371,1.4389752,
2.6319583,3.6718859,-2.3503689\\PG=C01 [X(C10H20N1O2)]\\@

(3 - H⁴) •

1\1\GINC-V1438\FOpt\UB3LYP\Gen\C10H19N1O2(3)\DMM574\17-Nov-2010\0\\#B3
LYP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\OMettempo4ra
d.freq\\0,3\C,-0.0313996618,-0.1057151897,-0.0039506841\C,-0.009848443
2,-0.0484435876,1.5381968055\N,1.4120115073,-0.0353494884,2.0282070274
\C,2.5463283887,0.6711589547,1.3394958546\C,2.3831465065,0.5817310156,
-0.1956574865\C,0.9661224414,0.8169513829,-0.624059579\C,-0.7403057257
,1.2084568935,2.0535886775\C,-0.67611319,-1.305895608,2.1172404031\O,1
.5629437716,-0.2127265425,3.2924131838\C,3.842402829,-0.0376234216,1.7
628260763\C,2.5858656155,2.1430217073,1.7996814462\O,0.6533500539,1.12
78984976,-1.9242378991\C,1.5204819958,2.0062059596,-2.6280908385\H,3.8
071328994,-1.0996098697,1.4978585718\H,4.6960466918,0.4195439853,1.249
8659825\H,3.9907648213,0.0414081186,2.8410645889\H,3.5232467574,2.6107
838539,1.4766124004\H,1.7575468225,2.7189781183,1.3766744002\H,2.53210
10403,2.1898330437,2.8908913521\H,-0.5688019796,1.3216977731,3.1278411
676\H,-0.3995551178,2.1117003767,1.5392971171\H,-1.8181449328,1.109669
2994,1.8810526716\H,-0.6983010202,-1.2644871679,3.207574164\H,-1.70241
81864,-1.3815008918,1.7411013854\H,-0.130406088,-2.2070597623,1.818436
6808\H,0.1748334491,-1.1448886439,-0.3239423623\H,-1.0406184846,0.1338
289202,-0.357322452\H,3.0827963911,1.2943590468,-0.6458139287\H,2.7070
404691,-0.424061681,-0.5287361727\H,1.0115759981,2.251246983,-3.562845
8803\H,1.6997497143,2.928594522,-2.0601900211\H,2.4833918149,1.5336080
818,-2.8611501019\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-597.5790079\\
S2=2.006714\\S2-1=0.\\S2A=2.000027\\RMSD=6.158e-09\\RMSF=4.444e-06\\Dipole=0.2344161,0.5328074,-1.1557831\\Quadrupole=2.4029986,0.9994328,-3.40243
14,1.6678864,-3.4932534,-0.1270355\\PG=C01 [X(C10H19N1O2)]\\@

(3 - H³) •

1\1\GINC-V1260\FOpt\UB3LYP\Gen\C10H19N1O2(3)\DMM574\17-Nov-2010\0\\#B3

LYP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\OMettempo3ra
d.freq\\0,3\C,0.0094197265,-0.003644431,-0.001748039\C,-0.000718838,0.
0115211751,1.5391894006\N,1.4026506633,0.0719819747,2.076116986\C,2.56
76965524,0.753858106,1.3771343093\C,2.3273748309,0.7703052816,-0.10004
52501\C,0.9521375041,1.0429851207,-0.6168698877\C,-0.7962237259,1.2123
960727,2.0948194772\C,-0.624853887,-1.2951745505,2.057366233\O,1.53133
22924,-0.0911080616,3.3409414194\C,3.8307123478,-0.0544544478,1.719266
5061\C,2.6972157989,2.1869298991,1.9552513132\O,0.8557772476,0.9209087
655,-2.02809457\C,1.4488379276,1.997311319,-2.7292615386\H,3.748293872
,-1.0777536772,1.3384437162\H,4.7058627992,0.4183453511,1.2609016149\H
,3.9716483248,-0.0974278564,2.8008676858\H,3.6131490136,2.6576587883,1
.5834927893\H,1.8510123611,2.8190379819,1.6690540217\H,2.7392120687,2.
1317371003,3.0470255897\H,-0.6971162424,1.2414453953,3.1833946122\H,-0
.4441376295,2.1673977263,1.6918885445\H,-1.8573025572,1.1107219229,1.8
411468264\H,-0.6395403558,-1.3053090844,3.1488998469\H,-1.6505520148,-
1.3886332183,1.6840454371\H,-0.0501457797,-2.1608820588,1.7118439207\H
,0.3285058604,-0.9877729931,-0.3646351547\H,-1.0110947992,0.1627961088
,-0.3672985254\H,3.0167593371,0.246970806,-0.7577773463\H,0.6120443126
,2.0519959406,-0.3171050678\H,1.3052683166,1.7996498296,-3.794658575\H
,0.9701185285,2.9568350574,-2.4753274566\H,2.5260041889,2.0838522293,-
2.5230769499\\Version=EM64L-G09RevA.02\State=3-A\HF=-597.5687582\S2=2.
008046\S2-1=0.\\$2A=2.00004\RMSD=7.107e-09\RMSF=6.621e-06\Dipole=-0.007
7742,0.5685894,-0.7906305\Quadrupole=3.4343761,1.7185941,-5.1529702,0.
6536795,-2.4935409,-0.3449461\PG=C01 [X(C10H19N1O2)]\\@

(3 - CH₂H) •

1\1\GINC-V1261\FOpt\UB3LYP\Gen\C10H19N1O2(3)\DMM574\17-Nov-2010\0\\#B3
LYP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\OMettempoCH3
rad.freq\\0,3\C,-0.0002482868,0.0124883959,0.0093394448\C,0.0222813762
, -0.0201981647,1.5500345629\N,1.4402858818,-0.1126197082,2.0409767328\
C,2.5701853206,0.6298128146,1.3852745008\C,2.4129093742,0.5779332804,-
0.1485691914\C,1.0087316107,0.9733985139,-0.6109650454\C,-0.6354299856
,1.2364035029,2.15919643\C,-0.7135718312,-1.2750815297,2.0446855044\O,
1.5842541701,-0.3610673481,3.2933474319\C,3.8794201872,-0.0931391995,1
.7902912649\C,2.610882685,2.0455122177,1.8960556746\O,0.8564291231,0.8
669877116,-2.0231422506\C,1.4276643606,1.9290573269,-2.7598284895\H,3.
8555497213,-1.1350492633,1.4507044667\H,4.7342803379,0.4086157391,1.32
56284937\H,3.9999692908,-0.0828189369,2.8739202963\H,3.1824983166,2.79
48732263,1.3553646514\H,2.3683454103,2.2344741406,2.9363346522\H,-0.55
35285045,1.1995053267,3.2493826869\H,-0.161954245,2.1597554425,1.81145
9804\H,-1.6967374732,1.2720538434,1.888526578\H,-0.7083087034,-1.32058
14769,3.1351217092\H,-1.750620119,-1.2554242732,1.6921315484\H,-0.2346
61065,-2.181539181,1.6595996012\H,0.2176542235,-0.9895080396,-0.382278
3669\H,-1.0109286277,0.2711942382,-0.3258717672\H,3.1759132808,1.22914
14077,-0.5907596911\H,2.6118171067,-0.4407653533,-0.5041891866\H,0.794

5716876,2.0095694126,-0.3015293744\H,1.1703184488,1.7595129067,-3.8087
866486\H,1.0212229817,2.9042699342,-2.446942479\H,2.5238525377,1.96679
84081,-2.6720904978\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-597.563662
9\\S2=2.007601\\S2-1=0.\\S2A=2.000035\\RMSD=6.132e-09\\RMSF=4.742e-06\\Dipol
e=0.1285401,0.7104871,-0.8007602\\Quadrupole=3.2525558,1.5475888,-4.800
1446,1.2803363,-2.702398,-0.0248884\\PG=C01 [X(C10H19N1O2)]\\@

4 (4-carboxyTEMPO)

1\\1\\GINC-V1264\\FOpt\\UB3LYP\\Gen\\C10H18N1O3(2)\\DMM574\\17-Nov-2010\\0\\#B3
LYP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\COOHtempo.a
4.freq\\0,2\C,-0.0085442133,0.0235515913,-0.0014796121\N,-0.0239221199
,0.0315793703,1.5010455993\C,1.1982076637,-0.0491532997,2.3689572208\C
,2.270312578,-0.934327208,1.7031448746\C,2.4642624216,-0.6297909335,0.
2048299265\C,1.138959508,-0.8632846188,-0.5212872365\O,-1.0543129358,0.
.5744558161,2.0441799082\C,0.7678670082,-0.691983178,3.6982552746\C,1.
7246758837,1.3763073374,2.639672679\C,0.1131886666,1.4751981937,-0.512
9138597\C,-1.3528539245,-0.5636739354,-0.4629780678\C,3.5654062675,-1.
5041633026,-0.3663694819\H,0.3411776105,-1.6857419433,3.5261286345\H,1.
.6371842794,-0.7962567436,4.3568168658\H,0.0152886643,-0.0773734081,4.
1951552066\H,2.5091805993,1.3485483156,3.4042281357\H,2.1454698431,1.8
448143472,1.7445648581\H,0.9048834406,2.0025525922,3.0021377107\H,-0.6
448635901,2.0959905795,-0.0275113079\H,1.0965414403,1.9107046043,-0.30
93743234\H,-0.0496825001,1.5056993795,-1.5960294382\H,-2.1823263471,0.
0595715529,-0.1240860825\H,-1.3725521786,-0.6229564287,-1.5567052354\H
, -1.4923557152,-1.5719531972,-0.0594336395\H,0.8693532818,-1.919666283
3,-0.4077345577\H,1.2515487105,-0.6906928185,-1.5973290821\H,3.2114849
532,-0.8069357168,2.2481764765\H,1.9787964828,-1.9882939244,1.80243065
31\H,2.7990920003,0.4086801688,0.0920218571\O,4.787978097,-1.123716679
2,0.0873513212\O,3.4163721535,-2.4419441556,-1.1182072294\H,5.42774139
28,-1.7479080156,-0.3044867107\\Version=EM64L-G09RevA.02\\State=2-A\\HF=
-672.2853011\\S2=0.753685\\S2-1=0.\\S2A=0.750009\\RMSD=9.661e-09\\RMSF=3.45
2e-06\\Dipole=1.0267146,0.1321998,-0.068097\\Quadrupole=1.0151916,-1.257
5709,0.2423794,1.2537243,3.944899,-4.1552018\\PG=C01 [X(C10H18N1O3)]\\@

(4 - H⁴) •

1\\1\\GINC-V1266\\FOpt\\UB3LYP\\Gen\\C10H17N1O3(3)\\DMM574\\17-Nov-2010\\0\\#B3
LYP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\COOHtempo4r
ad.freq\\0,3\C,0.0971958889,-0.3599937238,-0.0471152928\C,0.0292801308
, -0.1071875188,1.4838726588\N,1.4210351567,-0.0221780003,2.0484969232\C
,2.5960661805,0.5978348502,1.3441611237\C,2.5139998284,0.3057139539,-
0.1810769587\C,1.1328316822,0.4772901568,-0.7109993723\C,-0.7343866282
,1.1964288898,1.7909264057\C,-0.668150362,-1.2917076184,2.1680798223\O
,1.4957042658,-0.0350196088,3.3317532885\C,3.8651029037,-0.0468884172,
1.9202782685\C,2.6163018945,2.1165338615,1.6102117509\C,0.7641686884,1.
.3887789044,-1.775827692\O,-0.3751770399,1.5446167487,-2.2005197992\O,

1.8205654435, 2.088284526, -2.2893559813\H, 3.8402818077, -1.1343084359, 1.
7932001095\H, 4.7451230294, 0.3446213312, 1.3984266144\H, 3.955912328, 0.17
10770302, 2.9857740177\H, 3.5626534641, 2.5445824321, 1.2613595351\H, 1.804
7409115, 2.6360010665, 1.0921009992\H, 2.5235885146, 2.3003631237, 2.684203
6521\H, -0.6384473397, 1.4346635353, 2.8539220288\H, -0.360580384, 2.040297
524, 1.2037296911\H, -1.7963991574, 1.0717153633, 1.5530418454\H, -0.755523
4836, -1.1177386232, 3.2419326026\H, -1.6696243208, -1.4218190325, 1.743795
4221\H, -0.1024839718, -2.2167977641, 2.0147263543\H, 0.3528957362, -1.4202
523164, -0.2039421331\H, -0.8876581256, -0.1867076794, -0.4875131486\H, 3.2
361891347, 0.9371829408, -0.7026962874\H, 2.8164769487, -0.7420316568, -0.3
39521705\H, 1.4407246738, 2.6535603259, -2.9862566059\Version=EM64L-G09R
evA.02\State=3-A\HF=-671.6377585\S2=2.010487\S2-1=0.\S2A=2.000063\RMSD
=5.484e-09\RMSF=8.186e-06\Dipole=0.4748511, 0.0465588, -0.5956106\Quadrupole=1.3074549, 4.0119767, -5.3194316, 1.9708227, -4.6553236, 0.6115655\PG=C01 [X(C10H17N1O3)]\\@

(4 - H³) •

1\1\GINC-V1264\FOpt\UB3LYP\Gen\C10H17N1O3(3)\DMM574\17-Nov-2010\0\\#B3
LYP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\COOHtempo3r
ad.freq\0,3\c,0.0221004011,0.1709434092,0.0640395351\c,0.0237433329,0
.0060131134,1.5508688796\N,1.4285988367,0.0571407296,2.0948137232\c,2.
5912836592,0.7165523403,1.4145773528\c,2.4498767176,0.6011676097,-0.11
47620332\c,1.0432308117,1.0132212001,-0.6162727767\c,-0.8032902014,1.1
291298579,2.2375343467\c,-0.562913876,-1.3660062745,1.9385233814\o,1.5
405535008,-0.1167875127,3.3613578969\c,3.8613605676,-0.0281310634,1.85
90100907\c,2.6722679015,2.1873569691,1.8751147825\c,0.951547202,0.9100
110336,-2.1304860023\o,0.2295467738,0.1688570498,-2.758499846\o,1.8057
233212,1.776002487,-2.7337058994\H,3.8070520431,-1.0853376002,1.578884
3447\H,4.7383386991,0.4155663445,1.3750944848\H,3.9813718719,0.0336195
735,2.9419359892\H,3.5918323223,2.6517930715,1.5016437315\H,1.82541184
65,2.7837978194,1.5203038196\H,2.6799594377,2.2235800997,2.967981191\H
, -0.7085750896,1.0345265016,3.3231970663\H,-0.4563187074,2.1239159613,
1.9401651081\H,-1.8580175106,1.038849593,1.958341186\H,-0.5245546845,-
1.4975520508,3.0217662958\H,-1.6042654159,-1.4306920877,1.6056038375\H
,0.0031411429,-2.1746296262,1.4655861921\H,-0.7699829486,-0.2860351527
, -0.5177369785\H,3.219123396,1.2223915468,-0.5851696513\H,2.6323266144
, -0.4373349196,-0.4164327068\H,0.9106815342,2.0842311518,-0.38033082\H
,1.693884331,1.6408072797,-3.6936098469\Version=EM64L-G09RevA.02\Stat
e=3-A\HF=-671.6190745\S2=2.007961\S2-1=0.\S2A=2.000039\RMSD=4.947e-09\
RMSF=1.116e-05\Dipole=0.3012743,0.6815801,-0.7533299\Quadrupole=2.9263
417,0.8569854,-3.7833271,-0.1924003,-4.4421756,-1.28126\PG=C01 [X(C10H
17N1O3)]\\@

(4 - CH₂H) •

1\1\GINC-V1257\FOpt\UB3LYP\Gen\C10H17N1O3(3)\DMM574\17-Nov-2010\0\\#B3

LYP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\COOHtempoCH
3rad.freq\\0,3\c,-0.027330756,0.0273686149,0.0100133081\c,-0.025197062
7,0.0401929504,1.5546188933\N,1.3835551914,0.0343605594,2.0845986083\c
,2.5519028042,0.6915673625,1.4100323216\c,2.3917524162,0.6299583949,-0
.1221142252\c,0.9760014697,1.0050758109,-0.6022659094\c,-0.7581253147,
1.2926680452,2.1132768759\c,-0.7053615241,-1.1938834035,2.0670000371\o
,1.5002835223,-0.147894625,3.3501020427\c,3.8092206732,-0.0950330499,1
.8177586894\c,2.6760398239,2.1460694974,1.9115280399\c,0.9123590602,0.
9762336449,-2.118636088\o,0.3307917297,0.1565946235,-2.7943433493\o,1.
6198632136,1.9989766883,-2.6649467906\H,3.7217425494,-1.1447085439,1.5
184150626\H,4.6891559409,0.3347518406,1.3265619261\H,3.9505076832,-0.0
575084223,2.8993203035\H,3.6186358124,2.5837825447,1.5641967053\H,1.85
98940037,2.7830792868,1.5566428662\H,2.6680989053,2.1545662153,3.00487
39739\H,-0.6434310133,1.3194564944,3.1995777981\H,-0.3614263463,2.2251
352151,1.695940342\H,-1.8247950522,1.23860457,1.8716367767\H,-0.421531
2962,-1.6055733249,3.026321422\H,-1.6027693038,-1.5459418296,1.5691050
488\H,0.21284877,-0.9803105321,-0.3457163773\H,-1.0436501902,0.2430486
687,-0.3373149574\H,3.1396707448,1.2899221292,-0.5736828588\H,2.609871
4533,-0.3897573782,-0.4656899177\H,0.7583740059,2.0371334136,-0.300626
6259\H,1.5459675367,1.8922386129,-3.6322179155\\Version=EM64L-G09RevA.
02\\State=3-A\\HF=-671.6107152\\S2=2.007686\\S2-1=0.\\S2A=2.000035\\RMSD=3.5
28e-09\\RMSF=9.092e-06\\Dipole=0.215652,0.7811142,-0.7333669\\Quadrupole=
3.8530452,0.4157054,-4.2687506,-0.3483651,-3.722751,-1.7017708\\PG=C01
[X(C10H17N1O3)]\\@

5 (TEMPONE)

1\\1\\GINC-V1268\\FOpt\\UB3LYP\\Gen\\C9H16N1O2(2)\\DMM574\\17-Nov-2010\\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\tempone.freq
\\0,2\c,-0.004737225,-0.0931829034,-0.0110001939\c,0.0032410614,-0.042
2762171,1.5375662355\N,1.4202232237,-0.0487056414,2.0428157455\c,2.571
9858806,0.6546748706,1.3780316058\c,2.4259095025,0.5664248844,-0.16190
94018\c,1.0086996072,0.8603466322,-0.6118105156\c,-0.7221354523,1.2217
776876,2.0435839009\c,-0.6859889134,-1.2953060812,2.0990333655\o,1.552
9907037,-0.2496577667,3.3046338841\c,3.85781948,-0.0625952853,1.816765
3946\c,2.6149070658,2.127103059,1.8365147197\H,3.8145888558,-1.1267003
724,1.5618246194\H,4.7175953783,0.3833742725,1.3053521342\H,3.99897789
42,0.0257965122,2.8952878248\H,3.556112881,2.5889059342,1.5183479118\H
,1.7968395457,2.7171094146,1.4128891943\H,2.5562906796,2.1719163906,2.
9276425251\H,-0.5687136055,1.3242863416,3.1215259191\H,-0.3676691751,2
.1298206033,1.5469841861\H,-1.7972521827,1.1365058917,1.8506773573\H,-
0.7270571831,-1.2562946515,3.188871609\H,-1.705683819,-1.359231749,1.7
043419854\H,-0.1425216379,-2.2002726748,1.807730234\H,0.2490535073,-1.
1118498121,-0.334604415\H,-1.0039383338,0.1475767834,-0.3839668433\H,3
.1170547182,1.2659676315,-0.6398552621\H,2.6844240739,-0.450920145,-0.
4859402169\o,0.71384863,1.7771824461,-1.3538950626\\Version=EM64L-G09R

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evA.02\State=2-A\HF=-557.7286684\S2=0.753652\S2-1=0.\S2A=0.750009\RMSD
=7.341e-09\RMSF=8.403e-06\Di pole=0.1014917,-0.4067366,-0.1864686\Quadr
upole=6.0459314,0.7669022,-6.8128336,2.0050693,-2.5187657,6.2011623\PG
=C01 [X(C9H16N1O2)]\\@
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(5 - H³) •

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1\1\GINC-V1265\FOpt\UB3LYP\Gen\C9H15N1O2(3)\DMM574\17-Nov-2010\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\tempone3rad.
freq\\0,3\C,-0.1806962923,-0.2670763198,0.1778917079\C,0.0072136368,-0
.2814390566,1.6869578982\C,1.4534091223,0.0102370313,2.1329544171\N,2.
362418306,-0.9130348579,1.3836622677\C,2.2503103294,-1.1582360146,-0.0
870719769\C,0.9334568024,-0.6888372752,-0.6172880549\C,1.8471990394,1.
4734835034,1.8405580431\C,1.6107374856,-0.2850279153,3.6296238702\O,3.
4872608332,-1.2238572952,1.9169906823\C,2.3806410362,-2.6888454384,-0.
3080913128\C,3.410518355,-0.4369793573,-0.8178362732\O,-1.2528714399,0
.0759887459,-0.3450121699\H,1.5525608827,-3.2239027537,0.1666861625\H,
2.3806470023,-2.9205332577,-1.3776655609\H,3.3200033564,-3.0278751057,
0.136334491\H,3.3920641496,-0.6804932536,-1.8851074352\H,3.3340629749,
0.6490054568,-0.7097980751\H,4.3602415633,-0.7665250596,-0.3905303972\
H,2.9047625059,1.6278139973,2.0762455546\H,1.6805995133,1.7430517848,0
.7921531304\H,1.2511020268,2.1543506409,2.4584386499\H,2.6238288849,-0
.0629791525,3.9688643347\H,0.9023947127,0.3307727153,4.1940734131\H,1.
4041289846,-1.338377352,3.8433038065\H,-0.2904931589,-1.272658342,2.05
74650822\H,-0.6829324291,0.4442664433,2.1286239642\H,0.7947935414,-0.6
992936001,-1.695609599\\Version=EM64L-G09RevA.02\State=3-A\HF=-557.079
9952\S2=2.01945\S2-1=0.\S2A=2.000148\RMSD=8.676e-09\RMSF=7.432e-06\Di p
ole=0.3552687,-0.0047021,-0.0719241\Quadrupole=-7.8122103,3.6703565,4.
1418538,3.1030721,-7.1736895,3.2200536\PG=C01 [X(C9H15N1O2)]\\@
```

(5 - CH₂H) •

```
1\1\GINC-V1265\FOpt\UB3LYP\Gen\C9H15N1O2(3)\DMM574\17-Nov-2010\0\\#B3L
YP/gen 6D OPT IOP(2/17=4) Freq=noram an maxdisk=268435456\\temponeCH3ra
d.freq\\0,3\C,0.0000083028,0.0061305481,0.0053058771\C,0.0084916562,0.
0393497251,1.5211639677\C,1.455384204,0.0479843088,2.0898268399\N,2.31
42987881,-0.9461687784,1.3523347667\C,2.2025344702,-1.2553285465,-0.11
53495219\C,0.7186244884,-1.2047809995,-0.5565648581\C,2.0779435765,1.4
640627718,1.9439836355\C,1.4365687168,-0.3511765351,3.5332315304\O,3.4
611236342,-1.1786260529,1.8793858613\C,2.7539822264,-2.6744337923,-0.3
226370413\C,3.0453855217,-0.2465095035,-0.9224869538\O,-0.5104616462,0
.8675858424,-0.6838312079\H,2.2098965102,-3.3959607386,0.2957263494\H,
2.6407541971,-2.9608812483,-1.3737364276\H,3.810495787,-2.7191880913,-
0.0528644655\H,3.1303137249,-0.581492152,-1.9620936447\H,2.5994914382,
0.7523963332,-0.9318148365\H,4.048748158,-0.1831534263,-0.4923572752\H
,3.1363383433,1.4220444571,2.2128314311\H,1.9789575804,1.8497345291,0.
9235681806\H,1.5710204834,2.1626761877,2.617702449\H,2.2698448697,-0.8
```

995832957,3.9513960043\H,0.6940920964,0.0927960442,4.1880521094\H,-0.5
08383118,-0.8566676073,1.8882747555\H,-0.531778735,0.9209881565,1.8759
223552\H,0.6583630861,-1.1945923191,-1.6481768579\H,0.2072989712,-2.10
54554791,-0.1903500475\Version=EM64L-G09RevA.02\State=3-A\HF=-557.054
0693\S2=2.00762\S2-1=0.\S2A=2.000035\RMSD=5.561e-09\RMSF=7.879e-06\Dip
ole=-0.2467452,-0.326375,0.0594526\Quadrupole=-2.937245,1.1716624,1.76
55827,4.2049524,-6.0951445,4.9538737\PG=C01 [X(C9H15N1O2)]\\@

OH•

1\1\GINC-V1252\FOpt\UB3LYP\Gen\H1O1(2)\DMM574\12-Oct-2010\0\\#B3LYP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\OH.freq\\0,2\0,0.,-0.0164586177\H,0.,0.,0.9664586177\\Version=EM64L-G09RevA.02\HF=-5.7234548\S2=0.751967\S2-1=0.\S2A=0.750002\RMSD=7.618e-09\RMSF=2.480e-06\Dipole=0.,0.,0.6914211\Quadrupole=-0.7686378,0.0770273,0.6916106,0.,0.,0.\PG=C*V [C*(H1O1)]\\@

H₂O

1\1\GINC-V1255\FOpt\RB3LYP\Gen\H2O1\DM574\08-Sep-2010\0\\#B3LYP/gen 6D OPT IOP(2/17=4) Freq=noram maxdisk=268435456\\water.freq\\0,1\0,-0.027195303,0.,-0.0192300993\H,0.0216657632,0.,0.9482050696\H,0.9011995525,0.,-0.295637773\\Version=EM64L-G09RevA.02\State=1-A1\HF=-76.4089533\RMSD=1.144e-09\RMSF=6.397e-05\Dipole=0.6729165,0.,0.4758261\Quadrupole=0.3006297,-1.0239681,0.7233384,0.,-0.5978088,0.\PG=C02V [C2(O1),SGV(H2)]\\@

TS(1-H⁴)•

1\1\GINC-V1460\FTS\UB3LYP\Gen\C9H19N1O2(3)\DMM574\22-Dec-2010\0\\#B3LYP/gen 6D OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noram maxdisk=268435456\\tsfinal.freq\\0,3\C,0.0110641369,0.0533398995,-0.0622545463\N,0.1352250444,0.2106117104,1.4277958515\C,1.4097706774,0.0496810131,2.2057092239\C,2.2685311681,-1.0730477576,1.5862253987\C,2.3340463958,-1.0634456058,0.0693067345\C,0.9516495874,-1.0646192147,-0.5588442312\O,-0.7596772176,0.9477478678,1.9825466447\C,1.0156192103,-0.3457375289,3.6388814865\C,2.168871733,1.3938179416,2.2364805287\C,0.3151119454,1.4022368125,-0.7482078312\C,-1.4456503752,-0.3479986408,-0.3507675692\O,3.6979796569,0.9240085941,-0.8243733259\H,2.9558661634,-1.8784512537,-0.3181850717\H,0.4118592582,-1.2595978115,3.6375512274\H,1.9192074583,-0.5268550476,4.231790164\H,0.4338089209,0.4476649526,4.1106545151\H,2.9808625295,1.3425354198,2.9721828131\H,2.6038581911,1.6462378586,1.2662129061\H,1.4817814366,2.1895151248,2.5377379349\H,-0.2828850621,2.1876078342,-0.2769966792\H,1.37187297,1.6726435198,-0.690748629\H,0.0409481076,1.3470122876,-1.8081954843\H,-2.131621199,0.4411114549,-0.0386688733\H,-1.5703422437,-0.5248928056,-1.4248697182\H,-1.7108070044,-1.2654487768,0.1857556201\H,0.4942506095,-2.0399759459,-0.3263606596\H,1.0184382201,-1.006692283,-1.6512195489\H,3.2710019467,-1.0

314321452,2.0298657484\H,1.8432300782,-2.0449351067,1.8836415104\H,2.9
253858232,-0.0842601987,-0.332366707\H,4.4687515521,0.8224425529,-0.22
98608812\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-559.4455845\\S2=2.0100
9\\S2-1=0.\\S2A=2.000054\\RMSD=6.320e-09\\RMSF=4.402e-06\\Dipole=0.9541415,
-0.9915946,-0.0121421\\Quadrupole=0.9913566,0.6003969,-1.5917535,0.2155
291,5.7926814,0.7569299\\PG=C01 [X(C9H19N1O2)]\\@

TS (1-H³) •

1\\1\\GINC-V1249\\FTS\\UB3LYP\\Gen\\C9H19N1O2 (3) \\DMM574\\22-Dec-2010\\0\\#B3LY
P/gen 6D OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noram
an maxdisk=268435456\\ts3final.freq\\0,3\C,0.0042537003,0.0561936798,-
0.0562045985\N,0.1261443407,0.2063345979,1.4364869763\C,1.4202977191,0
.0542315144,2.2091444092\C,2.258679696,-1.0381521227,1.5465886348\C,2.
3898235777,-0.9269609932,0.0402310041\C,0.9784136586,-1.0275001573,-0.
5621393852\O,-0.7693699138,0.9268339997,2.0033380785\C,1.0560719937,-0
.3662384233,3.6407428965\C,2.1551279929,1.4102822697,2.2454360056\C,0.
2699229052,1.4204314781,-0.727112012\C,-1.4426745381,-0.3775142005,-0.
3436909515\O,4.4888713054,-0.9459739964,2.7912810532\H,3.020594863,-1.
7329318828,-0.3510082026\H,0.4741164041,-1.2943666261,3.6383123003\H,1
.9803609248,-0.5290887721,4.2047188905\H,0.4652865782,0.4071343978,4.1
343377202\H,3.0254924264,1.3334970331,2.9033758945\H,2.5077956162,1.72
00218628,1.2574514175\H,1.4767014698,2.1785149288,2.6267622464\H,-0.34
40312184,2.1885372101,-0.2485492223\H,1.3187729055,1.7231497442,-0.656
9707292\H,0.0040617212,1.3725709777,-1.7891739474\H,-2.1468195719,0.38
55842257,-0.0069866093\H,-1.5733828324,-0.5349701309,-1.4200127496\H,-
1.6762714189,-1.3135032,0.1746450926\H,0.5666366494,-2.0169571926,-0.3
228248987\H,1.0255637911,-0.9623772757,-1.6563121242\H,3.3600917924,-0
.9582122217,2.0474328173\H,1.8990499709,-2.0351344697,1.8327689374\H,2
.8688044412,0.0165552365,-0.2446785199\H,4.3558954358,-1.7825035875,3.
2806464871\\Version=EM64L-G09RevA.02\\State=3-A\\HF=-559.4456816\\S2=2.01
0375\\S2-1=0.\\S2A=2.000058\\RMSD=7.042e-09\\RMSF=7.341e-06\\Dipole=0.14026
82,-0.8518848,-0.6711207\\Quadrupole=-7.6464055,3.7553866,3.8910189,-0.
1366535,1.8040828,-2.7041861\\PG=C01 [X(C9H19N1O2)]\\@

TS (1-CH₂H) •

1\\1\\GINC-X79\\FTS\\UB3LYP\\Gen\\C9H19N1O2 (3) \\GXG501\\04-Mar-2011\\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noram maxdisk=1342177280\\ts12.freq\\0,3\C,0.0104751417
,0.0085686486,-0.0033942577\C,-0.0021512462,0.0078320912,1.5252437785\
C,1.4052715285,0.002251837,2.1556614939\N,2.2887517124,-0.9906096084,1
.4485573271\C,2.2189742452,-1.3135575694,-0.018051643\C,0.7482896254,-
1.2366542648,-0.4993658818\C,2.7031626665,-2.7466039498,-0.2139016903\
H,3.9576210052,-2.8292209436,-0.0440375368\O,5.1429818873,-2.677926710
6,0.2909864829\C,2.0639795821,1.3965670759,2.0888710038\C,1.3074103751
,-0.4433175873,3.6243364567\O,3.4017362584,-1.243711285,2.0442333471\C

,3.1238982749,-0.3455242592,-0.8110821552\H,-1.0177368885,0.0038750873
, -0.3847307474\H,2.5901364626,-3.0788134314,-1.2496002783\H,2.27443218
83,-3.460640149,0.4925862812\H,3.1286853207,-0.6340064988,-1.868224905
6\H,2.7794113407,0.6899600034,-0.7440945623\H,4.1480376384,-0.41290406
81,-0.439073521\H,3.1033150518,1.3284352425,2.4218677216\H,2.050889202
5,1.8169678326,1.0788919156\H,1.5310156338,2.0906302433,2.7483423217\H
,2.285029712,-0.4163513057,4.1083508585\H,0.6254188593,0.2250083411,4.
1614672341\H,0.9167923982,-1.4639878625,3.694014573\H,-0.5473766086,-0
.8818493467,1.8690260011\H,-0.5443195254,0.8774449142,1.9159227595\H,0
.7511025528,-1.2865124764,-1.5942668993\H,0.2103891749,-2.1258107393,-
0.1432703331\H,0.4805218766,0.9202716636,-0.3921697815\H,4.922212525,-
2.1972295964,1.1178953954\\Version=EM64L-G09RevB.01\\State=3-A\\HF=-559.
446548\\S2=2.010831\\S2-1=0.\\S2A=2.000061\\RMSD=8.781e-09\\RMSF=1.417e-06\\
Dipole=-1.8445215,0.8463279,-0.1687988\\Quadrupole=-4.9550098,1.2885283
,3.6664815,5.0192384,1.563926,0.441423\\PG=C01 [X(C9H19N1O2)]\\@

TS (2-H⁴) •

1\1\GINC-X134\Freq\UB3LYP\Gen\C9H19N1O3(3)\GXG501\04-Mar-2011\0\\#B3LYP
P/gen 6D INT(grid=ultrafine) IOP(2/17=4) Freq=noram an maxdisk=13421772
80\\ts24.freq\\0,3\C,-0.438957,-1.27706,0.40367\C,0.923703,-1.261091,-
0.352521\C,1.722752,0.01282,-0.159918\C,0.893011,1.265531,-0.411221\C,
-0.459833,1.283779,0.361963\N,-1.213228,-0.004736,0.17196\O,-2.67134,-
0.024576,0.191861\C,-0.261556,1.573533,1.864619\C,-1.31391,2.442584,-0
.189912\O,2.388924,-0.014468,1.081095\C,-0.253736,-1.52215,1.918925\C,
-1.269967,-2.461424,-0.12791\O,3.63299,0.018204,-1.849229\H,2.879194,0
.819829,1.169733\H,0.722262,-1.364372,-1.424078\H,1.527184,-2.12417,-0
.04877\H,1.476612,2.163937,-0.167422\H,0.594982,-0.990065,2.343958\H,-
2.275242,2.494304,0.332954\H,0.495711,0.95074,2.334977\H,0.05643,2.616
052,1.980838\H,-0.074055,-2.590175,2.08357\H,-1.207861,1.449171,2.4004
44\H,-1.164308,-1.247475,2.460353\H,-0.719342,-3.391506,0.04997\H,-1.4
63451,-2.380073,-1.198255\H,-2.225048,-2.531785,0.404433\H,-0.789461,3
.389154,-0.01928\H,-1.49629,2.342754,-1.260626\H,0.678372,1.315473,-1.
484073\H,2.583677,0.034956,-1.016291\H,4.129564,-0.69154,-1.396258\\Ve
rsion=EM64L-G09RevB.01\\State=3-A\\HF=-634.629615\\S2=2.010403\\S2-1=0.\\S2
A=2.000057\\RMSD=8.714e-09\\RMSF=1.372e-02\\ZeroPoint=0.2727567\\Thermal=0
.2880145\\Dipole=0.8709918,0.0975619,0.7701128\\PG=C01 [X(C9H19N1O3)]\\@

TS (2-H³) •

1\1\GINC-X114\FTS\UB3LYP\Gen\C9H19N1O3(3)\GXG501\02-Mar-2011\0\\#B3LYP
/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP
(2/17=4) Freq=noram an maxdisk=1342177280\\ts23.freq\\0,3\C,0.000890075
1,-0.0008052557,0.0010253443\N,-0.0024568635,-0.0139612845,1.503925496
9\C,1.2260623382,-0.001198695,2.3622218844\C,2.3944091313,-0.682516478
9,1.6549478293\C,2.5311295204,-0.4916145551,0.1493026752\C,1.195521130
3,-0.817611065,-0.5252238874\O,-1.0682159434,0.4264994311,2.0701503748

```
\C,0.8842345232,-0.746769944,3.6663167572\C,1.5964785602,1.4675564702,  
2.6963073224\C,0.0380046424,1.4611923368,-0.4931935157\C,-1.3111116664  
, -0.6584083487,-0.4575170329\O,3.5893241418,-1.2825966899,-0.362095870  
8\H,0.6033624419,-1.7827405655,3.4529602796\H,1.755202293,-0.749888623  
7,4.3309816735\H,0.0510355673,-0.2555270523,4.1715850417\H,2.389591903  
6,1.495313317,3.4509811593\H,1.9447414006,2.0150614343,1.8155268844\H,  
0.710761154,1.9706966209,3.093853604\H,-0.7606640273,2.0308728268,-0.0  
095245801\H,0.9917278023,1.9534115026,-0.2784382619\H,-0.1169456887,1.  
4929536283,-1.5773641643\H,-2.1732100217,-0.0898881868,-0.1040296486\H  
, -1.3350596024,-0.701816773,-1.5517792087\H,-1.3877071137,-1.678913354  
2,-0.0684788397\H,0.9970868491,-1.8861606155,-0.3713008277\H,1.2881632  
599,-0.6615125157,-1.6056655645\H,3.3385605913,-0.4954460277,2.1780695  
644\H,2.2505381709,-1.8830164403,1.736802978\H,2.8183100337,0.54900714  
64,-0.0570328406\H,3.3999186573,-2.1932936159,-0.0575524808\O,2.481885  
6662,-3.2223425732,1.4665937655\H,3.2246443537,-3.3569883652,2.0901794  
78\Version=EM64L-G09RevB.01\State=3-A\HF=-634.6595305\S2=2.010082\S2-  
1=0.\S2A=2.000055\RMSD=8.018e-09\RMSF=6.803e-07\Dipole=0.6982337,0.116  
8584,0.3392387\Quadrupole=-4.0551943,1.6045044,2.45069,-0.3423979,8.49  
80496,-2.7673054\PG=C01 [X(C9H19N1O3)]\\@
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TS (2-CH₂H) •

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1\1\GINC-V1309\FTS\UB3LYP\Gen\C9H19N1O3(3)\GXG501\03-Mar-2011\0\\#B3LY  
P/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IO  
P(2/17=4) Freq=noram an maxdisk=268435456\\ts22.freq\\0,3\C,-0.00125047  
34,-0.0013942201,-0.0016171521\C,0.0004067658,0.0040634562,1.525981195  
1\C,1.4073021848,0.0004703061,2.1562475224\N,2.2901332568,-0.994553066  
2,1.4516440353\C,2.2202756849,-1.3150236813,-0.015427456\C,0.749365166  
7,-1.2409124455,-0.4933097816\C,2.7062319199,-2.7470412607,-0.21471566  
83\H,3.9610902489,-2.8262771427,-0.0437272208\O,5.1468414351,-2.674291  
4837,0.2873743345\C,2.0642857917,1.3960092528,2.0884466502\C,1.3085269  
009,-0.4416749049,3.6260120541\O,3.4010801068,-1.2506457125,2.04868877  
09\C,3.1221557749,-0.3450275396,-0.8103877055\O,-1.3223242575,0.054899  
5592,-0.5305326096\H,2.5950391662,-3.0766236755,-1.2512569741\H,2.2782  
904727,-3.4633347025,0.4899788041\H,3.1177211597,-0.6277850718,-1.8688  
497662\H,2.7830902293,0.6916674598,-0.7362603221\H,4.1484688158,-0.419  
1573379,-0.4456369284\H,3.1008234837,1.3294994626,2.4303530264\H,2.059  
1525066,1.8142061647,1.0776216073\H,1.5252351288,2.0915059355,2.741068  
0976\H,2.2873207002,-0.4144812584,4.1076403437\H,0.6282837938,0.228837  
798,4.1621933449\H,0.9174475954,-1.461945334,3.6985059464\H,-0.5458754  
186,-0.8887242776,1.8667015266\H,-0.5512364661,0.8753315396,1.89635113  
99\H,0.733025558,-1.2778797889,-1.5875768528\H,0.2083544601,-2.1284365  
433,-0.1319512651\H,0.4776072953,0.9049280501,-0.3860684807\H,-1.80249  
03591,-0.7238398096,-0.2038741503\H,4.9315241845,-2.2004198089,1.11938  
9372\Version=EM64L-G09RevB.01\State=3-A\HF=-634.6545866\S2=2.010813\S  
2-1=0.\S2A=2.000061\RMSD=8.917e-09\RMSF=6.868e-07\Dipole=-1.5479506,0.
```

3944014,0.2352655\Quadrupole=-6.1989652,2.4362113,3.7627539,9.3678972,
-1.7621328,2.2794146\PG=C01 [X(C9H19N1O3)]\\@

TS (3-H⁴) •

1\1\GINC-V1308\FTS\UB3LYP\Gen\C10H21N1O3(3)\GXG501\03-Mar-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) I
OP(2/17=4) Freq=noramam maxdisk=268435456\\ts34.freq\\0,3\C,0.00096614
58,-0.0013734071,0.0004523793\N,0.0000873091,0.0019088409,1.5028385731
\C,1.2324344762,0.0013330398,2.3630453745\C,2.340846391,-0.8443371414,
1.7021875143\C,2.4828387603,-0.6305816866,0.2011369538\C,1.1675315387,
-0.8664226935,-0.5248567684\O,-1.0589054574,0.4774260076,2.0537064249\
C,0.8408082426,-0.638349332,3.706011389\C,1.6948429869,1.4547088437,2.
6059510662\C,0.0768401128,1.4488070327,-0.5242100368\C,-1.329330884,-0
.6319259514,-0.4463808445\O,3.6043159557,-1.3034195324,-0.3378326356\H
,0.4387261371,-1.6460078311,3.5549472837\H,1.724288181,-0.709147722,4.
3499517309\H,0.0805126983,-0.0386761221,4.2091907516\H,2.4522220719,1.
4717319749,3.3982162445\H,2.1367821885,1.9115335818,1.7174007774\H,0.8
398491397,2.0537802347,2.9318505048\H,-0.6804199311,2.0525490448,-0.01
607242\H,1.0584133498,1.9038219592,-0.3747833661\H,-0.1341707057,1.462
4296133,-1.5998669847\H,-2.1720589633,-0.0233244521,-0.114750631\H,-1.
351160297,-0.7072998718,-1.5391571343\H,-1.4453939781,-1.6364569183,-0
.0253659432\H,0.8947306236,-1.9251824465,-0.4056318881\H,1.2890101304,
-0.6834000337,-1.5987284129\H,3.295868088,-0.6338730406,2.1950387002\H
,2.1241750254,-1.9113810094,1.8650610216\H,2.7924313633,0.4999149655,0
.0321781994\C,3.4697759661,-2.6822716219,-0.6575353882\H,4.4700757703,
-3.0246082309,-0.9330288945\H,3.1197865771,-3.2743432044,0.1994871162\
H,2.793716865,-2.849619912,-1.505982142\O,3.5107084012,1.6552745638,-0
.3443608993\H,4.2674469091,1.1593212023,-0.7187266149\\Version=EM64L-G
09RevB.01\State=3-A\HF=-673.9608884\S2=2.009624\S2-1=0.\S2A=2.00005\RM
SD=3.305e-09\RMSF=9.712e-07\DIPOLE=0.790563,-1.2853434,-0.5611702\Quad
rupole=-3.3684398,1.0464902,2.3219496,-1.8771415,3.017505,1.6112698\PG
=C01 [X(C10H21N1O3)]\\@

TS (3-H³) •

1\1\GINC-V1263\FTS\UB3LYP\Gen\C10H21N1O3(3)\GXG501\03-Mar-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) I
OP(2/17=4) Freq=noramam maxdisk=268435456\\ts33.freq\\0,3\C,0.00022214
13,-0.0004634576,-0.0007861634\N,0.0006723815,0.006241915,1.5028798358
\C,1.2499566759,0.0009768069,2.3616022901\C,2.3322273039,-0.8028273955
,1.6512135641\C,2.5230783428,-0.4801800277,0.186936116\C,1.2054102462,
-0.803378611,-0.5331249816\O,-1.0510215127,0.4783343146,2.0623167542\C
,0.8846065853,-0.6775785289,3.6910560788\C,1.6834274844,1.4580887023,2
.6294867684\C,0.0106912477,1.4560180766,-0.5133214054\C,-1.3038877932,
-0.6843665839,-0.4444887765\O,3.6135175271,-1.273565314,-0.2814484612\
H,0.5222805988,-1.6966430995,3.5194854223\H,1.7718458922,-0.7263064849

,4.3307960043\H,0.1023036512,-0.1159030334,4.2044368277\H,2.5160527368
,1.4728905774,3.3391479585\H,2.0141660621,1.9689576525,1.7207421426\H,
0.8399287485,2.0117893422,3.0508267804\H,-0.7902982362,2.0177903551,-0
.0250472264\H,0.9587642963,1.9642479811,-0.3129576802\H,-0.159269424,1
.4740091246,-1.5957793773\H,-2.1698534767,-0.1270681227,-0.0822638551\
H,-1.3423164049,-0.7339960595,-1.538186698\H,-1.3600730632,-1.70366869
58,-0.0485031168\H,1.0194136385,-1.8779574174,-0.4135732722\H,1.289749
0904,-0.6094474405,-1.6090838535\H,3.4077683865,-0.5572651612,2.207107
4989\H,2.2111244169,-1.8837008427,1.7866222225\H,2.7790219887,0.582316
241,0.0588457975\C,4.123457125,-0.8893976489,-1.5474330397\H,5.0025546
706,-1.5115197672,-1.7328692651\H,3.4002563229,-1.055803068,-2.3577621
331\H,4.4245565102,0.169382689,-1.5559793058\O,4.6691211564,-0.3141871
446,2.3813262647\H,4.9674853525,-0.7549579636,1.5590915147\\Version=EM
64L-G09RevB.01\State=3-A\HF=-673.9628499\S2=2.010613\S2-1=0.\S2A=2.000
061\RMSD=6.768e-09\RMSF=9.919e-07\Dipole=0.2084032,-0.1615813,-1.51606
89\Quadrupole=-5.7162096,1.7614567,3.9547529,0.9315972,-3.240711,-0.74
5638\PG=C01 [X(C10H21N1O3)]\\@

TS (4-H⁴) •

1\1\GINC-V1310\FTS\UB3LYP\Gen\C10H19N1O4(3)\GXG501\03-Mar-2011\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noramman maxdisk=268435456\\ts44.freq\0,3\C,0.0000179891,-0.0000253786,0.0008181039\N,-0.0003191852,-0.0030876707,1.502367876\C,1.2322093788,-0.0009897841,2.3581063134\C,2.3444681935,-0.840198351,1.6943684645\C,2.487887869,-0.6254249964,0.1867324924\C,1.1682568068,-0.8522999492,-0.5332471089\O,-1.0577432297,0.4695670769,2.0588352821\C,0.8499888482,-0.6547156584,3.6974144558\C,1.6915879839,1.4515007372,2.6102990434\C,0.0685498291,1.4550552564,-0.5106665001\C,-1.3256854611,-0.6359629933,-0.4511954387\C,3.6210237888,-1.431441934,-0.4060584031\H,0.4505038636,-1.6621573388,3.5392493055\H,1.7356319944,-0.7273562329,4.3383486777\H,0.0894847308,-0.0615857782,4.207700463\H,2.4377738825,1.4670662235,3.4136312919\H,2.142935654,1.9079274281,1.7260552084\H,0.8325242109,2.0494930529,2.9269398082\H,-0.713236885,2.0435163163,-0.0220798824\H,1.0358670388,1.92557204,-0.3192765358\H,-0.1055525385,1.475836014,-1.5925341258\H,-2.1730921333,-0.0386222481,-0.1112210151\H,-1.3482727897,-0.6989156424,-1.5446105915\H,-1.4315837923,-1.6466772547,-0.0429834421\H,0.9216438543,-1.9182045909,-0.4267896644\H,1.2798855872,-0.6713203999,-1.6070318329\H,3.2903148495,-0.6418639164,2.2083707535\H,2.120397655,-1.9074631151,1.8449313233\H,2.8375935678,0.5085244969,-0.0126808361\O,4.8274593888,-1.0519578945,0.1003046139\O,3.5113860975,-2.314765987,-1.2253223856\H,5.4942647531,-1.6226016004,-0.3267331697\O,3.5125716974,1.6740785724,-0.3048354888\H,4.396093114,1.3817370912,0.0014692222\\Version=EM64L-G09RevB.01\State=3-A\HF=-748.0131073\S2=2.010153\S2-1=0.\S2A=2.000056\RMSD=7.276e-09\RMSF=7.826e-07\Dipole=1.3546002,-0.4697262,0.1355887\Quadrupole=4.5341013,-3.1888835,-1.3452178

, -0.0424432, 4.8136053, -2.0864015 \PG=C01 [X(C10H19N1O4)] \\@

TS (4-H³) •

1\1\GINC-V1449\FTS\UB3LYP\Gen\C10H19N1O4(3)\GXG501\03-Mar-2011\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IO P(2/17=4) Freq=noramman maxdisk=268435456\\ts43.freq\\0,3\C,0.0004438944,-0.0000349738,0.0004925312\N,0.0009511953,-0.00028421,1.5018050733\C,1.2265084069,0.0016382307,2.3661618112\C,2.3847739006,-0.7002819677,1.6602631573\C,2.5361153322,-0.3773759905,0.183368314\C,1.2255556385,-0.7654277609,-0.5370364645\O,-1.0662692832,0.4478571692,2.0578179546\C,0.8759209186,-0.7430509587,3.6676559434\C,1.6022858597,1.4675612884,2.7014763112\C,-0.0305997208,1.4584416852,-0.502216322\C,-1.2784142218,-0.7257894472,-0.450708316\C,3.7066847033,-1.1051319328,-0.4512526438\H,0.5932955677,-1.7775385336,3.4551947294\H,1.7461700343,-0.7516995074,4.3327816102\H,0.0459496306,-0.2445839075,4.1712269811\H,2.4019150051,1.4907002054,3.4494540796\H,1.9421823638,2.0219718546,1.8209772195\H,0.7219873851,1.971965479,3.1094007345\H,-0.8501876896,1.9923733969,-0.0137968782\H,0.9007781386,1.9944616414,-0.291889291\H,-0.1934189211,1.4799702724,-1.5855210387\H,-2.1633915835,-0.2006921897,-0.0868489465\H,-1.3127697003,-0.7684285952,-1.5449514482\H,-1.2974378553,-1.7484126626,-0.0609013438\H,1.0774139449,-1.8403599899,-0.3884421333\H,1.3071215232,-0.5760108918,-1.612831541\H,3.3126376612,-0.5956254557,2.2310466478\H,2.1488377703,-1.9176040318,1.726321576\H,2.7220256222,0.6959237235,0.0434591443\O,4.1650637943,-0.4502989272,-1.5410430656\O,4.1899756217,-2.1584933018,-0.0836630617\H,4.8805581623,-1.0002126828,-1.9141982769\O,2.0322723295,-3.1941223119,1.5667008528\H,2.883177786,-3.3069470923,1.0911862906\\Version=EM64L-G09RevB.01\\State=3-A\\HF=-748.0145924\\S2=2.010545\\S2-1=0\\.\\S2A=2.000059\\RMSD=1.793e-09\\RMSF=1.063e-06\\Dipole=1.1921194,0.8276479,-1.0644412\\Quadrupole=-0.1719992,-4.7964908,4.9684901,2.0440674,0.734846,2.6880029\\PG=C01 [X(C10H19N1O4)] \\@

TS (5-H³) •

1\1\GINC-V1460\FTS\UB3LYP\Gen\C9H17N1O3(3)\GXG501\03-Mar-2011\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IO P(2/17=4) Freq=noramman maxdisk=268435456\\tst.freq\\0,3\C,0.0000793378,-0.0001095726,-0.000045135\C,-0.0003151023,0.0006388321,1.5503323657\N,1.4141708947,0.0010438992,2.0655279707\C,2.5667596569,0.7506869001,1.4204249679\C,2.4096887732,0.6821078168,-0.1010487152\C,1.0091627929,0.9757877008,-0.5726214674\C,-0.7554584415,1.2303553707,2.0949813477\C,-0.6664701155,-1.2858974094,2.0622695865\O,1.5466780623,-0.2279324134,3.3187901122\C,3.8642662754,0.0494215652,1.8459342287\C,2.5700989475,2.2112245793,1.916228256\H,3.8519230362,-1.0051528562,1.5509662074\H,4.7154191178,0.5390192345,1.3619609174\H,3.9893906983,0.1021791445,2.9285645363\H,3.4627760048,2.7223295041,1.545992731\H,1.7024014957,2.7715855376,1.5566448418\H,2.5684667385,2.2212736348,3.0096692427\H,-0.60861

96946,1.2984945619,3.1763976774\H,-0.4192550722,2.1632632903,1.6333448
131\H,-1.8274300558,1.1272554561,1.8939287384\H,-0.7080032076,-1.28626
66046,3.1528713066\H,-1.6850460726,-1.3550147408,1.6657691916\H,-0.105
3611938,-2.1689079731,1.739154371\H,0.2642281065,-1.0045944695,-0.3572
441325\H,-0.9983010539,0.2463761056,-0.3722661031\H,3.1576524237,1.553
0968006,-0.6248863595\H,2.7659557053,-0.2702237251,-0.512494305\O,0.71
12106525,1.9017788038,-1.3065339568\O,3.5502739262,2.5750127458,-1.223
5591716\H,2.6770539947,2.8436336704,-1.5821224881\Version=EM64L-G09Re
vB.01\State=3-A\HF=-633.4554086\S2=2.010817\S2-1=0.\S2A=2.000062\RMSD=
9.431e-09\RMSF=6.388e-07\Dipole=-0.8086965,-0.7466003,0.0178181\Quadru
pole=2.9603603,2.0046427,-4.9650031,-1.2587266,1.7103318,6.5703373\PG=
C01 [X(C9H17N1O3)]\\@

Biradical (2)

1\1\GINC-V1260\FOpt\UB3LYP\Gen\C9H17N1O2(3)\GXG501\22-Feb-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram an maxdisk=268
435456\\hals2r.freq\\0,3\c,-0.026614337,-0.1534679794,0.0236253524\c,-
0.0079543544,-0.0557476944,1.5642384474\N,1.4127969123,-0.0484474212,2
.062156496\c,2.5618933778,0.6304239264,1.3680998713\c,2.4042973208,0.4
9870371,-0.1634531521\c,0.9955998888,0.7271266987,-0.6106765216\c,-0.7
24070344,1.2235029357,2.0435359324\c,-0.6920826178,-1.2896542992,2.172
123925\O,1.553635856,-0.2005559959,3.3306791534\c,3.8474604787,-0.0779
915179,1.8216453361\c,2.6098048328,2.1134816074,1.7893879073\O,0.75521
05813,0.9765886398,-1.9445489877\H,3.8035466811,-1.1472253684,1.589431
9301\H,4.7085384405,0.355229733,1.3003720634\H,3.9897169528,0.03313378
82,2.8977810311\H,3.554238785,2.5650777595,1.463744151\H,1.7903910831,
2.685307274,1.3442098159\H,2.5464619469,2.188923048,2.878487769\H,-0.5
528936536,1.3642629859,3.114565991\H,-0.372144333,2.1082953004,1.50519
26379\H,-1.8027277069,1.132850065,1.8716633862\H,-0.7185977924,-1.2208
911785,3.2609156895\H,-1.7174455643,-1.3622161274,1.7929049994\H,-0.15
62293296,-2.2045040689,1.8980976775\H,0.1557360669,-1.2047566699,-0.27
14503782\H,-1.029198435,0.1003121201,-0.3391139825\H,3.0978889863,1.20
67707131,-0.6402349513\H,2.7335491035,-0.5125895386,-0.4729687271\H,1.
514786728,1.4555514646,-2.3131484299\Version=EM64L-G09RevB.01\State=3
-A\HF=-558.2732301\S2=2.006681\S2-1=0.\S2A=2.000027\RMSD=6.252e-09\RMS
F=3.882e-06\Dipole=0.3505087,0.4251522,-0.9996154\Quadrupole=2.9078604
,0.8935473,-3.8014077,1.9881764,-4.568272,0.0182635\PG=C01 [X(C9H17N1O
2)]\\@

Alcohol (2)

1\1\GINC-V1265\FOpt\UB3LYP\Gen\C9H18N1O3(2)\GXG501\23-Feb-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram an maxdisk=268
435456\\hals2ad.freq\\0,2\c,-0.0009503451,0.0387294037,-0.0021011723\N
,0.0033317786,0.0068920036,1.4990803117\c,1.2363864065,0.0243327937,2.
3544522999\c,2.368732581,-0.7686120933,1.67031504\c,2.5424340349,-0.51

2631913,0.173071087\c,1.2146162293,-0.7387556763,-0.5512285655\o,-1.07
23125705,0.4224823743,2.0664859661\c,0.8757771122,-0.6761727473,3.6768
356172\c,1.6305913915,1.4870250605,2.6521885746\c,-0.0331254963,1.5039
527569,-0.4856509018\c,-1.2884666414,-0.6704211367,-0.4596777643\o,3.5
226562324,-1.4447061478,-0.2565903653\h,0.523997701,-1.6967640247,3.49
25477571\h,1.7610035389,-0.7254114305,4.3206041008\h,0.0868546921,-0.1
30365189,4.1969097121\h,2.4330055876,1.5119443546,3.3993690566\h,1.978
1527367,2.0055252787,1.7570091413\h,0.764240212,2.0171203298,3.0577993
138\h,-0.847796422,2.0306647193,0.0194090659\h,0.9090987381,2.01816748
9,-0.2913709014\h,-0.217433332,1.5327092556,-1.5660284558\h,-2.1686924
461,-0.1335162995,-0.1020556672\h,-1.3162486076,-0.7128750761,-1.55417
02668\h,-1.3284491278,-1.693738703,-0.0712521701\h,1.0133260268,-1.813
6373998,-0.4871716049\h,1.3385083376,-0.4911342575,-1.6130894546\h,3.3
155582248,-0.5624544813,2.1857987607\h,2.1808167382,-1.8418038743,1.78
56650451\o,2.9845701699,0.8024476287,-0.1332385727\h,3.6496455203,-1.2
91132412,-1.2082870269\h,3.8363211018,0.9193789384,0.3209618915\\Versi
on=EM64L-G09RevB.01\State=2-A\HF=-634.1530238\S2=0.753686\S2-1=0.\S2A=0.
750009\RMSD=7.009e-09\RMSF=7.336e-06\Dipole=1.0554938,-0.1276176,-0.
5588306\Quadrupole=-1.9444689,-1.3469564,3.2914254,2.9483163,2.7186674
,0.9861883\PG=C01 [X(C9H18N1O3)]\\@

TSa- (2)

1\1\GINC-V1334\FTS\UB3LYP\Gen\C9H20N1O4 (2)\GXG501\23-Feb-2011\0\\#B3LY
P/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IO
P(2/17=4) Freq=noraman maxdisk=268435456\hals2ts.freq\\0,2\c,-0.00181
16228,0.0417932484,0.0128068971\N,-0.0800287224,-0.012951301,1.5132766
497\c,1.1060055997,0.0099277407,2.438452359\c,2.2796220463,-0.77575543
45,1.805079464\c,2.4769817703,-0.396567862,0.3432654989\c,1.2462233255
, -0.7349446368,-0.4764403851\o,-1.1892937698,0.3889105531,2.0218635896
\c,0.6775275856,-0.697535943,3.7350541951\c,1.4880298154,1.4710500408,
2.7515976874\c,0.0215699794,1.512787005,-0.4507659882\c,-1.264108834,-
0.6490907909,-0.5296747991\o,3.6193047495,-1.6789467089,-0.1017694706\
H,0.3357246802,-1.717082198,3.5276075247\h,1.5287563185,-0.7492367772,
4.4225492622\h,-0.1370914863,-0.1537630489,4.2165723147\h,2.2242966361
,1.4945018216,3.5633640774\h,1.9262611644,1.9712275326,1.8859261947\h,
0.5965160783,2.0160140033,3.0751369077\h,-0.7964242269,2.0549815057,0.
032048619\h,0.9711651079,1.9973039827,-0.2161965307\h,-0.1221724136,1.
5610582709,-1.5365592706\h,-2.1589486919,-0.1073159128,-0.2187642813\h
, -1.2261392673,-0.677707961,-1.6242575548\h,-1.3368946045,-1.676152301
4,-0.1563973894\h,1.0552434516,-1.8102501456,-0.3986830734\h,1.4208605
937,-0.4855453705,-1.5291487513\h,3.1921228942,-0.5723237999,2.3746559
886\h,2.0740310192,-1.8484506142,1.8685889903\o,3.0851319658,0.7207535
358,0.0539440612\h,3.6248143907,-1.646461475,-1.0751320406\h,4.2738429
103,0.5493385156,0.4665394784\o,5.2433451115,-0.0885834671,0.671735149
7\h,5.9177640513,0.1761220114,0.025888547\h,4.5909133939,-1.0589020187

,0.2506450786\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-710.5395794\\S2=0
.753675\\S2-1=0\\.S2A=0.750009\\RMSD=9.414e-09\\RMSF=4.949e-05\\Dipole=1.12
30488,-0.4716772,-1.1400526\\Quadrupole=-1.8308888,-2.3572142,4.188103,
1.1391372,-2.2637005,1.7042075\\PG=C01 [X(C9H20N1O4)]\\@

O₂

1\\1\\GINC-V1249\\FOpt\\UB3LYP\\Gen\\O2 (3) \\GXG501\\29-Nov-2010\\0\\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramam maxdisk=268435456\\
\\o2.freq\\0,3\\0,0.,0.,0.8412923286\\0,0.,0.,-0.3732923286\\Version=EM64
L-G03RevE.01\\State=3-SGG\\HF=-150.3200401\\S2=2.006605\\S2-1=0\\.S2A=2.000
023\\RMSD=1.061e-09\\RMSF=4.350e-05\\Thermal=0\\.Dipole=0.,0.,0.\\PG=D*H [C
*(O1.O1)]\\@

Peroxy radical (2)

1\\1\\GINC-X118\\FOpt\\UB3LYP\\Gen\\C9H17N1O4 (3) \\GXG501\\04-Mar-2011\\0\\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramam maxdisk=1342
177280\\hals2p.freq\\0,3\\C,0.059000488,-0.061548124,-0.0167386236\\C,0.
0236025835,0.0224944634,1.5248258917\\N,1.4178523165,0.0378831356,2.081
2368095\\C,2.5855004428,0.7311923682,1.4418881422\\C,2.4982840354,0.5996
269876,-0.0935556578\\C,1.1155872184,0.7722938687,-0.7183247668\\C,-0.74
98488376,1.2589920022,2.0322438004\\C,-0.6600832207,-1.2477489175,2.062
5880495\\O,1.5087446105,-0.1445094973,3.349816027\\C,3.8562676366,0.0057
393136,1.9201857629\\C,2.6402790492,2.1993280196,1.9158727868\\O,1.10322
79658,0.4673635062,-2.0674415359\\H,3.8159390014,-1.0584629272,1.665118
2214\\H,4.7352282205,0.4464419188,1.4370732468\\H,3.9628394047,0.0946000
158,3.0023572999\\H,3.5706680544,2.6661719242,1.5728533118\\H,1.80772843
06,2.7947718518,1.5371238491\\H,2.6223874041,2.2216580059,3.0090486978\\
H,-0.666796842,1.3098917376,3.1214355019\\H,-0.3775674227,2.1910943692,
1.6034582884\\H,-1.8093659977,1.1676546153,1.7672945561\\H,-0.7336929971
, -1.2108563763,3.1504711472\\H,-1.6667557528,-1.3307936268,1.6385849127
\\H,-0.0914783642,-2.141961205,1.7864144068\\H,0.2666464161,-1.094492909
2,-0.3187583013\\H,-0.9246739968,0.19520625,-0.4231117067\\H,3.191614097
8,1.3095359056,-0.5600822258\\H,2.8207837386,-0.4058944332,-0.387261668
9\\H,1.6160884273,1.1747662666,-2.5035038427\\O,0.703139075,2.2238502462
, -0.573030103\\O,1.320775877,2.9673146797,-1.4692107234\\Version=EM64L-
G09RevB.01\\State=3-A\\HF=-708.6483187\\S2=2.006977\\S2-1=0\\.S2A=2.000029\\
RMSD=2.120e-09\\RMSF=4.627e-06\\Dipole=0.2020471,-0.2096856,-0.5301563\\Q
uadrupole=6.2023836,-1.209848,-4.9925356,1.6745804,-2.8439481,2.998793
5\\PG=C01 [X(C9H17N1O4)]\\@

TsB- (2)

1\\1\\GINC-X75\\FTS\\UB3LYP\\Gen\\C9H17N1O4 (3) \\GXG501\\05-Mar-2011\\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noramam maxdisk=1342177280\\hals2tso.freq\\0,3\\C,0.110173
474,-0.1277231762,-0.0568441336\\C,0.0429886853,0.0174880492,1.47908501

54\N,1.4251838975,0.0245533809,2.0639011526\C,2.6166247325,0.694761284
4,1.444455319\C,2.5909933569,0.5252297332,-0.0902436025\C,1.2482325633
,0.5513321292,-0.7785033337\C,-0.7148896223,1.2899323664,1.9144279821\
C,-0.6816734601,-1.2129413372,2.055221067\O,1.4840644356,-0.1343964754
,3.3377298844\C,3.8671953617,-0.0158780029,1.9940636777\C,2.660805732,
2.1782928565,1.8690115251\O,1.2235007048,0.579600078,-2.0614325554\H,3
.8269544585,-1.0904453926,1.7865277511\H,4.7621641292,0.3974299735,1.5
16095019\H,3.9446215063,0.1211512869,3.0734985209\H,3.6157680203,2.621
5515462,1.5642539497\H,1.8612431634,2.7704906645,1.4204970339\H,2.5820
239233,2.2405690433,2.9580966932\H,-0.6506858311,1.3894059444,3.001705
45\H,-0.3210674698,2.1961307174,1.4508981565\H,-1.7713989048,1.2043398
193,1.6355466534\H,-0.7907742824,-1.1240197468,3.1369519956\H,-1.67524
44169,-1.2976289621,1.6014574051\H,-0.1222486051,-2.1297280966,1.84092
19389\H,0.2400733196,-1.192161872,-0.3071189364\H,-0.8385310355,0.1751
918898,-0.5106091438\H,3.2558690408,1.2530076865,-0.5656256406\H,2.995
7012378,-0.4668173744,-0.3443736201\H,0.9207572162,1.7184298682,-2.300
9126992\O,0.7309609354,2.5252977269,-0.612058049\O,0.6368797498,2.8183
845997,-1.8692701508\\Version=EM64L-G09RevB.01\\State=3-A\\HF=-708.63049
07\\S2=2.008882\\S2-1=0.\\S2A=2.000048\\RMSD=7.828e-09\\RMSF=9.951e-06\\Dipo
le=0.0657265,-0.2664326,-0.2994835\\Quadrupole=6.9006673,0.3796542,-7.2
803215,1.8879354,-1.0107935,3.0879362\\PG=C01 [X(C9H17N1O4)]\\@

HOO•

1\1\GINC-V1252\FOpt\UB3LYP\Gen\H1O2(2)\DMM574\28-Oct-2010\0\\#B3LYP/ge
n 6D OPT IOP(2/17=4) Freq=noramman maxdisk=268435456\\ho2.freq\\0,2\O,-
0.0360039241,0.,0.0458710795\O,0.032225635,0.,1.3758922805\H,0.8994468
786,0.,-0.2584300267\\Version=EM64L-G09RevA.02\\State=2-A"\\HF=-150.8991
566\\S2=0.752677\\S2-1=0.\\S2A=0.750005\\RMSD=8.747e-09\\RMSF=2.327e-05\\Dip
ole=0.6777349,0.,-0.5813817\\Quadrupole=0.3877755,-0.2883036,-0.0994719
,0.,-1.2654171,0.\\PG=CS [SG(H1O2)]\\@

Biradical (3)

1\1\GINC-V1330\FOpt\UB3LYP\Gen\C10H19N1O2(3)\GXG501\22-Feb-2011\0\\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramman maxdisk=26
8435456\\hals3r.freq\\0,3\C,-0.0313259595,-0.1047864496,-0.0037190936\
C,-0.0101130629,-0.0478776504,1.5384587333\N,1.4115286793,-0.034140286
5,2.0290611588\C,2.5464320433,0.6712545986,1.3400872205\C,2.3827961806
,0.5820425536,-0.1952963387\C,0.9659792056,0.8182013281,-0.623437138\C
, -0.7413289549,1.2086184994,2.0538838796\C,-0.6752639324,-1.306511188,
2.1161584893\O,1.5623619768,-0.2117986249,3.2932013839\C,3.8422239549,
-0.03789518,1.7632730646\C,2.5866537077,2.1430835183,1.8003399103\O,0.
6531547219,1.1283601536,-1.9238386231\C,1.5204526225,2.00549182,-2.628
9656769\H,3.8059082481,-1.1004397572,1.5007835249\H,4.6953952237,0.417
6881655,1.2481816442\H,3.9916686387,0.0436252423,2.8411449129\H,3.5242
689039,2.6109908115,1.4780203776\H,1.7586084032,2.7192425938,1.3770840

004\H,2.5323984383,2.1894919588,2.8915586285\H,-0.5690459867,1.3224851
666,3.1279341149\H,-0.4012622085,2.1119275662,1.5390452517\H,-1.819268
3563,1.1094733743,1.8819452303\H,-0.6951043097,-1.2679043592,3.2066290
501\H,-1.7022088186,-1.3817480059,1.7417579743\H,-0.1297795249,-2.2066
535167,1.8137128604\H,0.1753441986,-1.1437969874,-0.3240760754\H,-1.04
0623673,0.1344483859,-0.35681441\H,3.082804336,1.2942091222,-0.6455713
221\H,2.705725066,-0.4240057795,-0.5286092162\H,1.0108290027,2.2504619
814,-3.5633477954\H,1.7012011134,2.9280391089,-2.0618419352\H,2.482557
271,1.5317365159,-2.8628212353\\Version=EM64L-G09RevB.01\\State=3-A\\HF=
-597.5789621\\S2=2.006713\\S2-1=0.\\S2A=2.000027\\RMSD=5.603e-09\\RMSF=2.75
4e-06\\Dipole=0.2352502,0.531988,-1.1569915\\Quadrupole=2.4027923,0.9975
729,-3.4003652,1.6664658,-3.4913574,-0.1258318\\PG=C01 [X(C10H19N1O2)]\\
\@

Alcohol (3)

1\1\GINC-V1337\FOpt\UB3LYP\Gen\C10H20N1O3(2)\GXG501\23-Feb-2011\0\\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram an maxdisk=26
8435456\\hals3ad.freq\\0,2\C,-0.0174565805,0.0307629713,-0.003926452\N
,0.0152721498,-0.0176780405,1.4943038139\C,1.2615982152,0.0712815827,2
.3252480146\C,2.4427302401,-0.6168305576,1.6050707261\C,2.556503158,-0
.3552723623,0.1010282202\C,1.2241952281,-0.6775182419,-0.5808660522\O,
-1.0739770556,0.3206606136,2.086666237\C,0.9780245139,-0.6859986262,3.
635560251\C,1.5558184014,1.550822162,2.6528872738\C,-0.1377330542,1.49
91089622,-0.4658411079\C,-1.2736426935,-0.7381706423,-0.4520351236\O,3
.4858032948,-1.2270681477,-0.5314212694\H,0.6955718353,-1.7244542172,3
.431753161\H,1.8766995771,-0.6868955137,4.2622983767\H,0.1626975913,-0
.2103507932,4.1832522896\H,2.3499354637,1.6117761665,3.4062859144\H,1.
8841087486,2.1056040779,1.7728901563\H,0.6533734357,2.0141529542,3.061
6512794\H,-0.9891643767,1.9654095961,0.0379229685\H,0.7640414057,2.071
8564579,-0.2429857328\H,-0.3126157084,1.5365888989,-1.5478909077\H,-2.
1747472182,-0.2546235915,-0.0712091477\H,-1.3177422208,-0.7659367081,-
1.5464600925\H,-1.2522857867,-1.7678668902,-0.0797498827\H,1.08935494,
-1.7620725872,-0.5066238916\H,1.3049985852,-0.4493678371,-1.6515001131
\H,3.367726945,-0.3133114722,2.1060371481\H,2.3495314131,-1.7030394261
,1.719152397\O,2.9626384553,0.9940823143,-0.077416161\C,4.8273258619,-
1.1750310796,-0.0586055293\H,5.4309459362,-1.7075741816,-0.7978821284\
H,5.184235716,-0.1422272592,0.0256544003\H,4.9411138393,-1.675799464,0
.912295784\H,3.0116675197,1.1443733702,-1.0368534539\\Version=EM64L-G0
9RevB.01\\State=2-A\\HF=-673.4572777\\S2=0.753683\\S2-1=0.\\S2A=0.750009\\RM
SD=9.654e-09\\RMSF=5.208e-06\\Dipole=1.0927556,-0.1314179,-0.6453127\\Qua
drupole=-1.7743096,-0.5240044,2.2983141,0.2516201,3.4976442,-2.6333084
\PG=C01 [X(C10H20N1O3)]\\@\n

TSa- (3)

1\1\GINC-V1485\FTS\UB3LYP\Gen\C10H22N1O4(2)\GXG501\23-Feb-2011\0\\#B3L

```
YP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) I
OP(2/17=4) Freq=noram maxdisk=268435456\\hals3ts.freq\\0,2\C,-0.1093
186276,0.0132564502,0.0411378743\N,-0.0175428731,-0.0466729375,1.54048
60613\C,1.2558189053,0.0876273137,2.3268683881\C,2.426852088,-0.573651
756,1.5564144905\C,2.4210993069,-0.192058364,0.0905999928\C,1.13810525
34,-0.6536969942,-0.5876120426\O,-1.0934004646,0.2506890138,2.17668671
97\C,1.0473428075,-0.6626883891,3.6531342452\C,1.5319084484,1.57773872
54,2.6150481254\C,-0.2704178829,1.4801313861,-0.4077087381\C,-1.357647
6875,-0.7875529287,-0.3656935171\O,3.5226576499,-1.36573877,-0.6888374
039\H,0.7802456856,-1.7090444143,3.4706911107\H,1.9718796339,-0.635901
2347,4.2403308336\H,0.2452873016,-0.2002589645,4.2309011708\H,2.337640
1997,1.6690069773,3.3528021704\H,1.8381442301,2.1157393384,1.715938250
3\H,0.6294739868,2.0373968049,3.0279945272\H,-1.0873822589,1.941963194
1,0.1542103284\H,0.6448874443,2.0554220606,-0.2557583467\H,-0.51763152
51,1.5153908449,-1.4749811015\H,-2.2574544032,-0.3294656606,0.04866071
88\H,-1.4382871047,-0.810939629,-1.4578383234\H,-1.2957265242,-1.81775
30928,0.0006304785\H,1.0586862676,-1.7401483632,-0.4857940555\H,1.1652
914527,-0.4162594206,-1.6555128256\H,3.3655226374,-0.264034681,2.02518
56297\H,2.3393996367,-1.6624728195,1.6358726572\O,2.9163838625,0.97739
40608,-0.2154005847\C,4.8258705515,-1.3779978116,-0.1063082958\H,5.525
4914842,-1.821169959,-0.8238205038\H,5.1565401156,-0.3607440947,0.1429
083414\H,4.8195922928,-1.9915370552,0.799032054\H,3.1736696562,0.88354
87234,-1.4283782993\O,3.5116278328,0.2972876116,-2.423723249\H,4.39033
90586,0.6143612874,-2.6856602167\H,3.6062395614,-0.7083064524,-1.68267
56647\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-749.8451133\\S2=0.753671\\
S2-1=0.\\S2A=0.750009\\RMSD=6.665e-09\\RMSF=9.279e-06\\Dipole=1.5904217,-0
.4368755,-0.3251506\\Quadrupole=2.9991389,-1.5119679,-1.4871711,-0.6699
885,1.8791255,-1.4339292\\PG=C01 [X(C10H22N1O4)]\\@
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CH₃OH

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1\\1\\GINC-V1340\\FOpt\\RB3LYP\\Gen\\C1H4O1\\GXG501\\22-Feb-2011\\0\\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram maxdisk=268435456
\\ch3oh.freq\\0,1\C,-0.0181793569,-0.0000159524,0.0064370713\H,0.01970
31172,-0.0321638113,1.1066797359\H,1.0089949566,0.0183690942,-0.367981
6639\O,-0.6519908347,1.1693569907,-0.4855686582\H,-1.564779739,1.16684
8822,-0.161313751\H,-0.4959889476,-0.9253700919,-0.3519205701\\Version
=EM64L-G09RevB.01\\State=1-A'\\HF=-115.7144055\\RMSD=3.367e-09\\RMSF=9.702
e-05\\Dipole=-0.3216225,-0.4401479,0.3832448\\Quadrupole=1.7168189,-0.94
36857,-0.7731332,-0.7251856,-0.389062,0.4425577\\PG=CS [SG(C1H2O1),X(H2
)]\\@
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Peroxy radical (3)

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1\\1\\GINC-X86\\FOpt\\UB3LYP\\Gen\\C10H19N1O4(3)\\GXG501\\04-Mar-2011\\0\\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noram maxdisk=1342
177280\\hals3p.freq\\0,3\C,-0.0601105089,0.0256338383,0.021591994\N,-0
```

.0154326952,-0.0671463266,1.5180084951\c,1.2323053166,0.0673728238,2.3
378323124\c,2.4300691543,-0.5877605149,1.612273334\c,2.5155929015,-0.3
795012352,0.1004144061\c,1.186203786,-0.6460502282,-0.5897912837\o,-1.
1107431477,0.214575413,2.1282308869\c,0.9897332983,-0.6960349542,3.652
8844124\c,1.4819414387,1.5558961882,2.663896835\c,-0.2184195951,1.5024
906947,-0.4006219077\c,-1.3028312927,-0.7569807995,-0.4406717852\o,3.4
475117401,-1.19491783,-0.5336665923\h,0.7317828869,-1.7415615233,3.453
6676018\h,1.8972603365,-0.6716106937,4.2662014424\h,0.1700772857,-0.24
21914281,4.2118893843\h,2.284118894,1.6440816446,3.4057415233\h,1.7746
597315,2.132291691,1.7847428202\h,0.5696301502,1.9861579266,3.08617390
22\h,-1.0823458191,1.9296049476,0.1164155918\h,0.6617654582,2.10498652
99,-0.1714208409\h,-0.3923681859,1.5627529479,-1.4807407152\h,-2.21216
17713,-0.2985471391,-0.049084523\h,-1.346971198,-0.7612952061,-1.53517
06348\h,-1.2619866625,-1.7937710441,-0.0904448025\h,1.0592936248,-1.73
37963888,-0.5643259994\h,1.2863918922,-0.3579952713,-1.6401070375\h,3.
3510734413,-0.2451989067,2.0955325335\h,2.3793018686,-1.6745480919,1.7
486221341\o,2.9347192131,1.0513701496,-0.0694366339\c,4.7992167389,-1.
1425293988,-0.077269391\h,5.3698444348,-1.7463146844,-0.7853253084\h,5
.1864878648,-0.1182012697,-0.0839846542\h,4.9110166566,-1.5717547353,0
.9260904168\o,3.0454738513,1.3911101993,-1.3428100234\\Version=EM64L-G
09RevB.01\State=3-A\HF=-747.9491275\S2=2.006936\S2-1=0.\S2A=2.000029\R
MSD=5.246e-09\RMSF=1.009e-05\Dipole=0.9102081,-0.6519895,0.2359707\Qua
drupole=0.4176883,0.2600828,-0.6777711,-2.6148314,6.8896584,0.9350728\
PG=C01 [X(C10H19N1O4)]\\@

TSb-(3)

1\1\GINC-V1331\FTS\UB3LYP\Gen\C10H19N1O4(3)\GXG501\06-Mar-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) I
OP(2/17=4) Freq=noramam maxdisk=268435456\hals3tso.freq\0,3\c,0.0079
677556,0.0114882388,0.0129854073\N,0.0054640938,-0.0558238446,1.513267
2111\c,1.2317134693,0.0363762491,2.3725894206\c,2.4158408736,-0.674945
2424,1.6823145504\c,2.5549004646,-0.421191684,0.1847021161\c,1.2516661
695,-0.7057256712,-0.5537528062\o,-1.0955412054,0.2797392735,2.0844550
682\c,0.9187280803,-0.7038675209,3.6854157478\c,1.535410608,1.51643732
8,2.6880617678\c,-0.0768579427,1.4850699411,-0.4387360276\c,-1.2470874
275,-0.73633841,-0.4711053929\o,3.5275364651,-1.3586613426,-0.36336103
05\h,0.62830112,-1.7411936165,3.4878676125\h,1.8061773454,-0.706768770
4,4.3278527563\h,0.0990416144,-0.2136376,4.2128516716\h,2.323722886,1.
5803721348,3.447043499\h,1.8713286413,2.0669672758,1.8076715146\h,0.63
25175523,1.9895361087,3.0841433274\h,-0.9208781296,1.9659274293,0.0639
517641\h,0.8362559964,2.0398623106,-0.2175070174\h,-0.2421322322,1.531
3304813,-1.5209745578\h,-2.1502817893,-0.2394653221,-0.1133277456\h,-1
.2610613941,-0.7585530678,-1.5662014317\h,-1.2526607886,-1.7675311913,
-0.1022103186\h,1.1018104925,-1.7900562416,-0.5095898366\h,1.38209039,
-0.4351543882,-1.6048543925\h,3.3483817211,-0.4002730311,2.1870292316\

H,2.2966279814,-1.7587359647,1.7870293401\O,3.0433366814,0.8989413652,
0.0235721346\C,4.7248353267,-0.8195862075,-0.763053883\H,5.2538420601,
-1.51786451,-1.4096423294\H,4.2726645799,0.3094302374,-1.3956823153\H,
5.3245260336,-0.3414784765,0.0213846845\O,3.3757540817,1.1131147848,-1
.3468919132\\Version=EM64L-G09RevB.01\\State=3-A\\HF=-747.9082529\\S2=2.0
09535\\S2-1=0\\.S2A=2.000051\\RMSD=6.271e-09\\RMSF=2.666e-05\\Dipole=1.0601
958,-0.7051036,-0.1407451\\Quadrupole=0.0922776,-1.2660516,1.1737739,-1
.9265812,3.9849324,1.6036284\\PG=C01 [X(C10H19N1O4)]\\@

CH₂O

1\\1\\GINC-X7\\FOpt\\RB3LYP\\Gen\\C1H2O1\\GXG501\\03-Mar-2011\\0\\#B3LYP/gen 6D
INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1342177280\\
ch2o.freq\\0,1\C,0.,0.,1.0522539354\O,0.,0.,-0.154294873\H,0.,0.938190
2021,1.6456704688\H,0.,-0.9381902021,1.6456704688\\Version=EM64L-G09Re
vB.01\\State=1-A1\\HF=-114.5004721\\RMSD=3.661e-09\\RMSF=1.734e-04\\Dipole=
0.,0.,0.8604581\\Quadrupole=0.1547925,0.0806527,-0.2354452,0.,0.,0.\\PG=
C02V [C2(C1O1),SGV(H2)]\\@

Biradical (4)

1\\1\\GINC-V1331\\FOpt\\UB3LYP\\Gen\\C10H17N1O3(3)\\GXG501\\22-Feb-2011\\0\\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\\hals4r.freq\\0,3\C,0.0965164043,-0.3614029333,-0.0481752286\C
,0.0296874008,-0.1080803495,1.4830815102\N,1.4213817,-0.0229748358,2.0
475139953\C,2.5958229023,0.596707031,1.3427231667\C,2.5150922338,0.299
7449308,-0.1810844232\C,1.134169511,0.4733035889,-0.7121330402\C,-0.73
40063869,1.1956807087,1.7898500771\C,-0.6676616931,-1.2921592059,2.168
4828363\O,1.4964038457,-0.0357714727,3.3307244399\C,3.8653959804,-0.04
45712023,1.9216909435\C,2.6135386337,2.1163008775,1.6036285768\C,0.766
0126959,1.3915274507,-1.7714545637\O,-0.3735732978,1.5518208582,-2.193
9700991\O,1.822829391,2.0925991925,-2.2817422698\H,3.8409326728,-1.132
5628154,1.7994818836\H,4.7453009482,0.3448481408,1.3980143227\H,3.9564
163571,0.1781143151,2.9861451568\H,3.558647869,2.5450748144,1.25227009
23\H,1.8003371728,2.63222337,1.0845186809\H,2.5218948447,2.3042977112,
2.6770359405\H,-0.6403253674,1.4336527069,2.8531767237\H,-0.3593268348
,2.0400289679,1.2038136917\H,-1.7956893142,1.0712622333,1.5501721649\H
, -0.7510494846,-1.1188935651,3.2427469317\H,-1.6707343825,-1.420501258
5,1.7474847879\H,-0.10389208,-2.218016279,2.0124888882\H,0.3492209753,
-1.4223386753,-0.2045733952\H,-0.8879179596,-0.1848804767,-0.488072175
3\H,3.2389276748,0.9279090367,-0.704498103\H,2.8150353236,-0.749198775
3,-0.3358237728\H,1.4430200629,2.6631720788,-2.9743496021\\Version=EM6
4L-G09RevB.01\\State=3-A\\HF=-671.6377985\\S2=2.010488\\S2-1=0\\.S2A=2.0000
63\\RMSD=9.994e-09\\RMSF=1.163e-05\\Dipole=0.4742039,0.0463509,-0.5951798
\\Quadrupole=1.3056653,4.02741,-5.3330753,1.983889,-4.6479926,0.6159677
\\PG=C01 [X(C10H17N1O3)]\\@

Alcohol (4)

```
1\1\GINC-V1275\FOpt\UB3LYP\Gen\C10H18N1O4(2)\GXG501\23-Feb-2011\0\\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\hals4ad.freq\\0,2\C,0.0166717111,0.0278073091,0.0201247828\N,
-0.0043691011,-0.0149648736,1.5188626106\C,1.2145500882,0.0287657615,2
.3910200423\C,2.3738635005,-0.7428869994,1.7230750609\C,2.5674823142,-
0.4560399452,0.2196661634\C,1.2424258181,-0.7437685218,-0.5163378726\O
,-1.0981621505,0.3726784964,2.0713068872\C,0.8506537749,-0.6863486314,
3.7053185162\C,1.5788357239,1.4964859913,2.7002655426\C,-0.016638291,1
.4952125994,-0.4575115494\C,-1.2569925899,-0.6880466397,-0.4661871737\
C,3.6666894392,-1.3703936206,-0.3357682239\H,0.5145498914,-1.710778204
8,3.5122825452\H,1.7295642594,-0.7254586125,4.3583065719\H,0.048882706
8,-0.1543507527,4.2199595062\H,2.3594783317,1.5288498497,3.4694673555\
H,1.9534451538,2.0187534694,1.8195831341\H,0.6930797483,2.01139508,3.0
833234132\H,-0.8506411489,2.0101673461,0.0279660865\H,0.9144057681,2.0
17900662,-0.2369405581\H,-0.1727685657,1.5268361753,-1.5422920129\H,-2
.1471204149,-0.1561191477,-0.1264219858\H,-1.2612080331,-0.7278692008,
-1.5610854206\H,-1.3006562356,-1.7122393313,-0.0804320847\H,1.04337770
3,-1.8183454261,-0.4408595199\H,1.3628947407,-0.5068259647,-1.57975976
87\H,3.3012898354,-0.5053473238,2.2568918168\H,2.1953009288,-1.8174320
034,1.8391625769\O,2.9972479846,0.8786364453,0.0022980718\O,3.41297425
65,-2.6849598569,-0.205878751\O,4.6806785822,-0.9403020247,-0.85031122
19\H,4.175327281,-3.1573895318,-0.5918046699\H,3.866102762,0.816759705
5,-0.439288219\\Version=EM64L-G09RevB.01\State=2-A\HF=-747.4961845\S2=
0.753676\S2-1=0.\S2A=0.750009\RMSD=4.573e-09\RMSF=7.540e-06\Dipole=0.9
723441,-1.0154859,-0.4915543\Quadrupole=-5.273372,3.7695423,1.5038297,
-2.894955,4.6003874,1.4606581\PG=C01 [X(C10H18N1O4)]\\@
```

TSa- (4)

```
1\1\GINC-V1269\FTS\UB3LYP\Gen\C10H20N1O5(2)\GXG501\25-Feb-2011\0\\#B3L
YP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) I
OP(2/17=4) Freq=noraman maxdisk=268435456\hals4ts.freq\\0,2\C,0.01245
28149,0.1252930002,-0.000072901\N,0.0032901285,-0.0596702238,1.4920764
955\C,1.2147116321,0.0239765598,2.3786004871\C,2.4476173867,-0.5715782
402,1.6352386087\C,2.4948719747,-0.071329188,0.2256302048\C,1.31358981
64,-0.4889108652,-0.6051980916\O,-1.1188156473,0.1752888559,2.07024975
36\C,0.9286078392,-0.8277515545,3.6250573414\C,1.4602366784,1.48836277
08,2.7917219629\C,-0.1182650307,1.6231291801,-0.3390562038\C,-1.194284
9804,-0.642208047,-0.5625386135\C,4.0746180484,-1.6992090727,-0.624710
2862\H,0.6881773826,-1.8583328632,3.3445272526\H,1.8114017655,-0.83866
71114,4.2730529375\H,0.0837687242,-0.4164440329,4.180162633\H,2.219412
3869,1.5292337468,3.5805492285\H,1.8123683428,2.1021515756,1.958935833
\H,0.53032759,1.9130170399,3.1804326789\H,-0.972342217,2.0415309585,0.
201013192\H,0.7784986576,2.1896104473,-0.0750425033\H,-0.2902685482,1.
7480260168,-1.4139420923\H,-2.1245087022,-0.222055673,-0.176060697\H,-
```

1.1967258175,-0.5731205611,-1.6554661031\H,-1.14841205,-1.6987425737,-
0.2799430557\H,1.2398003487,-1.578282255,-0.5969685616\H,1.4116383036,
-0.1556672901,-1.6412911475\H,3.363672702,-0.3024726426,2.1656454561\H
,2.355542675,-1.6609533704,1.6136741414\O,3.1626144934,0.9962480153,-0
.0227703857\O,3.3686193813,-2.8742828533,-0.7462279895\O,5.1730025681,
-1.7066635778,-0.0988517789\H,3.9416217142,-3.5786473186,-0.3710346487
\H,3.4335467424,0.9724976133,-1.1403100952\O,3.8368080433,0.4049379946
,-2.2235822207\H,3.8485620377,-0.5730935898,-1.6430795707\H,4.77624278
28,0.621207628,-2.3538911216\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-8
23.8242356\S2=0.753656\S2-1=0.\S2A=0.750009\RMSD=6.646e-09\RMSF=1.180e
-05\Dipole=-0.0247997,0.2310477,-0.1496704\Quadrupole=-7.6734316,4.160
8723,3.5125593,2.6947888,2.6268124,-2.6736592\PG=C01 [X(C10H20N1O5)]\\
@

HCOOH

1\1\GINC-V1341\FOpt\RB3LYP\Gen\C1H2O2\GXG501\22-Feb-2011\0\\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramam maxdisk=268435456
\hcooh.freq\\0,1\c,0.0543702606,0.,-0.0027628752\o,-0.0469921574,0.,1
.3407778477\H,0.8663113298,0.,1.6901002352\o,1.0881651692,0.,-0.621782
1635\H,-0.9527366848,0.,-0.4441663776\\Version=EM64L-G09RevB.01\\State=
1-A'\\HF=-189.755457\RMSD=6.413e-09\RMSF=2.072e-04\Dipole=-0.2543672,0.
,0.5011388\Quadrupole=0.023074,0.2317522,-0.2548262,0.,3.3480769,0.\PG
=CS [SG(C1H2O2)]\\@

Peroxy radical (4)

1\1\GINC-X74\FOpt\UB3LYP\Gen\C10H17N1O5(3)\GXG501\04-Mar-2011\0\\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramam maxdisk=1342
177280\\hals4p.freq\\0,3\c,-0.047783592,0.0296332722,0.0276875574\N,-0
.0345782168,-0.0472332261,1.5254901242\c,1.2010771443,0.0408305844,2.3
679714059\c,2.3789549312,-0.673947831,1.6678088103\c,2.5088716549,-0.4
469864329,0.1570345463\c,1.1840297979,-0.6920668382,-0.5580979029\o,-1
.1276157783,0.2889625328,2.1112942635\c,0.9042719955,-0.7015421037,3.6
838313959\c,1.5136436452,1.5190503074,2.6860075098\c,-0.1425238591,1.5
065347449,-0.4133938104\c,-1.3086144891,-0.7137903498,-0.4497429972\c,
3.6008936024,-1.380670597,-0.3979888232\H,0.6040534594,-1.7363405432,3
.4879193762\H,1.8012177199,-0.71117677,4.3128118365\H,0.0957822139,-0.
2077327147,4.2248441449\H,2.3139701051,1.5772643802,3.4325171581\H,1.8
364779086,2.077337255,1.8057445706\H,0.6178096941,1.9910847648,3.09888
24163\H,-0.9993913306,1.9723710375,0.0813122573\H,0.7556599736,2.07751
73929,-0.1722723397\H,-0.292961913,1.561196875,-1.4973964737\H,-2.2078
558829,-0.2191581804,-0.0794863014\H,-1.3334907598,-0.7282989841,-1.54
47206572\H,-1.3106128353,-1.7475534646,-0.0886503953\H,1.0214480901,-1
.7737305699,-0.5293592322\H,1.2960960039,-0.4219738709,-1.6125994403\H
,3.31518799,-0.392369535,2.160669741\H,2.2604413018,-1.756490068,1.800
1800713\o,2.9716886436,0.9411784986,-0.0307069566\o,4.8366080222,-0.95

```
8923054,-0.0651966262\O,3.3823378253,-2.4039627291,-1.0028269885\H,5.4
599420808,-1.6111115472,-0.4380822133\O,3.2513119902,1.1891959289,-1.3
002923049\\Version=EM64L-G09RevB.01\\State=3-A\\HF=-821.9858707\\S2=2.006
88\\S2-1=0.\\S2A=2.000029\\RMSD=8.087e-09\\RMSF=5.646e-06\\Dipole=0.7991828
,-0.459863,0.2510107\\Quadrupole=1.230472,-1.6112009,0.3807289,-3.07265
03,5.7814987,-1.0198476\\PG=C01 [X(C10H17N1O5)]\\@
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TSb-(4)

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1\\1\\GINC-X71\\FTS\\UB3LYP\\Gen\\C10H17N1O5(3)\\GXG501\\05-Mar-2011\\0\\#B3LYP
/gen 6D INT(grid=ultrafine) OPT=(TS, calcfc, noeigentest, maxcyc=200) IOP
(2/17=4) Freq=noraman maxdisk=1342177280\\hals4tso.freq\\0,3\c,0.05314
03162,0.050091318,0.0165204461\N,-0.0136345808,-0.0586359283,1.5099286
771\c,1.1758424443,0.0141628829,2.4215004072\c,2.3905487424,-0.6879396
973,1.7700608827\c,2.5849450028,-0.4158927453,0.2891748069\c,1.3064372
968,-0.6816533071,-0.5198238348\O,-1.1361485745,0.2744522938,2.0380901
788\c,0.8101050649,-0.7535854542,3.7042095534\c,1.468560488,1.48632452
49,2.7789205205\c,0.0149565477,1.5340108377,-0.4024369007\c,-1.1859992
307,-0.6690047522,-0.547027768\c,3.7183892515,-1.4774393464,-0.3736885
386\H,0.5273830229,-1.7855156683,3.4721283738\H,1.6716526209,-0.772489
0559,4.3802981454\H,-0.0285408697,-0.2728477585,4.2101553007\H,2.22449
41678,1.5329767608,3.5707898699\H,1.8411344017,2.0597881438,1.92723231
8\H,0.5513550163,1.9555378707,3.1454333243\H,-0.8474589679,2.013136793
6,0.0693854013\H,0.9175763474,2.0772048022,-0.1160841186\H,-0.09149410
76,1.6131949015,-1.48982282\H,-2.0957276988,-0.1697660207,-0.209667674
8\H,-1.1559044067,-0.6561016336,-1.6417704467\H,-1.2196732068,-1.70996
21218,-0.2096000302\H,1.1393240856,-1.7631003454,-0.4772439782\H,1.460
8442656,-0.413733539,-1.5675290633\H,3.2977065389,-0.4187534422,2.3209
576724\H,2.2819268947,-1.7721243628,1.8578364457\O,3.1260504728,0.8719
854408,0.1461136215\O,4.2360908027,-0.9936390305,-1.4304979168\O,3.825
3738191,-2.540448034,0.1953359351\H,3.8303110742,0.1948046973,-1.51326
09995\O,3.3839379582,1.2102069756,-1.1724587907\\Version=EM64L-G09RevB
.01\\State=3-A\\HF=-821.9617331\\S2=2.007257\\S2-1=0.\\S2A=2.000033\\RMSD=5.
194e-09\\RMSF=7.679e-06\\Dipole=-0.3365669,0.2998463,0.0798653\\Quadrupol
e=-5.5140876,-0.7305069,6.2445946,4.102217,7.7939928,-0.4311335\\PG=C01
[X(C10H17N1O5)]\\@
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CO₂

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1\\1\\GINC-V1266\\FOpt\\RB3LYP\\Gen\\C1O2\\GXG501\\02-Dec-2010\\0\\#B3LYP/gen 6
D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\
co2.freq\\0,1\c,0.,-0.4070327273,0.9060998182\O,0.,0.4022191135,0.0622
640269\O,0.,-1.2162845681,1.7499356094\\Version=EM64L-G03RevE.01\\State
=1-SGG\\HF=-188.5809394\\RMSD=1.134e-09\\RMSF=6.225e-06\\Thermal=0.\\Dipole
=0.,0.,0.\\PG=D*H [O(C1),C*(O1.O1)]\\@
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TS (2-O-H⁴)•

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1\\1\\GINC-X154\\Freq\\UHF\\Gen\\C9H19N1O3(3)\\GXG501\\22-Mar-2011\\0\\#N Geom=
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AllCheck Guess=TCheck SCRF=Check Test GenChk UHF/ChkBasis Freq\\ts24.2.f
req\\0,3\C,-0.0319261057,0.0305358054,-0.0100270465\N,0.0169798096,-0.
0206300884,1.4724737293\C,1.2511045379,-0.0471059304,2.2956462597\C,2.
3409504986,-0.854132739,1.5726728469\C,2.4615461965,-0.5166036426,0.09
45745072\C,1.1338783789,-0.7801309883,-0.598271714\O,-1.0115695989,0.4
127001064,2.0601197225\C,0.9111306349,-0.7474460092,3.6157909115\C,1.7
18446721,1.3863184942,2.5964877812\C,-0.0001501441,1.4905710576,-0.490
5006071\C,-1.352042875,-0.6106394524,-0.4513224023\O,3.5302115983,-1.1
939956554,-0.5226217128\H,0.4954156589,-1.7311869631,3.429857962\H,1.8
131394837,-0.8623623809,4.2088361798\H,0.1929715892,-0.1770450942,4.18
72810827\H,2.5398161946,1.3668491725,3.305621168\H,2.0605566726,1.9088
783354,1.7114024475\H,0.9060033271,1.9553661298,3.0308079457\H,-0.7809
292498,2.0576584096,0.0007914633\H,0.9470138226,1.9764216467,-0.289357
8097\H,-0.1700348429,1.5311973349,-1.561567772\H,-2.1998304164,-0.0322
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4413826807,-1.6141948502,-0.0514594037\H,0.9151672038,-1.8395652444,-0
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2.754123945,0.5213614878,-0.0299266634\H,3.2959757152,-2.3057524397,-0
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6\ZeroPoint=0.2926991\Thermal=0.3069849\Dipole=0.8196254,0.0445161,0.0
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(2-OH⁴)•

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P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramman maxdisk=1342
177280\\hals2or.freq\\0,3\C,-0.02385972,0.0187660038,-0.0123169396\N,-
0.002889015,-0.0048323518,1.4910361964\C,1.2425862654,-0.0100626975,2.
333441861\C,2.3567158842,-0.8157780022,1.6364690899\C,2.4936889322,-0.
5119029283,0.1368265854\C,1.1618068905,-0.7885705626,-0.5767947318\O,-
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6671657863\C,1.6796436342,1.4457819083,2.6023976195\C,0.0060529599,1.4
838791721,-0.4974884922\C,-1.3432706338,-0.6348406551,-0.4556970654\O,
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0.1203987403,4.1877443284\H,2.4760193323,1.4654322063,3.3546048112\H,2
.056739354,1.9447041021,1.7036773182\H,0.8273372357,2.0176282403,2.979
6619925\H,-0.7711022811,2.0540092643,0.0189841038\H,0.9693822089,1.969
4640477,-0.3103343771\H,-0.1856104015,1.5260183025,-1.575405744\H,-2.1
979602892,-0.0679194892,-0.0824508745\H,-1.3867946594,-0.6706957614,-1
.5496959329\H,-1.4151300122,-1.6578933014,-0.0720142596\H,0.9552480476
,-1.8619130808,-0.4758048356\H,1.2644605223,-0.5801242866,-1.647105121
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\RMSD=3.445e-09\RMSF=1.668e-05\Di pole=0.270272,0.1927974,-0.1442854\Qu
adrupole=-5.300147,2.6299959,2.6701511,3.6357705,6.1611853,-2.0048593\
PG=C01 [X(C9H17N1O2)]\\@