

Ring-Enlargement Reactions of Donor-Acceptor-Substituted Cyclopropanes: Which Combinations are Most Efficient?

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SUPPORTING INFORMATION

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Donor-Acceptor Cyclopropanes

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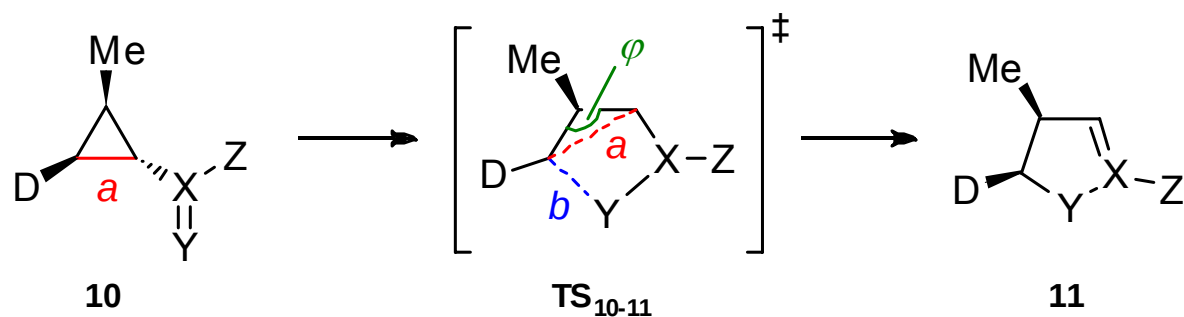


Table S1 (OMe)

Acceptor	10^a	11^a	TS₁₀₋₁₁^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-384.993777	-385.003563	-384.934969	154.40	-25.69	0.877	0.245	2.562	98.82
COMe	-424.297281	-424.308213	-424.236290	160.13	-28.70	0.923	0.250	2.526	99.03
COOH	-460.250112	-460.241583	-460.183078	176.00	22.39	0.927	0.267	2.471	99.85
COOMe	-499.531510	-499.528456	-499.466137	171.64	8.02	0.925	0.269	2.474	99.60
NO ₂	-476.203889	-476.217859	-476.143056	159.72	-36.68	0.932	0.228	2.464	99.73
NO	-400.974646	-401.030545	-400.948303	69.16	-146.76	0.893	0.146	2.790	100.00
CHNH	-365.090371	-365.113965	-365.026660	167.27	-61.94	0.927	0.310	2.603	100.60
CHNMe	-404.383111	-404.401773	-404.316937	173.74	-49.00	0.931	0.305	2.618	100.97
CHS	-707.955575	-707.983946	-707.918515	97.30	-74.49	0.889	0.176	3.102	100.37

Table S2 (SMe)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-707.984585	-707.984131	-707.918862	172.56	1.19	0.900	0.256	2.551	99.73
COMe	-747.290091	-747.288996	-747.220055	183.88	2.87	0.909	0.269	2.521	99.77
COOH	-783.242183	-783.221989	-783.165948	200.16	53.02	0.935	0.263	2.434	101.14
COOMe	-822.523442	-822.508962	-822.449054	195.30	38.02	0.935	0.272	2.443	100.83
NO ₂	-799.197353	-799.197375	-799.126193	186.83	-0.06	0.920	0.242	2.462	100.80
NO	-723.966735	-724.010603	-723.934838	83.74	-115.18	0.915	0.127	2.856	101.82
CHNH	-688.079488	-688.098829	-688.012054	177.05	-50.78	0.912	0.309	2.575	101.72
CHNMe	-727.369149	-727.386439	-727.302631	174.64	-45.39	0.914	0.307	2.599	102.02
CHS	-1030.949178	-1030.969211	-1030.902706	122.01	-52.60	0.865	0.187	3.119	101.27

Table S3 (SeMe)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-2711.317761	-2711.317394	-2711.249615	178.92	0.96	0.911	0.264	2.539	99.86
COMe	-2750.623316	-2750.622332	-2750.550892	190.15	2.59	0.919	0.280	2.510	99.81
COOH	-2786.575518	-2786.555215	-2786.496555	207.32	53.31	0.940	0.276	2.432	101.15
COOMe	-2825.856808	-2825.842168	-2825.779647	202.59	38.44	0.939	0.283	2.437	100.81
NO ₂	-2802.530779	-2802.530648	-2802.456939	193.87	0.34	0.930	0.256	2.461	100.59
NO	-2727.300434	-2727.343875	-2727.266355	89.47	-114.05	0.920	0.129	2.868	102.07
CHNH	-2691.412607	-2691.433422	-2691.342982	182.80	-54.65	0.922	0.315	2.558	101.82
CHNMe	-2730.702490	-2730.721851	-2730.634679	178.04	-50.83	0.925	0.335	2.625	102.48
CHS	-3034.282246	-3034.303001	-3034.233556	127.84	-54.49	0.878	0.198	3.117	101.24

Table S4 (NMe₂)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-404.399780	-404.401362	-404.358551	108.25	-4.15	0.907	0.188	2.753	101.69
COMe	-443.705234	-443.705570	-443.660014	118.73	-0.88	0.914	0.191	2.728	101.88
COOH	-479.658254	-479.636365	-479.609141	128.95	57.47	0.919	0.205	2.731	103.34
COOMe	-518.939315	-518.923129	-518.891862	124.59	42.50	0.922	0.199	2.713	103.22
NO ₂	-495.613340	-495.609484	-495.570213	113.23	10.13	0.923	0.178	2.702	102.60
NO	-420.383896	-420.422567	-420.365244	48.97	-101.53	0.879	0.127	2.825	100.85
CHNH	-384.494907	-384.510868	-384.448084	122.93	-41.90	0.918	0.236	2.787	103.30
CHNMe	-423.784446	-423.799018	-423.738849	119.72	-38.26	0.918	0.237	2.820	103.88
CHS ^b	-727.364105	-727.387310	-727.342585	56.50 ^b	-60.92 ^b	0.876	0.136	3.245	102.10

Table S5 (PMe₂)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-691.039513	-691.034142	-690.968370	186.78	14.10	0.919	0.284	2.533	99.29
COMe	-730.344962	-730.338683	-730.269619	197.81	16.48	0.924	0.298	2.502	99.13
COOH	-766.297887	-766.269723	-766.215449	216.44	73.94	0.930	0.275	2.422	100.97
COOMe	-805.578810	-805.558691	-805.498598	210.60	52.82	0.928	0.287	2.428	100.50
NO ₂	-782.252890	-782.244899	-782.176011	201.85	20.98	0.940	0.266	2.456	99.56
NO	-707.023218	-707.060675	-706.977120	121.03	-98.34	0.903	0.132	2.877	102.16
CHNH	-671.137980	-671.145313	-671.054300	219.70	-19.25	0.930	0.333	2.513	102.99
CHNMe	-710.430767	-710.434220	-710.345790	223.11	-9.06	0.931	0.328	2.546	103.45
CHS	-1014.003321	-1014.021231	-1013.950218	139.42	-47.02	0.894	0.231	3.121	99.30

Table S6 (Me)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-309.775520	-309.777575	-309.701267	194.95	-5.39	0.908	0.355	2.460	96.57
COMe	-349.080986	-349.079993	-349.002942	204.90	2.61	0.915	0.369	2.434	96.31
COOH	-385.043625	-385.013651	-384.954944	232.83	78.70	0.920	0.354	2.357	98.85
COOMe	-424.328422	-424.300411	-424.238497	236.10	73.54	0.922	0.359	2.348	98.94
NO ₂	-400.989298	-400.988669	-400.907206	215.53	1.65	0.929	0.352	2.379	95.96
NO	-325.759661	-325.801832	-325.714688	118.08	-110.72	0.887	0.196	2.780	97.85
CHNH	-289.873519	-289.889027	-289.796818	201.38	-40.72	0.919	0.398	2.502	98.52
CHNMe	-329.166260	-329.176151	-329.087830	205.92	-25.97	0.922	0.394	2.524	98.74
CHS	-632.739782	-632.761997	-632.682505	150.38	-58.33	0.878	0.289	3.018	96.75

Table S7 (Ph)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-501.497344	-501.497126	-501.428537	180.65	0.57	0.921	0.286	2.532	100.67
COMe	-540.802929	-540.801621	-540.730221	190.90	3.43	0.927	0.298	2.503	100.43
COOH	-576.755609	-576.735234	-576.675585	210.10	53.49	0.931	0.289	2.427	102.29
COOMe	-616.036691	-616.022060	-615.958635	204.94	38.41	0.931	0.297	2.428	101.73
NO ₂	-592.710915	-592.708462	-592.636045	196.57	6.44	0.937	0.268	2.459	100.87
NO	-517.481152	-517.523144	-517.444461	96.33	-110.25	0.899	0.122	2.919	102.07
CHNH	-481.595814	-481.609676	-481.523939	188.71	-36.39	0.932	0.325	2.567	102.40
CHNMe	-520.888580	-520.896614	-520.815635	191.52	-21.09	0.935	0.321	2.604	102.96
CHS	-824.461120	-824.482011	-824.411679	129.81	-54.85	0.894	0.223	3.130	100.64

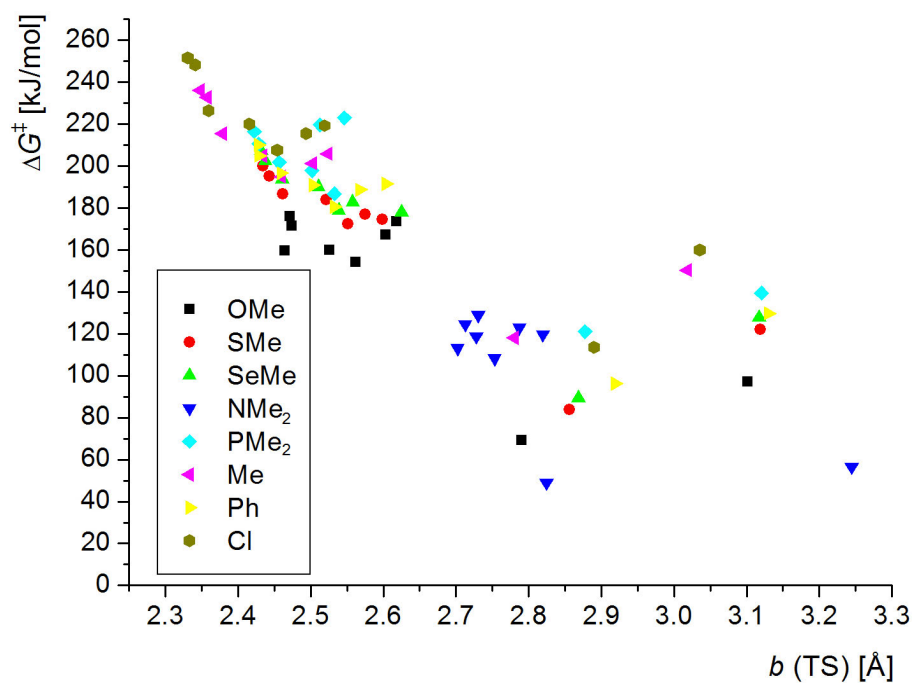
Table S8 (CI)

Acceptor	10 ^a	11 ^a	TS ₁₀₋₁₁ ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]	WBI <i>a</i> (10)	WBI <i>a</i> (TS ₁₀₋₁₁)	<i>b</i> (TS) [Å]	ϕ (TS) [°]
CHO	-730.109947	-730.115573	-730.030920	207.49	-14.77	0.927	0.347	2.454	98.54
COMe	-769.416272	-769.421019	-769.332467	220.03	-12.46	0.933	0.366	2.415	98.23
COOH	-805.377923	-805.352553	-805.283393	248.18	66.61	0.937	0.356	2.341	100.35
COOMe	-844.663126	-844.639968	-844.567283	251.64	60.80	0.939	0.362	2.331	100.46
NO ₂	-821.320972	-821.328156	-821.234684	226.55	-18.86	0.942	0.339	2.360	97.71
NO	-746.092487	-746.141310	-746.049247	113.53	-128.18	0.908	0.151	2.890	100.67
CHNH	-710.210003	-710.237321	-710.127945	215.44	-71.72	0.936	0.393	2.493	100.19
CHNMe	-749.502965	-749.527859	-749.419425	219.34	-65.36	0.939	0.392	2.519	100.38
CHS	-1053.073784	-1053.099242	-1053.012836	160.02	-66.84	0.903	0.273	3.036	98.99

^a Energies are given in Hartree^b Values to generate Figure 4

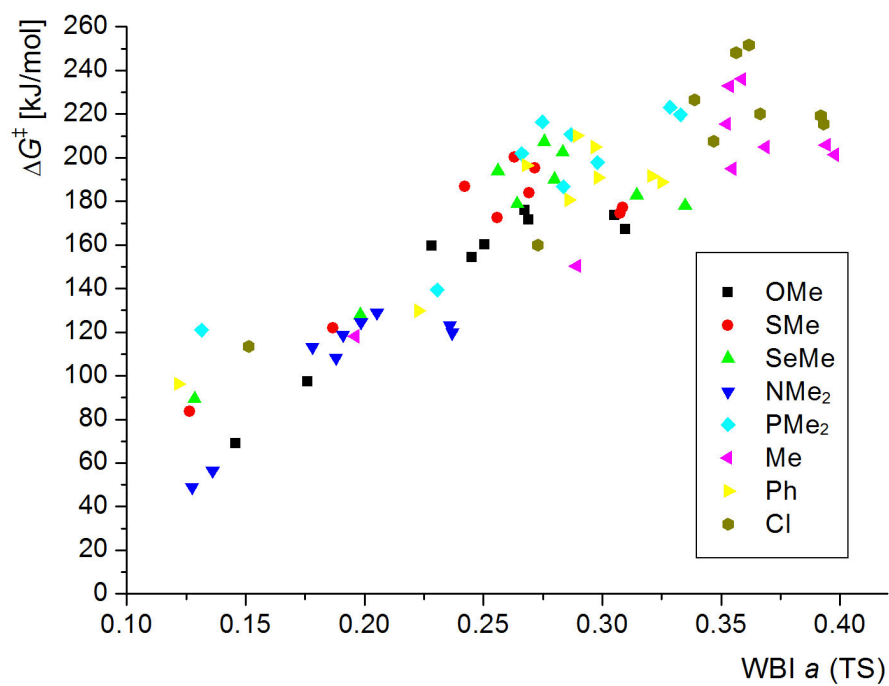
Graphic S1

Length b of the Transition State vs. Activation Barrier $\Delta G^\ddagger$



Graphic S2

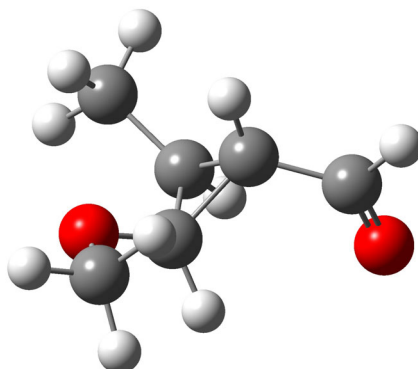
WBI of distance a of the Transition State vs. Activation Barrier $\Delta G^\ddagger$



Donor-Acceptor Cyclopropanes

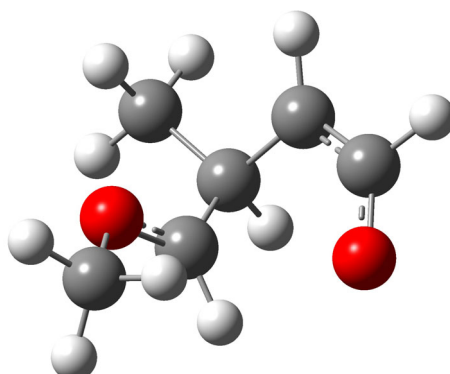
OMe-Donor

10 (MeO/CHO)



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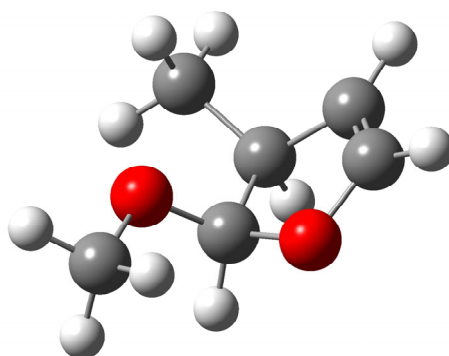
TS₁₀₋₁₁ (MeO/CHO)



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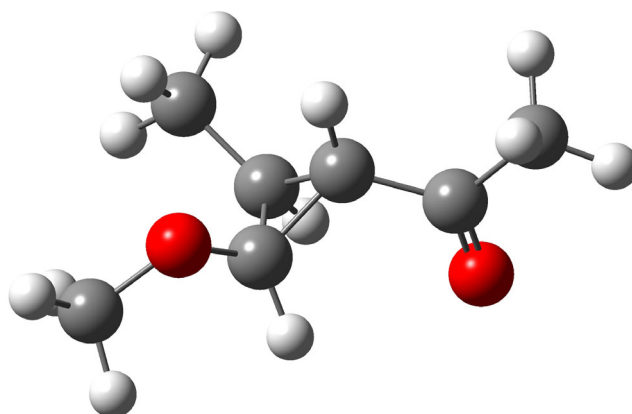
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11 (MeO/CHO)



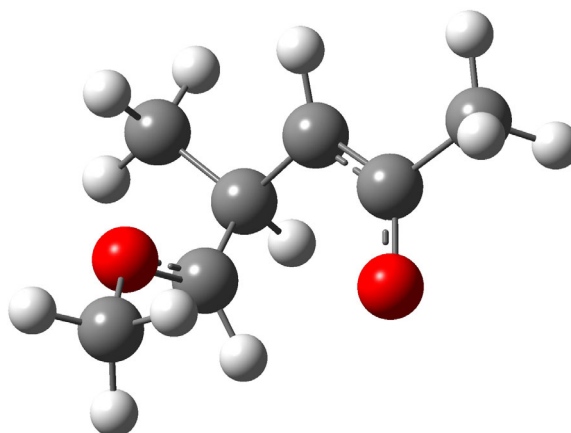
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10 (MeO/COMe)



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4,-0.5081061128\H,0.8292124621,-1.579603101,-1.5336640575\C,-0.9473743
428,-0.4428945343,-0.9167981745\H,-1.8628109488,-0.6165133818,-0.36048
02507\H,0.8649973567,-3.1342493397,0.4943878735\H,-0.6351587719,-3.420
8498178,-0.3888466646\H,0.8474038874,0.2679289667,3.1138919807\H,1.678
1173391,-0.8668846634,2.0169971795\C,-1.0656540672,0.1791859798,-2.265
7587268\C,-2.4658650698,0.5166145431,-2.7378463641\H,-2.9454493935,1.2
126266968,-2.0416732099\H,-2.4275140358,0.9623910643,-3.7309398831\H,-
3.0882644212,-0.3840214011,-2.7638571838\O,-0.0852291261,0.4049378283,
-2.9482363695\H,1.856718964,0.8923441159,1.7854883842\H,-0.6438875531,
-2.4218602589,1.0714040209\Version=AM64L-G03RevC.02\State=1-A\HF=-424
.4766823\RMSD=3.968e-09\RMSF=2.756e-06\Thermal=0.\Dipole=-0.2549165,-0
.3920543,0.7137119\PG=C01 [X(C7H12O2)]\

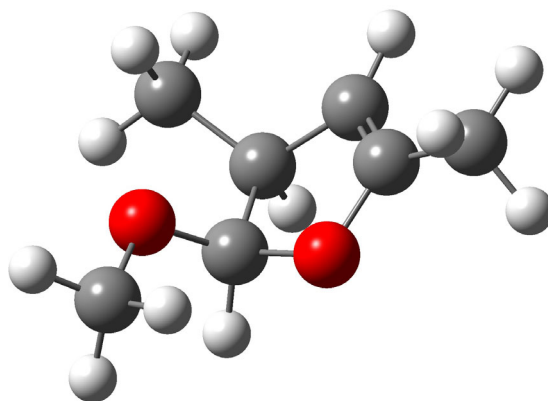
TS₁₀₋₁₁ (MeO/COMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\11-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\
\DA_O_COR_TS\0,1\C,0.0027223365,-0.1033946464,-0.1487997

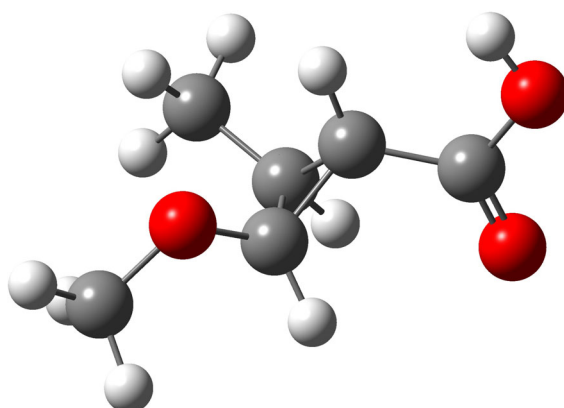
938\C,-0.0804150531,-0.276398042,2.3730743174\C,0.7583436492,-0.112165
 4799,1.102240399\H,1.3567297059,0.8046925023,1.1503586036\C,1.63953277
 81,-1.3414838935,0.8427066485\H,1.6149096235,-2.1297026917,1.587399064
 4\H,-0.7130902971,0.5960400223,2.5531828649\H,0.5876186275,-0.39736617
 62,3.2282440532\C,2.3418192488,-1.4490648369,-0.3524785966\C,3.4722289
 976,-2.4678182511,-0.4424161422\H,3.5500332871,-3.1090247518,0.4377084
 607\H,3.3352459684,-3.0901660821,-1.3311345713\H,4.4187565557,-1.93426
 44197,-0.5696611986\O,2.1273903915,-0.7221629036,-1.3663641758\H,-0.71
 84303406,-1.1598432579,2.3139861914\O,-1.0350910027,-0.8729514773,-0.3
 195861612\C,-1.4924016477,-1.066658252,-1.6751657424\H,-2.4671186729,-
 1.5406308985,-1.5980317677\H,-1.5748172404,-0.1058836269,-2.18727826\H
 ,-0.7851843313,-1.7121211909,-2.1946551233\H,0.3072698707,0.5099819203
 ,-0.9868042466\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-424.4133338\\RMS
 D=2.492e-09\\RMSF=1.053e-06\\Thermal=0.\\Dipole=-1.7028227,0.245248,0.076
 7352\\PG=C01 [X(C7H12O2)]\\@

11 (MeO/COMe)



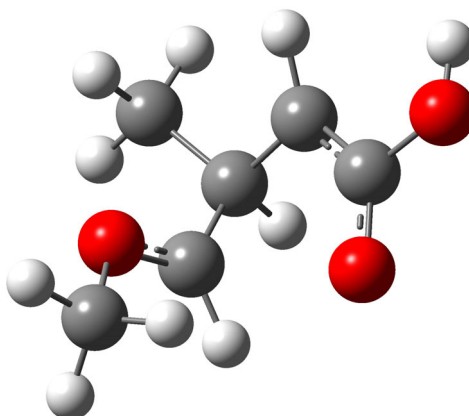
1\\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2\TSCHEI\18-Dec-2009\
 0\\# opt freq rb3lyp/6-311g(d)\\DA_O_COR_2\\0,1\C,0.0625542973,0.107822827
 3,0.089676736\O,0.0719697599,-0.330087291,1.4117493991\C,1.3680589119,
 -0.4036069885,1.9884767069\C,-2.3457083217,-0.8498235306,0.2658022653\
 C,-1.380768505,0.0765590489,-0.4795735004\H,-1.3201745774,-0.260304842
 3,-1.5242411356\C,-1.7340429767,1.5460990055,-0.441964696\H,-2.7205284
 464,1.9459254057,-0.6310018142\H,-2.0096846301,-1.8894400614,0.2324617
 951\H,-3.3363142927,-0.8043762679,-0.195653905\H,1.2414037742,-0.81091
 34009,2.9908811073\H,2.0195873324,-1.0708878163,1.4079415178\C,-0.6444
 467651,2.2613761284,-0.1696488643\C,-0.4241144788,3.7266691506,-0.0444
 315758\H,-0.0583366436,3.9786528009,0.9559207581\H,0.3330327691,4.0655
 204908,-0.7586005382\H,-1.3475716014,4.2769347809,-0.2286650409\O,0.48
 86294684,1.4887775373,0.0126445191\H,1.8326013325,0.5840025823,2.04967
 77167\H,-2.43862715,-0.560411114,1.3123852\H,0.7898325374,-0.461868593
 3,-0.5007179943\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-424.489555\\RMS
 D=2.998e-09\\RMSF=5.289e-06\\Thermal=0.\\Dipole=0.132397,-0.0004778,-0.10
 09596\\PG=C01 [X(C7H12O2)]\\

10 (MeO/COOH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\22-Dec-2009\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COOH_1\0,1\C,0.0254254846,0.01594033
39,-0.00069969\O,0.0206355789,0.0171931244,1.3923492582\C,1.3305684592
,-0.0066080679,1.9441428564\C,-0.1142454279,-2.6096983374,-0.063247420
7\C,-0.0839744318,-1.2697113307,-0.7602395505\H,0.5807278074,0.8307635
023,-0.4632574197\H,0.3715225591,-1.2499507797,-1.7458953815\C,-1.2960
265443,-0.3364039759,-0.6472926777\H,-2.0637270324,-0.6505032512,0.054
351168\O,-0.9356851863,0.8213736204,-2.6947609341\H,0.8918252456,-3.03
42055351,0.0041120417\H,-0.7367332697,-3.3244778073,-0.6086176159\H,1.
2142388556,0.0080044052,3.0272925296\H,1.8773474511,-0.9097955113,1.64
92958864\O,-3.0325129871,0.7045537574,-1.9686795152\C,-1.7032685464,0.
4374186268,-1.8533887791\H,1.9070326701,0.8736299107,1.6331124121\H,-0
.5061554098,-2.5213219836,0.9516694746\H,-3.5191306499,0.3456227511,-1
.2164103596\\Version=AM64L-G03RevC.02\State=1-A\HF=-460.4072526\RMSD=
8.466e-09\RMSF=4.133e-06\Thermal=0.\Dipole=0.1237174,-0.8906454,1.35496
67\PG=C01 [X(C6H10O3)]\
```

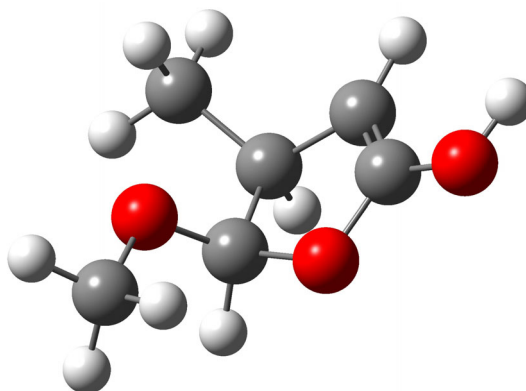
TS₁₀₋₁₁ (MeO/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\07-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\
\DA_O_COOH_TS\0,1\C,-0.3105376512,0.0213236989,0.5751562
544\C,0.4544019324,-0.121637486,2.9809221275\C,0.8302657085,0.00681293
86,1.5004884352\H,1.4091826743,0.9241020325,1.3404500985\C,1.557706971
```

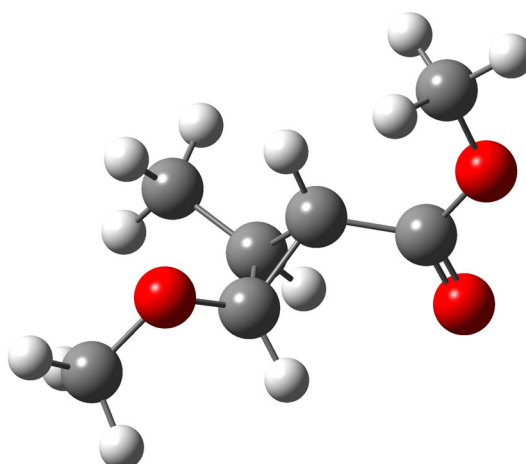
8,-1.2340439896,0.9979706825\H,1.7071867164,-2.0418081931,1.7079939067
 \O,1.0848811426,-0.8210220567,-1.2820545708\H,-0.0624509808,0.76961321
 64,3.3442215529\H,1.3661264316,-0.2523366959,3.5673794076\O,2.53475012
 03,-2.447100833,-0.7999075123\C,1.6781215584,-1.4502266327,-0.38530930
 02\H,-0.1862579042,-0.9886050131,3.1510043401\H,3.0751007995,-2.724217
 2513,-0.050636823\O,-1.3416888912,-0.7489458632,0.7423109826\C,-2.2214
 373508,-0.906792721,-0.3998047178\H,-2.9566155671,-1.6501199301,-0.105
 2484572\H,-2.7109832755,0.0434126495,-0.6217229227\H,-1.6303863246,-1.
 2498251945,-1.2470272888\H,-0.3160681176,0.6635591479,-0.2972839101\\V
 ersion=AM64L-G03RevC.02\State=1-A\HF=-460.3376352\RMSD=6.976e-09\RMSF
 =8.709e-06\Thermal=0.\Dipole=-1.5249417,0.5130714,1.1646005\PG=C01 [X(C
 6H10O3)]\\

11 (MeO/COOH)



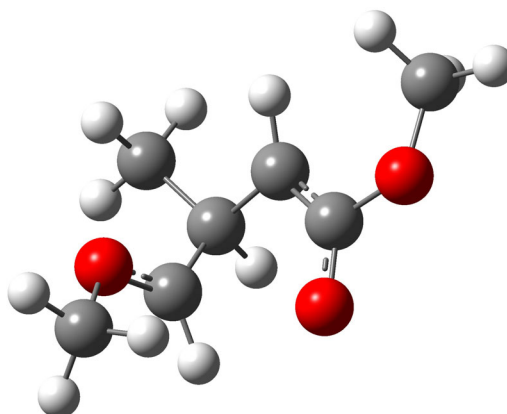
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\22-Dec-2009\
 0\\# opt freq rb3lyp/6-311g(d)\\DA_O_COOH_2\\O,1\C,0.010521252,-0.01044270
 71,-0.004182777\O,0.0024793343,0.0189522383,1.3822676773\C,1.295996854
 7,0.0045641183,1.9737457458\C,-2.4764692811,-0.5991784574,0.4331934802
 \C,-1.4404930882,-0.0645393188,-0.5588599302\H,0.6613892494,-0.8135177
 203,-0.3673589688\H,-1.4340344708,-0.7282914454,-1.4356489346\C,-1.636
 1298435,1.3723955307,-0.9902357401\H,-2.5754264192,1.8076027329,-1.300
 3689876\O,0.5914231291,1.2168877595,-0.5294045063\H,-2.2514280095,-1.6
 259169939,0.7343082091\H,-3.4675392506,-0.5981193392,-0.0295687228\H,1
 .144214419,-0.0402294955,3.0513174862\H,1.8645618876,-0.8779976249,1.6
 5162241\O,-0.0524580126,3.2323520982,-1.250301508\C,-0.4491300468,1.98
 39432608,-0.9472275881\H,1.8579929104,0.9062718628,1.7185109687\H,-2.5
 140544007,0.0161773975,1.3318609815\H,-0.8097268143,3.7241604914,-1.58
 79675317\\Version=AM64L-G03RevC.02\State=1-A\HF=-460.3998274\RMSD=7.59
 6e-09\RMSF=2.431e-05\Thermal=0.\Dipole=-0.3327593,-0.07382,-0.1598728\
 PG=C01 [X(C6H10O3)]\\

10 (MeO/COOMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\18-Dec-2009\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COOR_1\0,1\C,0.1368869928,-0.0793479
651,-0.0428934037\O,0.0231550421,0.0227679372,1.3427083483\C,1.2838736
634,0.1440560257,1.9871018548\C,0.2160151939,-2.7031828587,0.088964972
5\C,0.1924804646,-1.4189395547,-0.706066453\H,0.6602594582,0.744610962
,-0.5258650311\H,0.7207732349,-1.4284193076,-1.6544850963\C,-1.0995605
137,-0.5903750508,-0.7527137008\H,-1.8817239826,-0.9218381167,-0.08299
48311\O,-0.6258093757,0.3999432984,-2.8489594208\H,1.2451624001,-3.021
9907274,0.2804840962\H,-0.2824832985,-3.5120061444,-0.4527441532\H,1.0
832455833,0.2339273053,3.0543362382\H,1.9155302494,-0.7340770917,1.808
7162135\O,-2.7657904966,0.2833938858,-2.3301266855\C,-1.4562001682,0.0
599889526,-2.043955119\C,-3.8068231799,-0.0327241463,-1.4026950947\H,-
3.8755292382,-1.1091108343,-1.2243043636\H,-3.6773896934,0.4947022187,
-0.4545811779\H,-4.7257060112,0.3068777827,-1.8765834033\H,1.818711509
3,1.0395632101,1.6459910311\H,-0.2793654014,-2.5836769187,1.0543321904
\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.7167548\RMSD=4.948e-09\R
MSF=6.784e-05\Thermal=0.\Dipole=-0.2310442,-0.6430942,1.3338513\PG=C01
[X(C7H12O3)]\
```

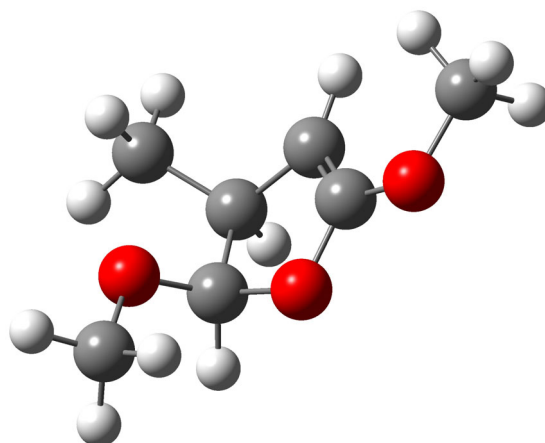
TS₁₀₋₁₁ (MeO/COOMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\11-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\
DA_O_COOR_TS\0,1\C,-0.1509116452,-0.0672007112,0.067813
7419\C,0.1234780445,0.0469700592,2.5791674522\C,0.7839330998,-0.017915
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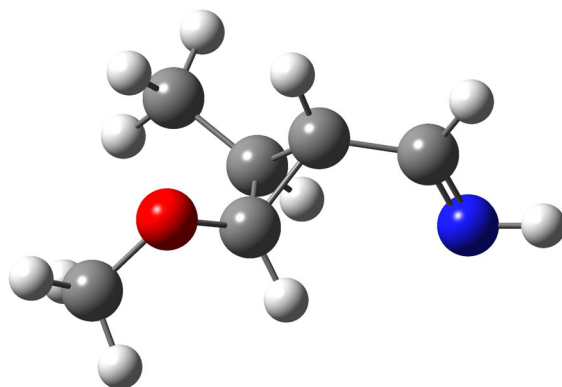
5208,1.1983930284\H,1.443361259,0.8460737651,1.0553374164\C,1.51226375
9,-1.3395223175,0.983694164\H,1.4818337267,-2.0511159182,1.7991003993\
O,1.5879669143,-1.0948802572,-1.3604183729\H,-0.3958924198,0.995746317
5,2.7334093669\H,0.8948250243,-0.0503627157,3.3459076161\O,2.787299846
5,-2.7419103343,-0.4973489557\C,1.9286302612,-1.685178958,-0.312420694
9\C,3.3824395593,-3.3690981669,0.6295522525\H,3.8571629551,-2.63787306
14,1.290044094\H,2.6491976915,-3.9475324606,1.2033778793\H,4.134474450
8,-4.0512609347,0.2331616108\H,-0.5923535144,-0.766054841,2.7125610144
\O,-1.2425545819,-0.7700015131,0.1093774324\C,-1.8940379494,-1.0247557
653,-1.1600160079\H,-2.7266750296,-1.6858507166,-0.9373993779\H,-2.257
8162717,-0.0864762236,-1.583279067\H,-1.1798022914,-1.5022644525,-1.82
86227032\H,0.0552088183,0.4629446904,-0.8536259519\\Version=AM64L-G03
RevC.02\State=1-A\HF=-499.6486831\RMSD=9.037e-09\RMSF=3.545e-06\Ther
mal=0.\Dipole=-1.6510173,0.5095754,0.708209\PG=C01 [X(C7H12O3)]\

11 (MeO/COOMe)



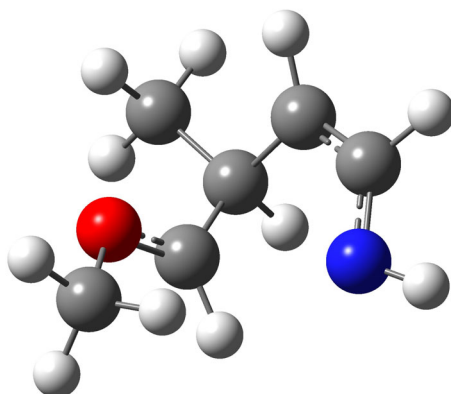
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\18-Dec-2009\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COOR_2\0,1\C,0.5543800325,-0.3587088
899,0.0707752312\O,1.0246437362,-0.4301679912,1.375292734\C,0.79224407
56,0.743742278,2.1431894775\C,2.0789700219,-2.4476804659,-0.1244960393
\C,0.9054206659,-1.656173365,-0.7076564126\H,0.9018186666,0.5625078222
, -0.4104371862\H,1.1691183026,-1.3640146898,-1.7345327756\C,-0.4276447
175,-2.3720068366,-0.6957560758\H,-0.582293301,-3.3917399058,-1.011500
7761\O,-0.8955128534,-0.2707746046,0.0623295874\H,3.000312831,-1.85892
25112,-0.1252261382\H,2.2563811227,-3.3439916439,-0.7257884046\H,1.264
9884896,0.5809977467,3.1108794892\H,1.2440055129,1.6223373053,1.663427
6135\O,-2.6777468241,-1.6030067634,-0.0815579159\C,-1.3567551852,-1.51
29803868,-0.2606417591\C,-3.2587311078,-2.8553755748,-0.4303456851\H,-
3.0887852652,-3.0815327621,-1.487520511\H,-2.8448335631,-3.6600292752,
0.1850859042\H,-4.3250615787,-2.756222345,-0.2400342074\H,-0.277140143
1,0.9212474034,2.2814599462\H,1.8751213406,-2.754671536,0.9011377685\\
Version=AM64L-G03RevC.02\State=1-A\HF=-499.715115\RMSD=8.535e-09\RM
SF=4.066e-06\Thermal=0.\Dipole=-0.0436277,-0.2708633,-0.1941501\PG=C01 [X
(C7H12O3)]\

10 (MeO/CHNH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1O1\TSCHNEI\27-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHNH_1_1\0,1\C,0.0498641045,-0.035
9029753,-0.0458409299\O,0.0454955355,-0.1290703137,1.3463563023\C,1.34
04265192,0.0242113726,1.9076319515\C,0.3777923653,-2.6338535286,-0.273
3715337\C,0.1763861019,-1.2685782131,-0.8880289393\H,0.4556712436,0.89
32977479,-0.445596364\H,0.6303513669,-1.1040508444,-1.861377094\C,-1.1
814267404,-0.5680948978,-0.7445813014\H,-1.8945405623,-1.055136433,-0.
0873312232\H,1.4424204871,-2.8780316839,-0.2017625089\H,-0.098123907,-
3.4128695553,-0.8760089171\H,1.2274580873,-0.0606724191,2.9883452969\H
,2.0308155582,-0.7504339232,1.5530046479\C,-1.749221319,0.1823248939,-
1.8854596435\H,1.7633486516,1.0085838316,1.6681142548\H,-0.0419162258,
-2.6804045043,0.7333101615\N,-1.007568032,0.7676184944,-2.7381969671\H
,-2.8469141839,0.1989177999,-1.9375287314\H,-1.5683856218,1.2393780124
,-3.4473180554\\Version=AM64L-G03RevC.02\State=1-A\HF=-365.2545055\RMS
D=7.921e-09\RMSF=1.053e-05\Thermal=0.\Dipole=-0.1329438,-0.1490525,0.0
877526\PG=C01 [X(C6H11N1O1)]\\
```

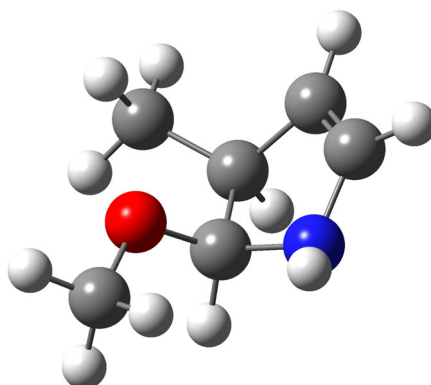
TS₁₀₋₁₁ (MeO/CHNH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H11N1O1\TSCHNEI\10-Jan-2010\
0\# opt=(ts,noeigentest,calcfc) b3lyp/6-311g(d) scf=tight Int=ultrafine freq\
\DA_O_CHNH_TS\0,1\C,-0.0673887603,-0.1313555057,-0.0
411039897\C,-0.0336641821,-0.0540145097,2.4900770896\C,0.7488944925,-0
.0697079454,1.1734815833\H,1.3887656007,0.816953672,1.1011222068\C,1.5
732128211,-1.3487774693,1.0235523686\H,1.4545285111,-2.0950597909,1.80
```

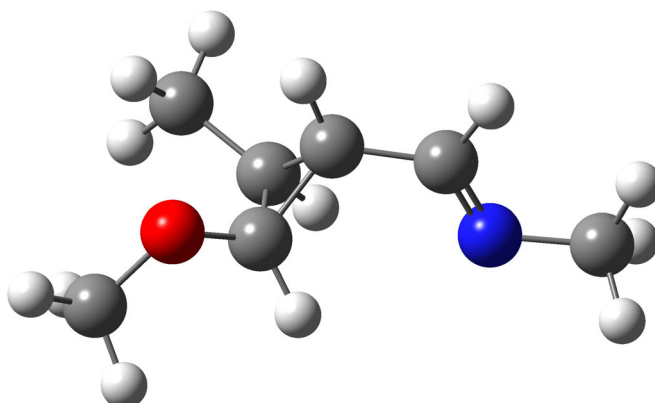
52561204\H,-0.5977486832,0.873862814,2.6104809774\H,0.6660685937,-0.14
 36568269,3.324281812\C,2.2122466201,-1.6884785261,-0.165289997\H,-0.73
 27384096,-0.8909403544,2.5418271719\N,1.9097624513,-1.2034437014,-1.35
 15080317\H,3.0233181206,-2.4263160237,-0.0627936046\H,2.6655337686,-1.
 3596955591,-2.0200285932\O,-1.1015743489,-0.9316866109,-0.1428507542\C
 ,-1.5765343156,-1.1783282118,-1.4829989785\H,-2.3202572117,-1.96647899
 83,-1.3973281045\H,-2.0370459019,-0.2729548764,-1.8870191825\H,-0.7365
 138625,-1.4960657885,-2.0993744761\H,0.2211394013,0.4126265863,-0.9310
 128328\\Version=AM64L-G03RevC.02\State=1-A\HF=-365.1881092\RMSE=9.696e
 -09\RMSE=4.304e-06\Thermal=0.\Dipole=-0.9010002,0.311911,-0.3253484\PG
 =C01 [X(C6H11N1O1)]\\

11 (MeO/CHNH)



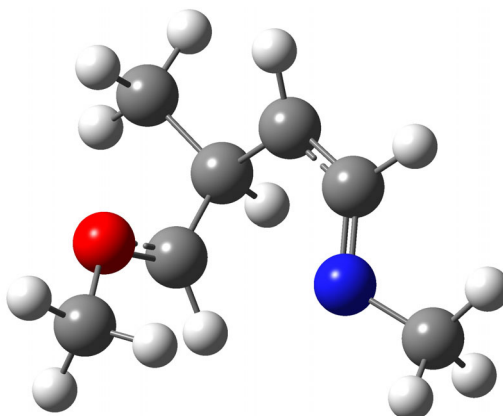
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1O1\TSCHNEI\26-Dec-2009\
 0\# opt freq rb3lyp/6-311g(d)\DA_O_CHNH_2\0,1\C,0.0269964835,0.032512
 3841,-0.0364064502\O,0.0313073935,0.1732180838,1.3783714591\C,1.288878
 6279,-0.0342104783,1.9856301226\C,-2.4256586227,-0.6672087848,0.457311
 1514\C,-1.441979683,-0.0552623596,-0.5406438319\H,-1.4253004858,-0.684
 5129391,-1.4431182415\C,-1.7199865656,1.3772551794,-0.9520462222\H,-2.
 6949153801,1.7603149586,-1.2193211636\H,-2.147479737,-1.691779713,0.72
 02510609\H,-3.428953371,-0.6973863581,0.0223263554\H,1.1298229272,-0.0
 147918198,3.063788286\H,1.7170458244,-1.006794981,1.7051424533\C,-0.56
 26132629,2.0361774204,-1.0272341919\H,2.0153191153,0.7513151063,1.7323
 879863\H,-2.465414293,-0.0835406615,1.3767764739\H,0.6208052603,-0.851
 6274638,-0.2985068553\N,0.5453853117,1.2148136723,-0.7341548306\H,1.33
 80214758,1.6658957303,-0.295562779\H,-0.3893606506,3.0603892097,-1.334
 3632547\\Version=AM64L-G03RevC.02\State=1-A\HF=-365.2797506\RMSE=3.032
 e-09\RMSE=2.538e-06\Thermal=0.\Dipole=0.5999241,0.0196889,0.1743525\PG
 =C01 [X(C6H11N1O1)]\\

10 (MeO/CHNMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHNR_1_1\0,1\C,-0.078852833,-0.002
7068563,0.0021968764\O,-0.0723331222,-0.0431465663,1.3975091484\C,1.23
64069884,0.0410485654,1.940433104\C,0.0809218297,-2.6243646113,-0.1276
567557\C,-0.0395190755,-1.273612194,-0.7937318469\H,0.3842521589,0.881
5204707,-0.4354412534\H,0.4168968919,-1.1769466716,-1.7750182226\C,-1.
346302937,-0.4800558629,-0.6658796099\H,-2.0810082649,-0.8975127482,0.
0151450373\H,1.1277837341,-2.9374036815,-0.0616096281\H,-0.4568250902,
-3.392740173,-0.6908412045\H,1.1303388682,0.0142608466,3.0249109434\H,
1.865264397,-0.7970079768,1.6167651453\C,-1.8897697158,0.2591700975,-1.
8269919061\H,1.7266719212,0.9801967248,1.652178534\H,-0.3234915564,-2.
6023869692,0.8861647583\N,-1.1456327022,0.7921478225,-2.7036005512\H,
-2.9888502931,0.3245329864,-1.887474921\C,-1.7708470222,1.5028646211,-
3.8005227771\H,-1.4531345987,1.0600580255,-4.7494522643\H,-2.871305545
8,1.4985521403,-3.7605970742\H,-1.4252490117,2.5411840224,-3.805257691
3\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5746368\RMSE=9.851e-09\
RMSF=2.796e-06\Thermal=0.\Dipole=0.0355779,-0.101875,-0.0117862\PG=C01
[X(C7H13N1O1)]\
```

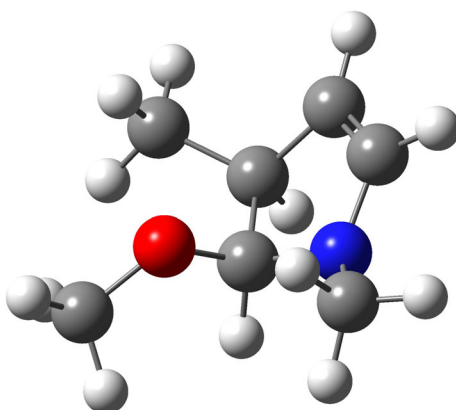
TS₁₀₋₁₁ (MeO/CHNMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\10-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight integral=
(grid=ultrafine)\DA_O_CHNR_TS\0,1\C,-0.0601509867,-0.1384803485,-0.0
388708257\C,0.0042647616,-0.0304042209,2.4895567801\C,0.7735395856,-0.
1124895181,1.167065143\H,1.4607353422,0.7365345416,1.0776760052\C,1.52
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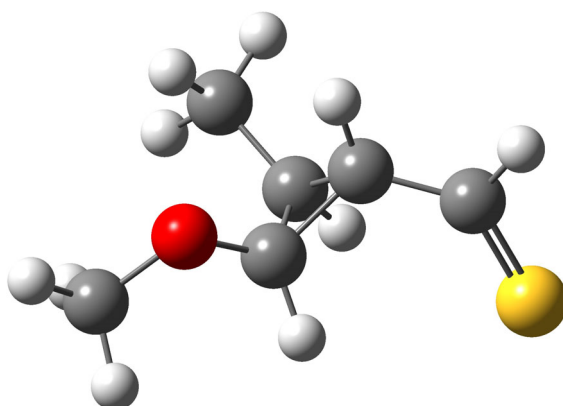
27761329,-1.4352170678,1.0307316746\H,1.371701712,-2.1660690744,1.8214
819324\H,-0.5036497438,0.9305858808,2.5997153519\H,0.7049864738,-0.147
9795257,3.3195371989\C,2.1288699132,-1.8262677445,-0.1597344449\H,-0.7
417678973,-0.8243200556,2.5601401672\N,1.8640747381,-1.3372072441,-1.3
485946618\H,2.8946629095,-2.6151566942,-0.0687288249\O,-1.1355480074,-
0.8874621991,-0.1186346019\C,-1.6528319274,-1.111883969,-1.4447527523\
H,-2.4667726753,-1.8237417384,-1.3336035185\H,-2.0311060129,-0.1750840
393,-1.8627105675\H,-0.8586458261,-1.5203072557,-2.0685337864\H,0.2333
328144,0.3931541747,-0.9345185301\C,2.8502046299,-1.5296135998,-2.3929
798339\H,3.5315056282,-2.3713112885,-2.1858382948\H,2.358541017,-1.719
0031551,-3.3539688797\H,3.4798708726,-0.6383744186,-2.5297535378\\Vers
ion=AM64L-G03RevC.02\State=1-A\HF=-404.5056881\RMSD=9.340e-09\RMSF=2.8
89e-06\Thermal=0.\Dipole=-1.0241484,0.4522615,-0.3184547\PG=C01 [X(C7H
13N1O1)]\\

11 (MeO/CHNMe)



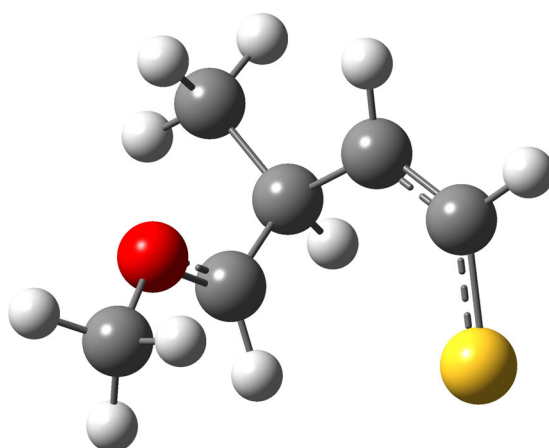
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C7H13N1O1\TSCHNEI\06-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHNR_2\0,1\C,0.1258722824,0.260868
3547,0.0389466838\O,0.1864252972,0.4009558392,1.461388639\C,0.99461295
19,-0.5487063773,2.1276330829\C,-1.9671794146,-1.2097999664,0.53721642
41\C,-1.2478553581,-0.2986686173,-0.4580825534\H,-1.0457587936,-0.8721
737793,-1.3752480816\C,-1.9891654402,0.9701716053,-0.8271552968\H,-3.0
373166411,1.0173546065,-1.0871840479\H,-1.4078912057,-2.130739177,0.72
91208943\H,-2.943936624,-1.50178368,0.1414093372\H,1.0292058038,-0.253
3875705,3.1767475517\H,0.5852331847,-1.5645386899,2.0634382067\C,-1.11
34461183,1.9772379452,-0.8750093137\H,2.0186126988,-0.5591297609,1.729
3318886\H,-2.1241847252,-0.6988091969,1.4877337806\H,0.9731188227,-0.3
590950225,-0.2795872214\N,0.1974944953,1.5768209883,-0.5790586574\H,-1
.2910373635,3.0092731522,-1.1530186453\C,1.1727513449,2.5313959041,-0.
0834554464\H,0.97304364,2.864174917,0.9418768816\H,2.1682795523,2.0807
319409,-0.1091327454\H,1.1890059674,3.4023398294,-0.7426723388\\Versio
n=AM64L-G03RevC.02\State=1-A\HF=-404.5952433\RMSD=3.888e-09\RMSF=2.5
91e-06\Thermal=0.\Dipole=0.4781454,-0.1714156,0.0485335\PG=C01 [X(C7H13N
1O1)]\\

10 (MeO/CHS)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNEI\27-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHS_1\0,1\C,0.090246894,-0.0779129
278,-0.0557200028\O,0.0341988205,-0.1402749337,1.3325547947\C,1.306341
6984,0.0426763537,1.9424301852\C,0.3647690869,-2.6789960247,-0.2278109
014\C,0.2155788551,-1.3180504078,-0.8636676451\H,0.5048339032,0.843381
0897,-0.4652975064\H,0.6810593724,-1.1824230379,-1.8364265505\C,-1.156
1507673,-0.5989582675,-0.7688988138\H,-1.8694914288,-1.0713375976,-0.1
011407325\H,1.4223214522,-2.9461782725,-0.1377267684\H,-0.1203603647,-
3.4518089256,-0.8297546809\H,1.1469545323,-0.0146551703,3.0185271699\H
,2.016474199,-0.734843483,1.6378678914\H,1.7268932713,1.0248126678,1.6
93246374\H,-0.0702009787,-2.6993121196,0.7726763781\C,-1.7208174737,0.
1114681772,-1.9098573648\S,-0.9092301172,0.9266826041,-3.0761141503\H,
-2.8106872433,0.0790980633,-1.9679649703\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-708.1046988\RMSD=4.975e-09\RMSF=1.065e-05\Thermal=0.\Dipole
=0.4424136,-0.7063307,0.9762133\PG=C01 [X(C6H10O1S1)]\
```

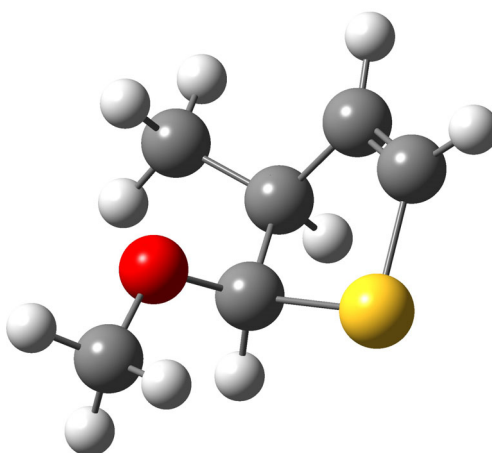
TS₁₀₋₁₁ (MeO/CHS)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNEI\27-Jul-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultr
afine\DA_O_CHS_TS\0,1\C,0.1802736462,-0.0431482181,-0.0586293339\C,-
0.0108889618,0.2522769512,2.2197436646\H,0.6910273284,0.7856603786,2.8
567207579\C,-1.3528495854,0.4388892446,2.3424220959\H,-1.6684406079,0.
9611967295,3.2481192133\C,0.621238212,-0.6868851815,1.1773935849\H,0.1
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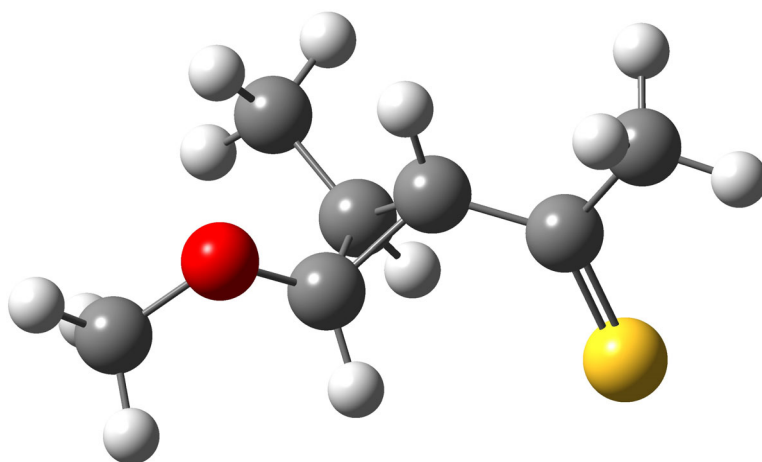
333621244,-1.6654434478,1.2362826297\C,2.1386022524,-0.8005341581,1.35
 11688889\H,2.576710111,-1.4734821736,0.610541135\H,2.6239556973,0.1729
 913115,1.2603407469\H,2.3569329834,-1.1970230403,2.3446272048\O,0.8012
 161799,1.0012279067,-0.5162835813\C,0.1581551317,1.7736170611,-1.55644
 16283\H,0.9486941089,2.3389595922,-2.0420211102\H,-0.3357741802,1.1117
 982291,-2.2691941387\H,-0.5657098619,2.4414475233,-1.0907694088\H,-0.7
 211792415,-0.3636355786,-0.5707787351\S,-2.6110226208,-0.0619692064,1.
 2934986381\\Version=AM64L-G03RevC.02\State=1-A\HF=-708.0660674\RMSD=2.
 709e-09\RMSF=1.190e-05\Thermal=0.\Dipole=2.2167363,0.5661533,-1.624582
 2\PG=C01 [X(C6H10O1S1)]\

11 (MeO/CHS)



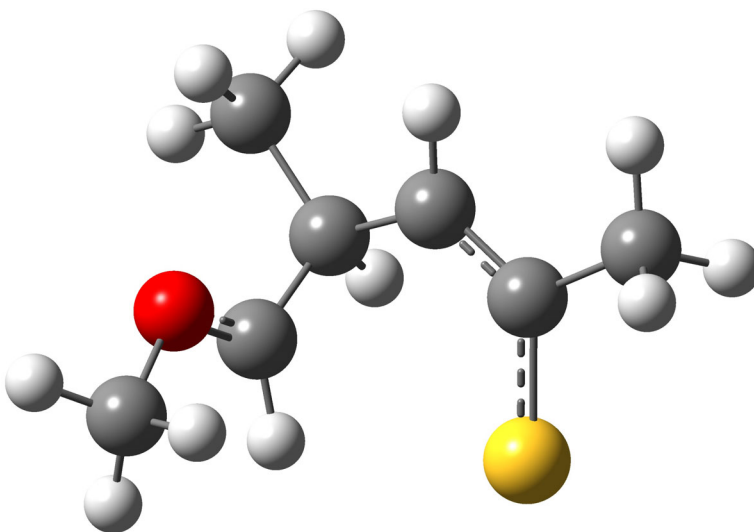
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNEI\27-Jul-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_O_CHS_2\0,1\C,0.0419498371,0.1684568
 828,0.0395432007\O,0.0945065829,-0.0540929577,1.4148834568\C,1.3950706
 575,-0.2792675525,1.9302048885\C,-2.2986309134,-0.8636861838,0.2981173
 728\C,-1.426882279,0.1580503107,-0.4384719295\H,-1.392640973,-0.118802
 945,-1.5034982182\C,-1.9194765258,1.5855765264,-0.3617621565\H,-2.9783
 129,1.8200504155,-0.3362622647\H,-1.8966250995,-1.8753869965,0.1993158
 734\H,-3.309078642,-0.8654294928,-0.1203711786\H,1.2780024549,-0.50697
 94771,2.9888203957\H,1.8781578527,-1.1283446974,1.4278747615\C,-0.9648
 981379,2.5116824533,-0.3853016151\H,2.0250039915,0.6099313862,1.819547
 046\H,-2.3645862104,-0.630558248,1.3606520141\H,-1.1023029652,3.585509
 5596,-0.3824699248\H,0.6581289977,-0.5634688302,-0.4956941461\S,0.6936
 021336,1.8729257093,-0.4354941703\\Version=AM64L-G03RevC.02\State=1-A\
 HF=-708.1342514\RMSD=3.070e-09\RMSF=3.404e-06\Thermal=0.\Dipole=-0.083
 2637,-0.469898,0.0494795\PG=C01 [X(C6H10O1S1)]\

10 (MeO/CSMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O1S1\TSCHNEI\19-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CSR_1\0,1\C,0.0040815956,0.0060086
85,-0.0303174889\O,0.0098999459,0.0547450675,1.361344459\C,1.323727406
2,0.0455394216,1.904726336\C,-0.1751387996,-2.6119844444,-0.0047154345
\C,-0.1268940096,-1.2951606254,-0.742276453\H,0.5540343992,0.805166918
7,-0.526624691\H,0.3107746983,-1.3123351297,-1.7366960966\C,-1.3415235
048,-0.3438623813,-0.6514304546\H,-2.0824088057,-0.6386065011,0.086192
0211\H,0.8258354948,-3.0484683288,0.0687521878\H,-0.811048816,-3.33351
28017,-0.5248336541\H,1.2140693949,0.0922468913,2.9876858519\H,1.86771
38464,-0.8668054592,1.6335053293\H,1.8993491848,0.9153602182,1.5641982
719\H,-0.5582303737,-2.4865735227,1.0095031824\C,-1.8577836097,0.37752
2746,-1.8240514282\S,-0.907939919,0.9181215351,-3.0569772979\C,-3.3483
037414,0.593431907,-1.8156444254\H,-3.6401373927,1.1556131676,-0.92051
67759\H,-3.6844522964,1.1292728483,-2.7005382779\H,-3.8677051951,-0.37
07142595,-1.7588064301\\Version=AM64L-G03RevC.02\State=1-A\HF=-747.43
44051\RMSE=4.747e-09\RMSE=3.027e-06\Thermal=0.\Dipole=0.034266,-0.632
4594,0.9854609\PG=C01 [X(C7H12O1S1)]\

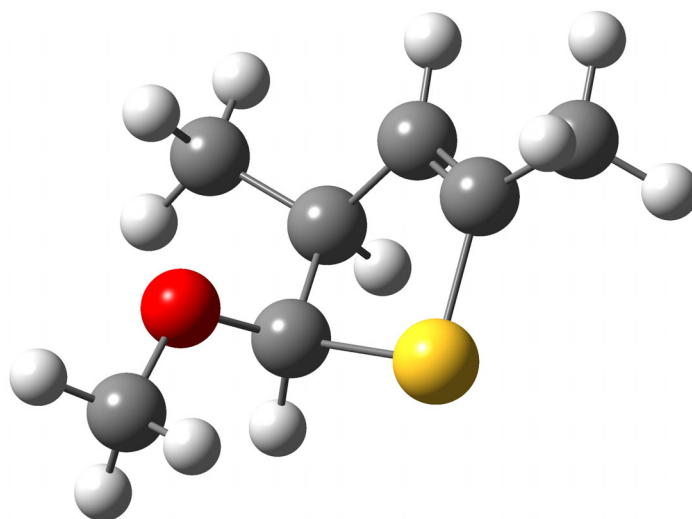
TS₁₀₋₁₁ (MeO/CSMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O1S1\TSCHNEI\19-Aug-2010\

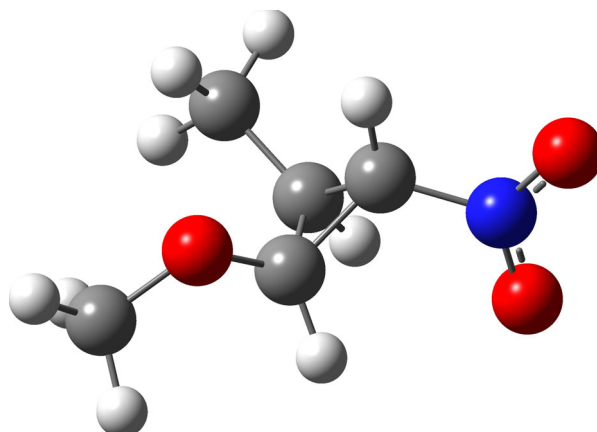
0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultrafine\\DA_O_CSR_TS\\0,1\\C,0.0916098518,-0.0475567413,-0.0374750156\\C,0.0364984861,0.2998223634,2.2344336385\\H,0.8248826584,0.7847772657,2.8057486894\\C,-1.2774246587,0.6066910485,2.4455799289\\C,0.5206468548,-0.7158607345,1.1917297193\\H,-0.0623808678,-1.6373689971,1.2890614298\\C,2.0253531158,-0.9814726176,1.2980882561\\H,2.3577253801,-1.7062284004,0.5511639042\\H,2.6030761584,-0.0644412194,1.1673928416\\H,2.2485551449,-1.3843563063,2.2879399277\\O,0.7900066033,0.9268390802,-0.534116072\\C,0.186098988,1.7434028356,-1.5635387623\\H,-0.4245188668,2.5057102619,-1.0809615767\\H,1.0090331664,2.1965903899,-2.1093992563\\H,-0.4244407006,1.1284511882,-2.2260801552\\H,-0.8501330333,-0.2933057871,-0.5155556272\\S,-2.5862269402,0.1132022146,1.4275608082\\C,-1.6271459863,1.4092870077,3.6828565713\\H,-2.1449053287,2.3317650437,3.4088703918\\H,-2.3175249553,0.8353557419,4.3067962251\\H,-0.7471913198,1.6633862973,4.2799479725\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-747.3913184\\RMSD=9.245e-09\\RMSF=8.513e-06\\Thermal=0.\\Dipole=2.1287578,0.4777915,-1.6330444\\PG=C01 [X(C7H12O1S1)]\\

11 (MeO/CSMe)



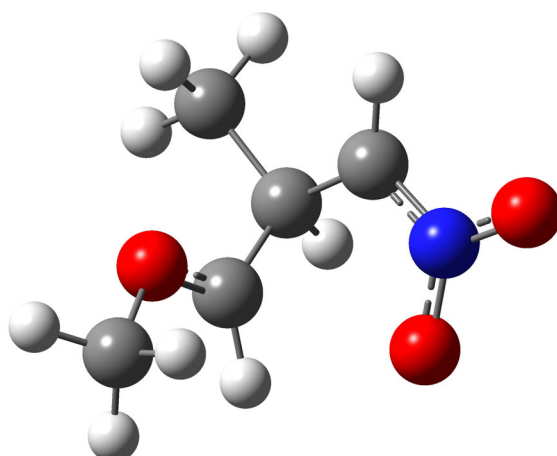
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H12O1S1\\TSCHNEI\\19-Aug-2010\\0\\# opt freq rb3lyp/6-311g(d)\\DA_O_CSR_2\\0,1\\C,0.0008510587,-0.0001694058,-0.0009899124\\O,-0.0018411724,0.0028794764,1.3945853511\\C,1.2837758706,0.0005594642,1.9893615941\\C,-2.2316315927,-1.2301470891,0.3284855\\C,-1.4302039654,-0.2444223054,-0.5275465852\\H,-1.3092129479,-0.6787637263,-1.5320160735\\C,-2.0664735816,1.1147571924,-0.6919877397\\H,-3.1453986288,1.228067713,-0.7383234229\\H,-1.7254264217,-2.1963177663,0.4029614047\\H,-3.2141050188,-1.4040373694,-0.119596034\\H,1.1315805013,-0.0640301859,3.0659937426\\H,1.8734213725,-0.8637305876,1.6543918447\\C,-1.2297020147,2.1426763385,-0.8315574486\\H,1.8313771126,0.9204334402,1.7568288147\\H,-2.3750226452,-0.8469925047,1.3386770428\\H,0.7161884035,-0.7379011385,-0.3835886637\\S,0.4960009528,1.6619174693,-0.7222079279\\C,-1.5592651875,3.5812198638,-1.0735772783\\H,-1.1162718544,3.9410622511,-2.0080405324\\H,-2.6402477514,3.7235766213,-1.1367677658\\H,-1.1743672987,4.2170269905,-0.2702453301\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-747.4629342\\RMSD=7.041e-09\\RMSF=2.871e-05\\Thermal=0.\\Dipole=-0.0698608,-0.2870716,0.0847974\\PG=C01 [X(C7H12O1S1)]\\

10 (MeO/NO₂)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O3\TSCHNEI\18-Dec-2009\0\# opt freq rb3lyp/6-311g(d)\DA_O_NO2_1\0,1\C,0.2100580015,-0.0726674958,-0.0868184857\O,0.0227420098,0.1740538209,1.2668184064\C,1.2426942529,0.1731166741,1.9999518738\C,-0.1284182996,-2.674480106,0.2385478543\C,0.1039052969,-1.4690638627,-0.6427479273\H,0.8754657992,0.614423386,-0.6072058595\H,0.688612713,-1.6283473505,-1.5434809033\C,-1.0305318971,-0.4746020777,-0.8344923928\H,-1.9549099149,-0.5963056389,-0.2887048587\H,0.8235286176,-3.135380445,0.5163459544\H,-0.7251395838,-3.4306037765,-0.2778946722\H,0.9825631543,0.3866255295,3.0356672193\H,1.7466543244,-0.7983901385,1.943408872\O,-0.2767693517,0.3054860069,-2.8764845388\H,1.9241650897,0.9498816213,1.6321598985\H,-0.6468354461,-2.4002663862,1.1588691324\N,-1.2567166885,0.0994734736,-2.1684455317\O,-2.4152239211,0.3308716331,-2.4803510236\Version=AM64L-G03RevC.02\State=1-A\HF=-476.3490289\RMSD=9.708e-09\RMSF=7.503e-06\Thermal=0.\Dipole=0.9711309,-0.7677789,1.3695353\PG=C01 [X(C5H9N1O3)]\

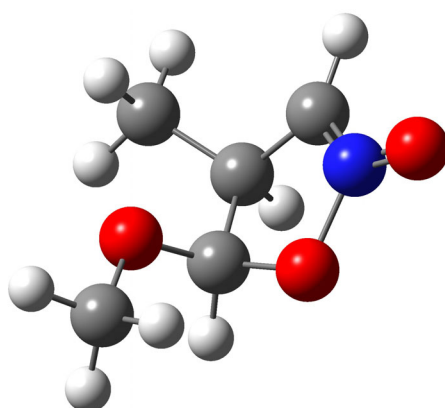
TS₁₀₋₁₁ (MeO/NO₂)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O3\TSCHNEI\11-Jan-2010\0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight integral=g rid=ultrafine\DA_O_NO2_TS\0,1\C,0.0262437681,-0.1583410699,-0.1125975065\C,-0.1038963709,-0.2086634611,2.418163679\C,0.76518843,-0.0756362293,1.162966347\H,1.317714006,0.870711262,1.170022713\C,1.6856787403,-

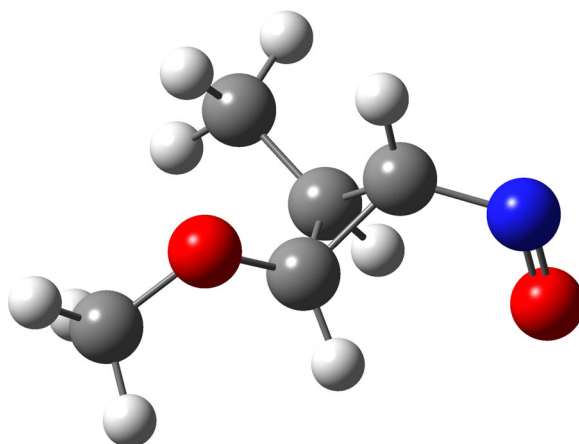
1.2541883572,1.0004344142\H,1.7068937262,-2.0904773803,1.6820434169\H,
 -0.7814594587,0.6412023534,2.5235703691\H,0.542391001,-0.2424210254,3.
 2970783863\O,2.2867031286,-0.4691109254,-1.043127587\H,-0.6973603081,-
 1.1240305569,2.3963909587\N,2.4811551685,-1.3223520754,-0.0985693755\O
 ,3.3807780747,-2.1765825172,-0.1793361273\O,-0.9293005903,-1.018976732
 7,-0.2674679574\C,-1.3938485002,-1.2919559811,-1.6100588514\H,-2.40064
 54298,-1.6864355345,-1.5056274288\H,-1.3959479365,-0.3764413606,-2.203
 5138843\H,-0.7313680714,-2.0334888426,-2.0552580066\H,0.2560054314,0.4
 838189513,-0.9533687793\\Version=AM64L-G03RevC.02\State=1-A\HF=-476.28
 56515\RMSD=5.735e-09\RMSF=1.471e-05\Thermal=0.\Dipole=-3.1264618,0.809
 3402,0.125315\PG=C01 [X(C5H9N1O3)]\\

11 (MeO/NO₂)



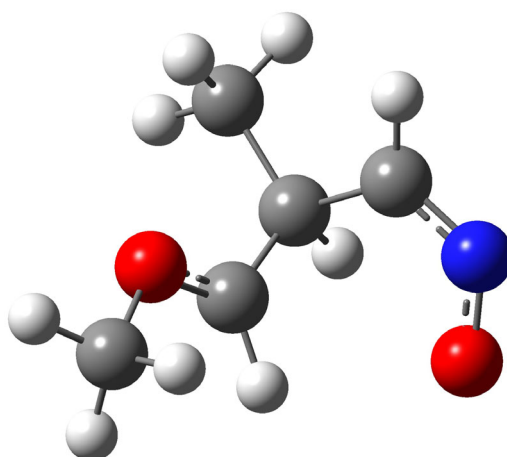
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O3\TSCHNEI\18-Dec-2009\
 0\# opt freq rb3lyp/6-311g(d)\DA_O_NO2_2\0,1\C,0.0514248227,0.11154100
 24,0.0136965405\O,0.0786258948,-0.1738206569,1.3758282468\C,1.38786017
 39,-0.2110722595,1.9351249574\C,-2.3635528764,-0.808344773,0.276480816
 3\C,-1.4123439891,0.1169082953,-0.4836910662\H,-1.4051022798,-0.178021
 7835,-1.5429698049\C,-1.7244607633,1.5759602649,-0.3812133066\H,-2.682
 5668109,2.0705708299,-0.4141901\H,-2.0510693181,-1.8506014578,0.177336
 8339\H,-3.3760641875,-0.7259503628,-0.1274142557\H,1.269518852,-0.4889
 666481,2.981147817\H,2.0081061809,-0.9624540261,1.4289034176\O,0.54428
 52659,1.4177009776,-0.2675727615\H,1.8745007834,0.7644304685,1.8656707
 917\H,-2.3877999364,-0.5621450971,1.337108186\N,-0.6571516614,2.309751
 2864,-0.2608400608\O,-0.4298727103,3.4974801052,-0.1811605334\H,0.7044
 423081,-0.5723400146,-0.5428107913\\Version=AM64L-G03RevC.02\State=1-A
 \HF=-476.3635381\RMSD=4.550e-09\RMSF=7.442e-06\Thermal=0.\Dipole=-0.39
 01053,-1.4353741,-0.0697826\PG=C01 [X(C5H9N1O3)]\\

10 (MeO/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\26-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_NO_1\0,1\C,0.1883473129,0.097385746
1,0.039146408\H,0.4592823234,0.2158395805,1.0895048012\C,1.3827627922,
-0.0335918013,-0.892924855\H,1.3129189188,0.4453506562,-1.8614769738\C
,0.4551396738,-1.2246389194,-0.5909904976\H,0.9424287947,-1.9398741923
,0.0681881721\C,-0.4061736411,-1.7822286583,-1.6976531725\H,-1.1854418
151,-2.4315601911,-1.2871057251\H,-0.8979950198,-0.9850793271,-2.25744
77969\H,0.1862794616,-2.377816078,-2.3966706952\N,2.712470276,0.006690
1453,-0.3412316131\O,2.8284624451,-0.5244740716,0.7456481225\O,-0.8358
042959,0.9143987947,-0.4181234106\C,-2.0408704071,0.7534550852,0.32194
27719\H,-1.8913271763,1.0051726774,1.379067271\H,-2.7653896073,1.44214
18775,-0.1105093693\H,-2.4245414204,-0.2708093592,0.2514413725\Versio
n=AM64L-G03RevC.02\State=1-A\HF=-401.1134383\RMSE=7.186e-09\RMSE=3.
953e-06\Thermal=0.\Dipole=-1.3891949,-0.3191023,-0.1764794\PG=C01 [X(C5H9
N1O2)]\

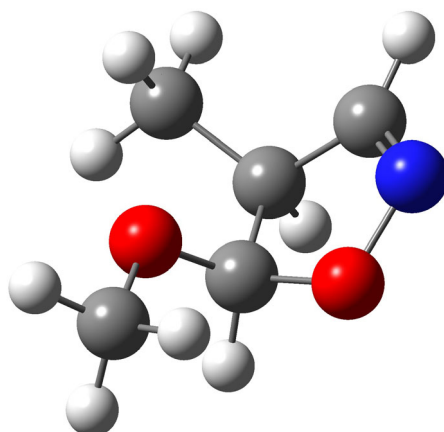
TS₁₀₋₁₁ (MeO/NO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\26-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=t
ight\DA_O_NO_TS\0,1\C,0.0868010424,-0.3072922374,-0.2182562954\C,-0.
0252544823,0.169775948,2.0473714813\H,0.8288921303,0.3472107958,2.6898
989356\O,-1.989814813,0.8475436242,1.243549119\C,0.0188725638,-1.03615
00337,1.0206497432\H,-0.9666347196,-1.5074077388,1.095776712\C,1.17710

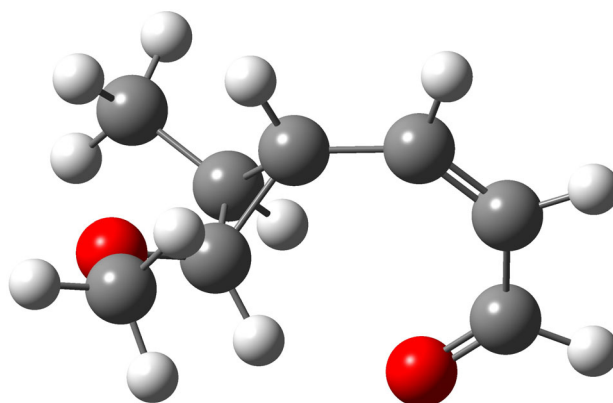
91495,-1.9776318967,1.3410033069\H,1.2060685832,-2.8187541412,0.644783
 6931\H,2.1377547291,-1.4619753996,1.2858098573\H,1.0613952253,-2.37405
 54618,2.3513583794\H,-0.8184982961,0.0857517867,-0.6708863097\N,-1.089
 2834405,0.8900554518,2.127636499\O,1.2489330566,0.0599314119,-0.714333
 4875\C,1.2319465907,1.0366118603,-1.7707328651\H,0.9657287957,2.012184
 1061,-1.3601536183\H,2.2398167048,1.0603612499,-2.1766201833\H,0.52023
 42082,0.7452481761,-2.5461359399\\Version=AM64L-G03RevC.02\State=1-A\H
 F=-401.0851002\RMSD=3.703e-09\RMSF=6.242e-06\Thermal=0.\Dipole=1.66081
 59,-0.5804707,-1.6351792\PG=C01 [X(C5H9N1O2)]\\

11 (MeO/NO)



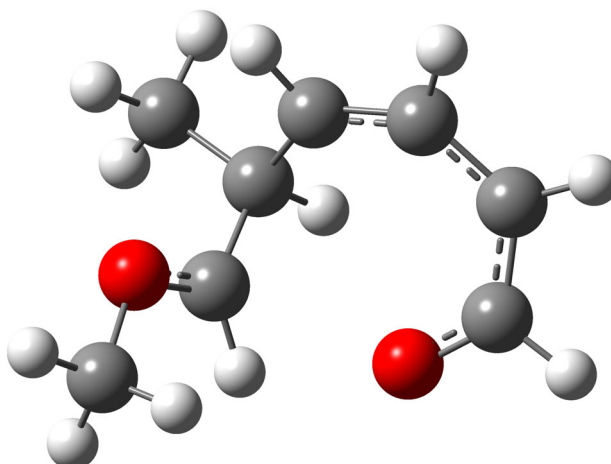
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C5H9N1O2\TSCHNEI\26-Jun-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_O_NO_2\0,1\C,0.0583989512,-0.07222324
 13,-0.0769317969\C,-0.0627852249,-0.1715495715,2.5239008181\C,0.795974
 9375,-0.0032077561,1.2698043653\H,1.3298911187,0.9551848434,1.32265416
 07\C,1.8181171032,-1.0849262823,1.0252535135\H,-0.7972703174,0.6325553
 999,2.6054280755\H,0.5635037214,-0.1426246561,3.4195602458\O,0.9941507
 437,-0.7235478766,-0.9602695679\H,-0.6035304,-1.1169077978,2.505852717
 5\H,-0.1507651526,0.9006456191,-0.5367562063\H,2.4643127567,-1.5317953
 533,1.7724502094\N,1.9198633674,-1.4652232691,-0.1835750001\O,-1.11166
 87738,-0.8143840914,0.0630482704\C,-1.867707722,-0.9365619459,-1.13641
 36311\H,-1.3095145655,-1.4821097454,-1.9005729777\H,-2.7717599505,-1.4
 862658875,-0.8785484427\H,-2.1443991909,0.0518212653,-1.5269753448\\Ve
 rsion=AM64L-G03RevC.02\State=1-A\HF=-401.1719015\RMSD=7.861e-09\RMSF=1
 .178e-05\Thermal=0.\Dipole=-0.5228371,0.7045539,0.7162049\PG=C01 [X(C5
 H9N1O2)]\\

10 (MeO/CHCHCHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H12O2\TSCHNEI\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_Acryl_1\0,1\C,-0.2771883207,-0.29000
60952,0.0331093018\H,-0.2340219086,-0.4148882424,1.1100843331\C,1.0768
421343,-0.0774505083,-0.6927488107\H,0.947198312,0.5521576331,-1.56799
56578\C,2.39136314,0.0752135147,-0.0710332349\C,0.2578865382,-1.381648
0948,-0.8057569146\H,0.6597418406,-2.2080822982,-0.2330485074\C,-0.357
7552506,-1.7425591883,-2.1377433934\H,-1.1595071589,-2.4741444555,-1.9
984671163\H,-0.7932021862,-0.8712207954,-2.6285809649\H,0.3856171128,-
2.1842708958,-2.8072960019\H,3.0173423451,0.7865899287,-0.6098161283\O
,-1.3644078965,0.4274872067,-0.4460464777\C,-1.4934250158,1.7105170425
,0.1451511987\H,-0.6253148046,2.3429245933,-0.0796918066\H,-2.39003664
11,2.1639784154,-0.2764199531\H,-1.6036827138,1.6376386145,1.234380471
7\C,2.9992762178,-0.4743054092,1.0095477206\H,4.0238373149,-0.16298101
34,1.1998570708\C,2.4945862544,-1.4462771053,1.9800170612\O,1.36826886
7,-1.9002831544,2.0633660288\H,3.2632329567,-1.7751039153,2.7130892186
\\Version=AM64L-G03RevC.02\State=1-A\HF=-462.5538049\RMSD=7.331e-09\
RMSF=1.134e-05\Thermal=0.\Dipole=0.5459875,0.8319416,-0.3781237\PG=C01
[X(C8H12O2)]\
```

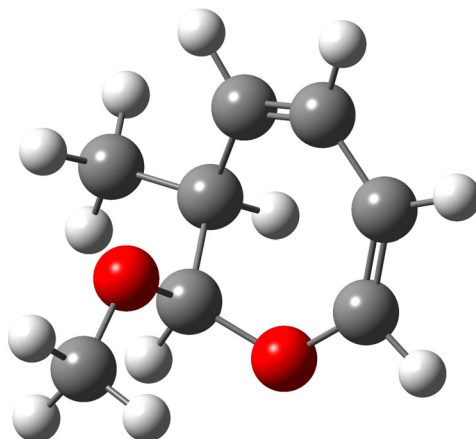
TS₁₀₋₁₁ (MeO/CHCHCHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H12O2\TSCHNEI\17-Aug-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=ti
ght\DA_O_Acryl_TS\0,1\C,0.1612865853,0.0946721334,-0.2254844284\H,0.3
```

526111754,0.4310080131,0.7811897399\C,1.441538612,-0.044390419,-2.2068902201\H,0.7993903897,-0.2388029818,-3.0640379904\C,2.4426818519,0.8723126251,-2.3842596191\C,1.0534687646,-0.8262593064,-0.9669629924\H,1.9248981567,-0.9868204272,-0.3353420377\C,0.3873338339,-2.1672660147,-1.3119106082\H,0.1129048866,-2.7254737333,-0.4121590612\H,-0.5145529837,-2.0191053852,-1.9108927635\H,1.0850377956,-2.7743081365,-1.8939998831\H,2.5826624018,1.1457984615,-3.4319357668\O,-0.9709799818,0.4552958688,-0.7715574366\C,-1.7416684952,1.4530498537,-0.073032578\H,-1.172514959,2.382671128,-0.034823721\H,-2.6539649786,1.5844004901,-0.6484448148\H,-1.9766175804,1.1102733756,0.9365273162\C,3.2947976892,1.5691234055,-1.4927344893\H,4.0913126702,2.159092986,-1.9369370623\C,3.0184697009,1.8257984246,-0.1479440436\O,2.1060794799,1.3154442834,0.5560443384\H,3.6397079677,2.6114987175,0.3244323318\\Version=AM64L-G03RevC.02\State=1-A\HF=-462.5105868\RMSD=5.539e-09\RMSF=4.797e-06\Thermal=0.\Dipole=-1.7962309,-0.1629562,0.1122678\PG=C01 [X(C8H12O2)]\\

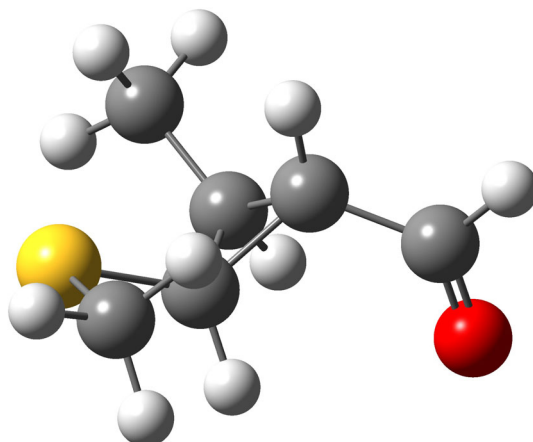
11 (MeO/CHCHCHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H12O2\TSCHNEI\03-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_O_Acryl_2\0,1\C,0.2304628863,-0.0026036571,0.1856802591\H,0.0924741353,-0.4520995824,1.1773393902\C,1.7576378773,-0.0204392392,-1.8340233018\H,2.128004337,-0.8053246027,-2.4881702174\C,1.4402230821,1.1676074915,-2.3668018304\C,1.6251596333,-0.3612513097,-0.3718759287\H,2.3350517251,0.2464685983,0.2045875585\C,1.9262331958,-1.842965258,-0.1081557229\H,1.8843748514,-2.0785535142,0.9588238997\H,1.2060033006,-2.4813494469,-0.6257852858\H,2.9261621889,-2.102613118,-0.4642945932\H,1.615110181,1.3151058749,-3.429966687\O,-0.7345597673,-0.4787852511,-0.6962670815\C,-2.0636916886,-0.4486655593,-0.1932115255\H,-2.404230453,0.5758275031,-0.0201831283\H,-2.6904677698,-0.9156925888,-0.9517515713\H,-2.1455171204,-1.0159353543,0.7432747115\C,0.8798040183,2.3039823195,-1.6597911088\H,0.9095065786,3.2592305246,-2.1763458293\C,0.3117873279,2.3592225445,-0.4408856114\H,-0.0364069642,3.3086528299,-0.0474427135\O,0.0619176322,1.389731569,0.4774560327\\Version=AM64L-G03RevC.02\State=1-A\HF=-462.5784578\RMSD=3.596e-09\RMSF=4.464e-06\Thermal=0.\Dipole=-0.2147295,-0.1735288,0.2352565\PG=C01 [X(C8H12O2)]\\

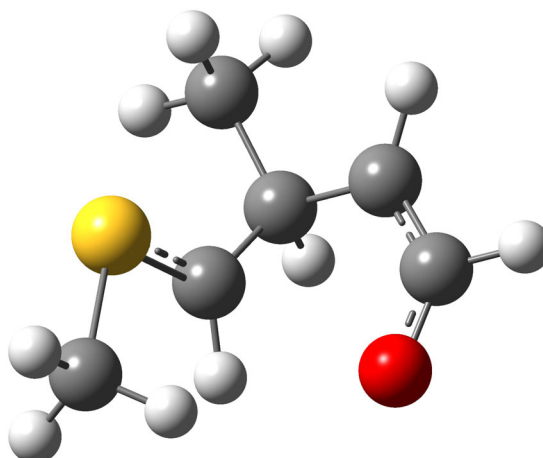
SMe-Donor

10 (MeS/CHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNEI\15-Jan-2010\
0\# opt=tight freq rb3lyp/6-311g(d) int=ultrafine\DA_S_CHO_1\0,1\C,-0
.0645085893,-0.1026999071,-0.0917314082\C,0.1617879384,0.1103165084,2.
6545674469\H,1.0127415951,-0.077743302,-0.2261283646\C,-0.7744214243,1
.1785026008,-0.568499899\H,-1.658035685,1.4767616379,-0.0137844871\C,0
.0723482612,2.2651227175,-1.105145457\H,-0.2292937005,1.1270269948,2.5
996471085\H,-0.0907016002,-0.3164232653,3.6255422512\H,1.246862079,0.1
242686642,2.5471865961\C,-0.8661668855,-0.1340932921,-1.3477563766\H,-
0.2509720365,-0.1297891684,-2.2438144455\C,-2.1907202232,-0.8491878632
,-1.4862812703\H,-2.0348255003,-1.9099670895,-1.7038859066\H,-2.792239
1696,-0.7813773483,-0.5785812065\H,-2.7698232414,-0.4227436333,-2.3098
324426\O,1.0936924868,2.0874170546,-1.7315841542\H,-0.2820596331,3.296
7694128,-0.8930874895\S,-0.6097160242,-0.9575859244,1.3893655748\Vers
ion=AM64L-G03RevC.02\State=1-A\HF=-708.132361\RMSD=8.536e-09\RMSF=1.
141e-06\Thermal=0.\Dipole=-0.6620621,0.172478,0.5233787\PG=C01 [X(C6H10O
1S1)]\
```

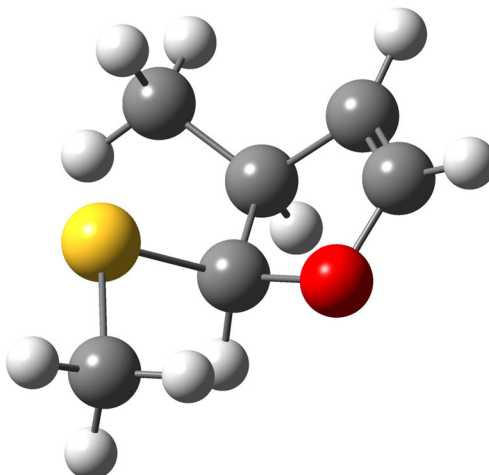
TS₁₀₋₁₁ (MeS/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNEI\17-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight integral=
grid=ultrafine\DA_S_CHO_TS\0,1\C,0.3059787124,-0.3373576401,-0.16677
```

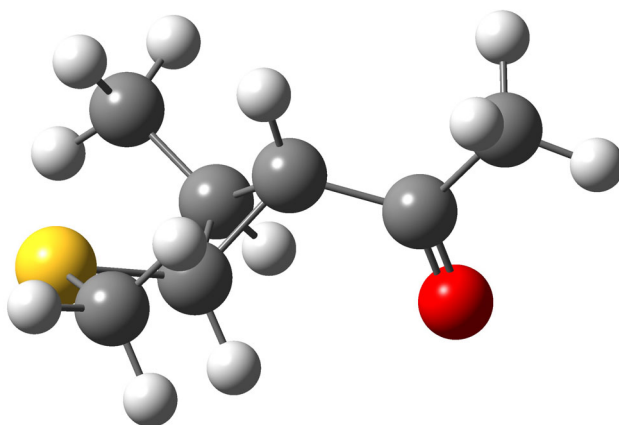
87791\C,0.0695094765,0.0638879056,2.0835254958\H,0.7355116841,0.101103
6408,2.9408355651\C,-0.824961197,1.0885584976,1.8217434538\H,-1.090540
1659,1.7107685865,2.7011557752\O,-1.3796127737,1.3565479617,0.72562095
95\C,0.2591541185,-1.093692461,1.0926775476\H,-0.6166885331,-1.7524797
038,1.0738285197\C,1.5094973752,-1.9106639899,1.4363461008\H,1.6746565
556,-2.7111630115,0.7119525948\H,2.4053001083,-1.2849823447,1.46966106
36\H,1.3859037297,-2.3602520514,2.4239072538\H,-0.6121166801,-0.207361
3413,-0.7205539711\S,1.6690382127,0.4298814204,-0.8369114916\C,0.86993
954,1.4370393614,-2.1398290103\H,0.0689578499,2.0154947382,-1.68404237
51\H,1.6339209987,2.1047006914,-2.5357428929\H,0.4885734536,0.80502867
61,-2.9407448939\\Version=AM64L-G03RevC.02\State=1-A\HF=-708.0639541\R
MSD=8.565e-09\RMSF=7.375e-06\Thermal=0.\Dipole=1.0167591,-0.5748106,-0
.9990556\PG=C01 [X(C6H10O1S1)]\\

11 (MeS/CHO)



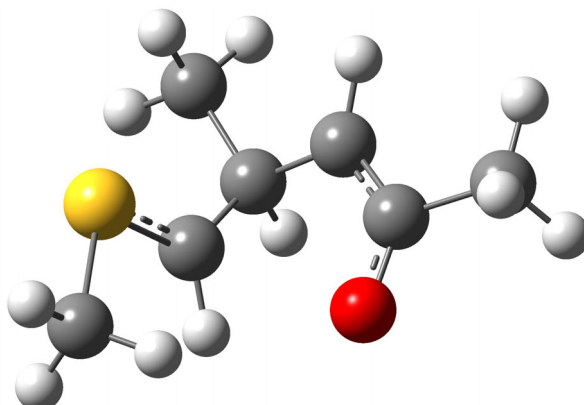
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1S1\TSCHNE\17-Jan-2010\
0\\# opt freq b3lyp/6-311g(d)\\DA_S_CHO_2\0,1\C,-0.2273241885,0.0441835
381,0.1823766985\C,0.2072384291,-0.132315077,2.7760819661\C,0.78407543
91,0.0210345212,1.3660635281\H,1.3365620166,0.9719849796,1.336838121\C
,1.7062676171,-1.0959017201,0.9170975562\H,2.4796837798,-1.5411846614,
1.5263050813\H,-0.4853805783,0.6767886546,3.0188535071\H,1.0176448564,
-0.1063835951,3.5098682419\C,1.4429602702,-1.3827027553,-0.3520617859\
O,0.4223719344,-0.6492758257,-0.9060175601\H,-0.3191299895,-1.08094350
38,2.8993679257\H,1.9027080541,-2.0896067266,-1.0288203056\H,-0.445025
8763,1.0489795249,-0.1777568819\S,-1.8370120171,-0.7666558758,0.575073
667\C,-2.646849745,-0.5047006687,-1.040285512\H,-2.0542168161,-0.95236
42563,-1.836252115\H,-3.6173183393,-0.9986070368,-0.9931110282\H,-2.80
05452699,0.5575271666,-1.2395527179\\Version=AM64L-G03RevC.02\State=1-
A\HF=-708.1338012\RMSD=2.618e-09\RMSF=1.981e-05\Thermal=0.\Dipole=0.27
98188,0.3022583,-0.0434178\PG=C01 [X(C6H10O1S1)]\\

10 (MeS/COMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O1S1\TSCHNEI\17-Jan-2010\
0\# opt freq rb3lyp/6-311g(d) geom=connectivity\DA_S_COR_1\0,1C,0.00
73955208,0.5369792951,0.3545906197\C,0.2371170094,-0.2198824936,2.8866
506231\C,0.8225441621,0.1277101141,1.5367340103\H,0.4794658457,1.25692
77044,-0.3068483374\H,1.7924053266,0.6170637903,1.5689114082\C,0.69024
57339,-0.8378759488,0.3622658038\H,0.039059376,-1.691769671,0.51909970
18\H,0.0543962702,0.6850248633,3.4738528246\H,0.9307164583,-0.84793804
07,3.452770737\C,1.8636216623,-1.0276090951,-0.5378925421\C,2.05307429
8,-2.4127102203,-1.1251774441\H,1.1782627329,-2.7032904014,-1.71637329
54\H,2.9402504789,-2.4301288638,-1.7567937346\H,2.157027257,-3.1559216
677,-0.3277233956\O,2.6271075914,-0.1148404728,-0.7868285958\H,-0.7094
877719,-0.7555334852,2.7994892357\S,-1.7801984227,0.683056466,0.457922
7061\C,-2.2146972959,0.3081954322,-1.2762169956\H,-1.9051221562,-0.701
6184378,-1.54848729\H,-3.2998143018,0.3805831585,-1.3542432975\H,-1.76
36571688,1.0299600013,-1.9580915769\\Version=AM64L-G03RevC.02\State=1-
A\HF=-747.4658402\RMSD=8.281e-09\RMSF=4.704e-06\Thermal=0.\Dipole=-0.4
597673,-0.867996,-0.0487064\PG=C01 [X(C7H12O1S1)]\
```

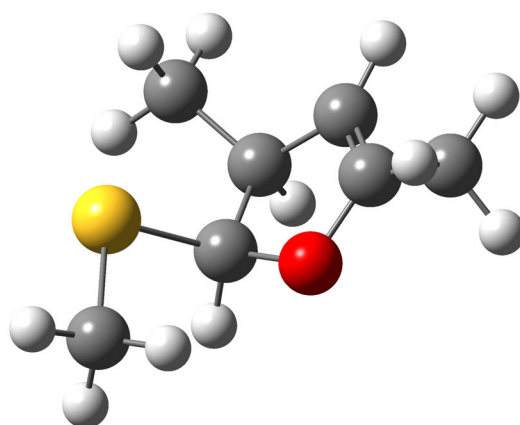
TS₁₀₋₁₁ (MeS/COMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O1S1\TSCHNEI\17-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_S_COR_TS\0,1C,-0.2238949549,0.1938585163,0.3995410979\C,0.2
21725215,0.0198470044,2.9019066584\C,0.7743052787,0.085769484,1.474068
3264\H,1.4693004971,0.92920951,1.3876858342\C,1.439716131,-1.234827992
1,1.0785307888\H,1.5200288417,-1.994475235,1.8494482158\H,-0.290331046
```

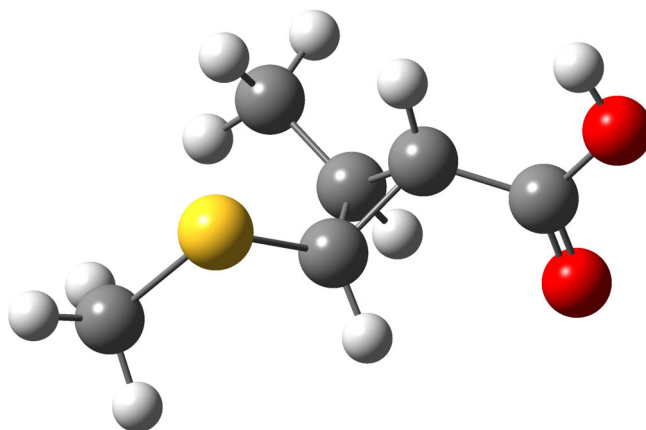
8,0.9449710443,3.1754446853\H,1.0468307658,-0.1369649167,3.6001554717\
C,1.8158274633,-1.4756307446,-0.2407229108\C,2.7996854287,-2.609016736
6,-0.5129645164\H,3.0527955029,-3.1884802764,0.3766129325\H,2.38377685
21,-3.2775084432,-1.2720444284\H,3.7190896005,-2.18634266,-0.927949497
1\O,1.4258594546,-0.7947095061,-1.2302214173\H,-0.4776392662,-0.811039
3112,3.027300303\H,0.0197332916,0.7837226372,-0.4713463686\S,-1.744358
197,-0.5714566341,0.3484190634\C,-2.2178681521,-0.2430331306,-1.388676
0311\H,-1.4119860366,-0.5809853094,-2.0368996112\H,-3.1199663151,-0.82
11164138,-1.5845454414\H,-2.4241755441,0.8153259287,-1.5427477329\\Ver
sion=AM64L-G03RevC.02\State=1-A\HF=-747.3930433\RMSD=5.735e-09\RMSF
=1.886e-06\Thermal=0.\Dipole=-1.2631474,0.4727153,0.3998141\PG=C01 [X(C7H
12O1S1)]\\

11 (MeS/COMe)



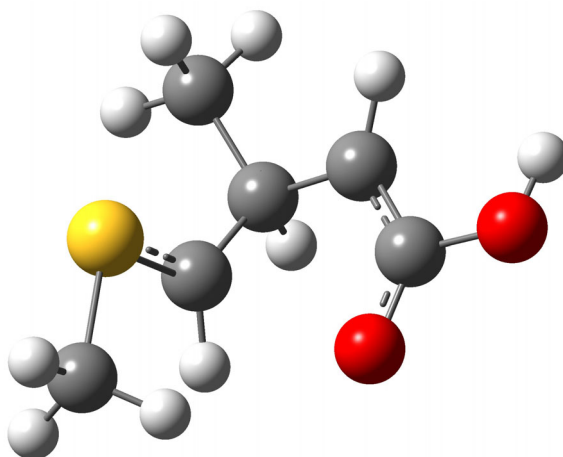
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C7H12O1S1\TSCHNEI\17-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_COR_2\0,1\C,-0.2312402883,-0.00091
87701,0.2666994941\C,0.2223555864,-0.0541445654,2.8599813645\C,0.78734
58355,0.0516296573,1.4410209375\H,1.3137035438,1.015559658,1.367206599
1\C,1.7289986469,-1.059814068,1.0305658251\H,2.5121692541,-1.462137706
,1.6576795619\H,-0.4864218152,0.7493135795,3.0737227494\H,1.0359351287
,0.0195042491,3.5871196977\C,1.4814056167,-1.4127009067,-0.2291686245\
C,2.1271044622,-2.4017473181,-1.1314516499\H,1.4069645002,-3.162139401
6,-1.4487088148\H,2.5005738909,-1.9123093922,-2.0364244405\H,2.9621899
179,-2.8953762509,-0.6332277524\O,0.4342902371,-0.708534271,-0.7965377
79\H,-0.2824183817,-1.0081363208,3.0253883279\H,-0.4881155955,0.982344
0756,-0.1263662704\S,-1.8118735363,-0.8509514335,0.7026004286\C,-2.643
5980916,-0.6687434606,-0.9122945977\H,-2.0424005145,-1.12066295,-1.699
3957621\H,-3.5961844276,-1.1936480664,-0.840907421\H,-2.8355350044,0.3
806296698,-1.1440599935\\Version=AM64L-G03RevC.02\State=1-A\HF=-747.46
64193\RMSD=6.789e-09\RMSF=4.374e-06\Thermal=0.\Dipole=0.3503634,0.1986
051,-0.1875769\PG=C01 [X(C7H12O1S1)]\\

10 (MeS/COOH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2S1\TSCHNEI\18-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_COOH_1\0,1\C,-0.0556071374,-0.2547
358184,-0.3382122414\C,-0.1522985276,0.1579556084,2.2880340394\C,0.600
9237554,-0.0034053191,0.989041182\H,0.4454029181,0.1700513295,-1.20185
85444\H,1.5108070475,0.5840553272,0.9029659344\C,0.7238862967,-1.37474
16578,0.3359250703\H,0.126669957,-2.1633304042,0.7862978432\O,2.783372
2949,-0.969369252,-0.7921844956\H,-0.4158758488,1.2068634185,2.4530798
684\H,0.4622291956,-0.1630594239,3.1336395621\O,2.3699605841,-3.067701
9922,-0.1920494565\C,2.0375850176,-1.7518000954,-0.2689415784\H,-1.075
9647449,-0.4229803097,2.297448697\H,1.6696980258,-3.5761069539,0.23556
08066\S,-1.8259738206,-0.500266146,-0.5569046403\C,-2.3767551527,1.241
5329311,-0.6329816506\H,-1.9009706142,1.7643828986,-1.4632347882\H,-3.
4537924308,1.2226768177,-0.8016367501\H,-2.1714993747,1.763067054,0.30
17198891\Version=AM64L-G03RevC.02\State=1-A\HF=-783.3956684\RMSD=9.48
3e-09\RMSF=9.645e-06\Thermal=0.\Dipole=-1.1798406,0.1663351,0.9759323\
PG=C01 [X(C6H10O2S1)]\
```

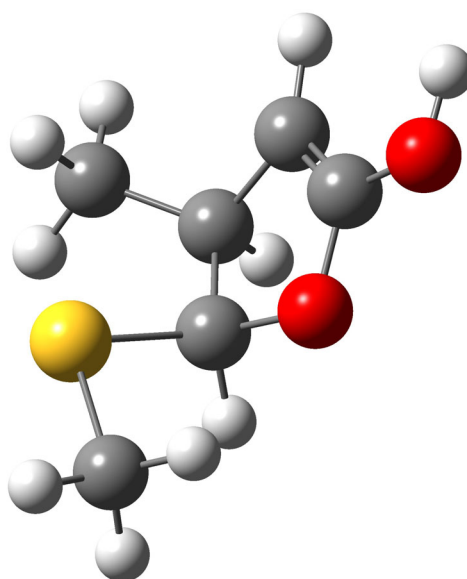
TS₁₀₋₁₁ (MeS/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2S1\TSCHNEI\18-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_S_COOH_TS\0,1\C,-0.293183594,0.173458391,0.3881062288\C,0.26
91469538,0.0118219851,2.8658230941\C,0.7670862183,0.052061,1.414619929
3\H,1.4472168618,0.9052622375,1.2975841024\C,1.4112889748,-1.262577786
```

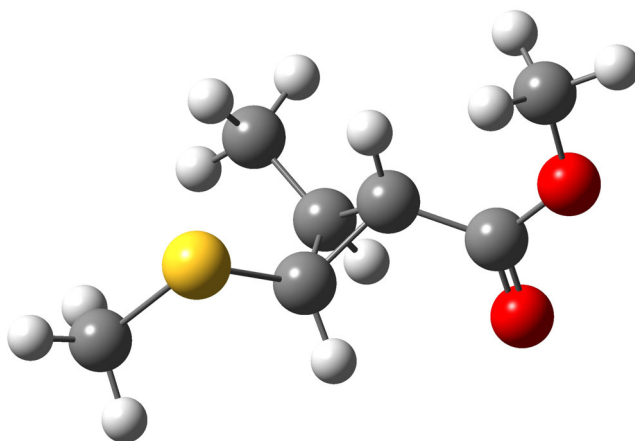
9,1.0165211374\H,1.5233947918,-2.0283068659,1.7780677454\O,1.095008578
3,-0.9071491239,-1.2945922531\H,-0.2193572665,0.9466391704,3.148467154
9\H,1.1216963794,-0.1456145409,3.5302533034\O,2.3984395161,-2.60967979
53,-0.6815174134\C,1.5936164364,-1.5437244954,-0.3464636999\H,-0.43299
4067,-0.8097408709,3.029381921\H,2.8703667814,-2.9064395482,0.10537712
08\H,-0.1293825224,0.8317272389,-0.4532339774\S,-1.792328321,-0.623037
1921,0.3865362223\C,-2.3604962472,-0.2493808356,-1.3119089177\H,-1.579
5457762,-0.5578999036,-2.0039972198\H,-3.2612981193,-0.8382413889,-1.4
793343286\H,-2.5917175482,0.8091177258,-1.4237298615\\Version=AM64L-G0
3RevC.02\State=1-A\HF=-783.3163117\RMSD=6.557e-09\RMSF=8.820e-06\Therm
al=0.\Dipole=-1.2864651,0.6950811,0.9702476\PG=C01 [X(C6H10O2S1)]\\

11 (MeS/COOH)



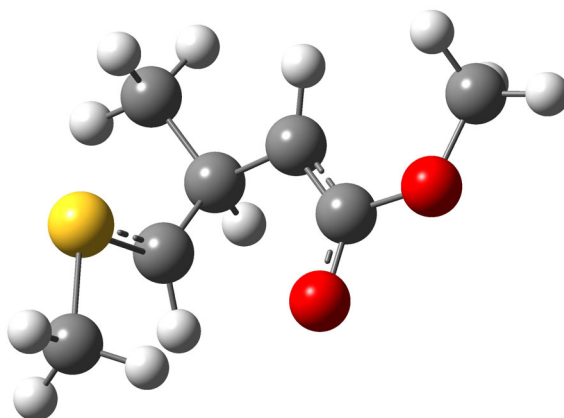
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2S1\TSCHNEI\29-Jul-2010\
0\\# opt freq rb3lyp/6-311g(d)\\DA_S_COOH_3\\0,1\C,-0.1540152399,0.21915
70795,0.304246354\C,0.2529606978,0.0072369085,2.8928020757\C,0.8463290
353,0.0203501524,1.4818958516\H,-0.1903261959,1.2437573643,-0.06315344
65\H,1.5625087109,0.8553522657,1.4358199915\C,1.521624026,-1.264169531
8,1.0495750086\O,0.3631025285,-0.5782117558,-0.7872964837\H,-0.2660348
487,0.9410319872,3.1227692263\H,1.0548796641,-0.1142313898,3.626487844
2\O,1.5628434323,-2.4346158538,-1.1113225085\C,1.206647487,-1.48668370
15,-0.2295465005\H,-0.4479250452,-0.8185640718,3.030846975\S,-1.875604
6185,-0.298526638,0.6997089001\C,-2.6271865255,0.0888117925,-0.9187340
543\H,-2.1237228179,-0.4647390023,-1.7093465117\H,-3.6697967717,-0.224
7608677,-0.8674908371\H,-2.590318252,1.1596182098,-1.1276148878\H,2.18
72414739,-1.8539124857,1.6633206376\H,2.2046221781,-3.0214647551,-0.69
52235068\\Version=AM64L-G03RevC.02\State=1-A\HF=-783.3762062\RMSD=
3.144e-09\RMSF=7.243e-06\Thermal=0.\Dipole=0.5926101,0.025544,0.231171
3\PG=C01 [X(C6H10O2S1)]\\

10 (MeS/COOMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2S1\TSCHNEI\18-Jan-2010\0\# opt freq rb3lyp/6-311g(d)\DA_S_COOR_1\0,1C,-0.074701542,-0.0686707641,-0.3606218816\C,-0.0863011794,-0.0922609141,2.2998902625\C,0.6125171027,0.0505747236,0.968558287\H,0.3301100333,0.5462367974,-1.1573246262\H,1.439500274,0.7546982418,0.9506578402\C,0.8623440184,-1.1782216488,0.0980022803\H,0.3801439985,-2.0861589357,0.4354764251\O,2.7604386589,-0.3039975557,-1.0191446384\H,-0.4472300499,0.8787615311,2.6521231777\H,0.6000935659,-0.480980833,3.0574442657\O,2.7545540332,-2.4928048002,-0.7586206605\C,2.1801893772,-1.2728210354,-0.5999122926\C,2.1222529653,-3.6964533181,-0.3152818107\H,1.9852112118,-3.705548659,0.769026105\H,1.1639197425,-3.8568945683,-0.8151126158\H,2.8053481647,-4.4967324143,-0.5924375443\H,-0.9439440044,-0.7646110003,2.2406871977\S,-1.8133692938,-0.4919697704,-0.5625037402\C,-2.5645565379,1.1618453207,-0.3540747133\H,-2.1865321229,1.8579927868,-1.1035349699\H,-3.63831313,1.0397106369,-0.4991988096\H,-2.3828692149,1.5571378792,0.64526904\Version=AM64L-G03RevC.02\State=1-A\HF=-822.7050918\RMSD=4.428e-09\RMSF=2.164e-05\Thermal=0\Dipole=-0.9286668,-0.4399266,0.969985\PG=C01 [X(C7H12O2S1)]\

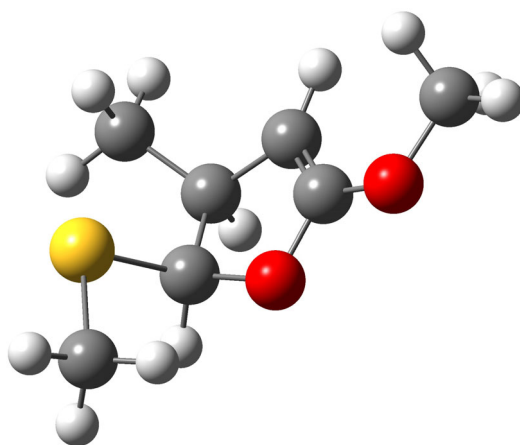
TS₁₀₋₁₁ (MeS/COOMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O2S1\TSCHNEI\18-Jan-2010\0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra fine\DA_S_COOR_TS\0,1C,-0.2674820888,0.1698389105,0.4300595035\C,0.2325050995,0.0789854771,2.9253226903\C,0.763896728,0.0851590378,1.4867

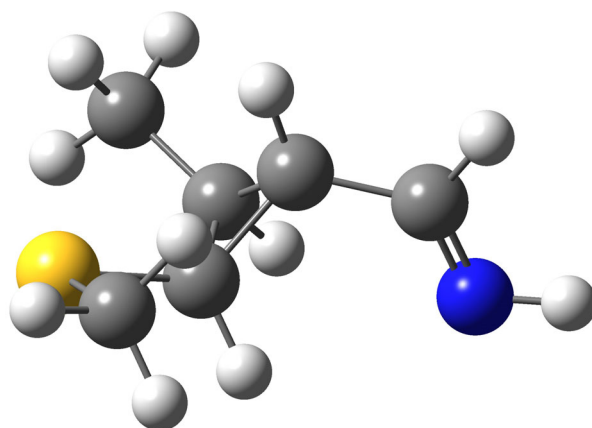
038002\H,1.4442464138,0.9364537345,1.3608095644\C,1.424205257,-1.23647
 51167,1.1354616122\H,1.5097555549,-1.9750935089,1.9225324459\O,1.22865
 04694,-0.8878200912,-1.1865462997\H,-0.2676775442,1.0178071971,3.17242
 30601\H,1.0694790143,-0.0571659794,3.613878704\O,2.4981369203,-2.58106
 24071,-0.5468806315\C,1.6822962851,-1.5284621246,-0.2141133359\C,3.218
 165512,-3.2628841201,0.4707219635\H,3.784333409,-2.5663159182,1.095731
 0227\H,2.552117385,-3.8570880605,1.1064833598\H,3.9033892284,-3.935539
 8814,-0.0447010405\H,-0.469754066,-0.7417752314,3.0932661629\H,-0.0787
 556457,0.7967581068,-0.4292218867\S,-1.7629230562,-0.6357720283,0.4074
 708145\C,-2.2774410339,-0.3227812738,-1.3206186733\H,-1.4702145117,-0.
 6412105465,-1.977107595\H,-3.1647266971,-0.9285196416,-1.4997354006\H,
 -2.5178429515,0.7285657473,-1.4731522669\\Version=AM64L-G03RevC.02\\Sta
 te=1-A\\HF=-822.6274722\\RMSD=8.125e-09\\RMSF=4.793e-06\\Thermal=0.\\Dipole
 =-1.2574247,0.5272129,0.8363631\\PG=C01 [X(C7H12O2S1)]\\

11 (MeS/COOMe)



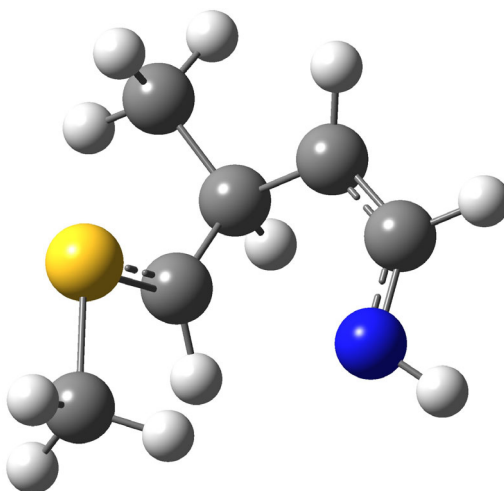
1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H12O2S1\\TSCHNEI\\18-Jan-2010\\
 0\\# opt freq rb3lyp/6-311g(d)\\DA_S_COOR_2\\0,1\C,-0.1756203863,0.09883
 20959,0.3080346749\C,0.2170579749,0.0324798394,2.9062583827\C,0.822431
 7477,0.1053946605,1.5024053029\H,-0.3859258916,1.0924443759,-0.0855062
 178\H,1.3888837638,1.0474371304,1.4385212131\C,1.7146110978,-1.0571893
 865,1.1203332766\H,2.4550801931,-1.5023142908,1.766013515\O,0.49057992
 74,-0.6201941526,-0.7524427002\H,-0.4551818989,0.8716675537,3.10143689
 42\H,1.0157662346,0.0680660032,3.6525238285\O,1.977836964,-2.261583416
 3,-1.004746201\C,1.4650410634,-1.3681767978,-0.1571136935\C,3.03112327
 45,-3.0669467829,-0.4831400671\H,3.8783666478,-2.4467370035,-0.1751954
 703\H,2.6809249604,-3.6567411828,0.3692397811\H,3.3317083289,-3.729156
 7231,-1.2917947346\H,-0.337528453,-0.895356985,3.0606204775\S,-1.78789
 85744,-0.7028783079,0.6988094663\C,-2.5689351969,-0.5009116801,-0.9393
 989141\H,-1.9638823741,-0.9804078321,-1.7068788816\H,-3.5416513758,-0.
 9901192693,-0.8895595684\H,-2.7160232456,0.553187879,-1.1820568117\\Ve
 rsion=AM64L-G03RevC.02\\State=1-A\\HF=-822.6916907\\RMSD=8.724e-09\\RMSF
 =8.120e-06\\Thermal=0.\\Dipole=0.6250448,0.0053332,0.1234923\\PG=C01 [X(C7H
 12O2S1)]\\

10 (MeS/CHNH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1S1\TSCHNEI\19-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_CHNH_1\0,1\C,0.0188098395,-0.04346
4191,-0.0055558274\C,0.0205276347,0.007151763,2.6475914695\C,0.7278582
908,-0.0371544247,1.3121105676\H,0.5340757701,0.4679520352,-0.81301139
68\H,1.6776957757,0.4898336865,1.2772041667\C,0.7355594695,-1.31139150
44,0.476105485\H,0.0923456168,-2.1112680538,0.8282756219\H,-0.23943404
01,1.0356776605,2.9160288985\H,0.6684107878,-0.3873317509,3.4356548975
\C,1.9736099321,-1.7323544119,-0.2156092594\H,-0.9012739089,-0.5769790
904,2.6445757243\N,2.8062224191,-0.8864721551,-0.674984881\H,2.1135340
252,-2.8189877807,-0.3047334112\H,3.594334598,-1.3532884305,-1.1228290
061\S,-1.7744421533,0.0317020364,-0.1012639203\C,-2.0334023938,-0.8959
622884,-1.6532292104\H,-1.6677249259,-1.9197356284,-1.5628550783\H,-3.
1081456655,-0.9164740453,-1.8363669901\H,-1.5424538125,-0.4012870906,-
2.4921256478\Version=AM64L-G03RevC.02\State=1-A\HF=-688.2439128\RMSE=
7.188e-09\RMSF=1.240e-05\Thermal=0.\Dipole=0.1873044,-0.9207267,-0.167
965\PG=C01 [X(C6H11N1S1)]\
```

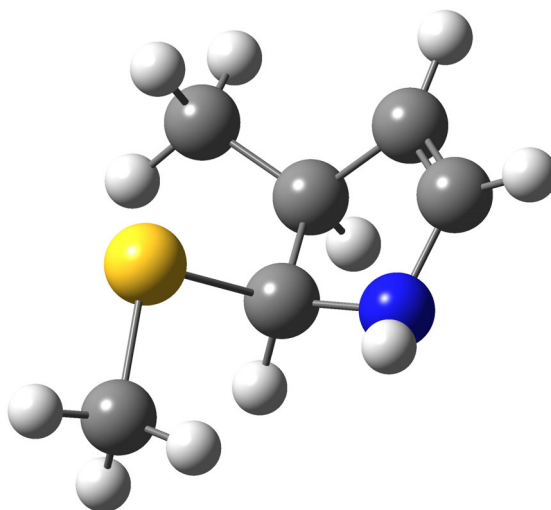
TS₁₀₋₁₁ (MeS/CHNH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H11N1S1\TSCHNEI\19-Jan-2010\
0\# opt=(ts,noeigentest,calcfc) b3lyp/6-311g(d) scf=tight int=ultrafine
freq\DA_S_CHNH_TS\0,1\C,-0.256902819,0.1798812231,0.3467838558\C,0.2
443287,0.0028007543,2.838682624\C,0.7685018547,0.0465579576,1.39832851
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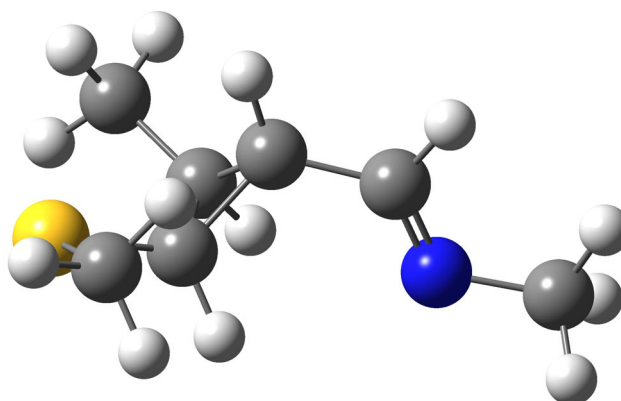
52\H,1.467220526,0.885314664,1.2962250725\C,1.4383346291,-1.2674275254
 ,1.0127139577\H,1.4723622465,-2.0470589086,1.7701837809\H,-0.237611965
 2,0.9426724875,3.1156878754\H,1.0789118079,-0.173968296,3.5218134088\C
 ,1.784241582,-1.5650541814,-0.299333777\H,-0.4768740361,-0.806437393,2
 .9811923969\N,1.2650898107,-0.9937377305,-1.3667260747\H,2.5482672385,
 -2.3490159977,-0.4144723138\H,1.8665722757,-1.1254112985,-2.1825837316
 \H,-0.0582117859,0.83104394,-0.491100264\S,-1.7370150208,-0.675520466,
 0.2524877831\C,-2.2166936468,-0.2731581372,-1.4636712206\H,-1.3770797,
 -0.5278588682,-2.1083391068\H,-3.0800648648,-0.8907894369,-1.708204176
 2\H,-2.4837726463,0.7788754592,-1.5613285177\\Version=AM64L-G03RevC.02
 \State=1-A\HF=-688.1694612\RMSD=6.954e-09\RMSF=2.505e-06\Thermal=0.\Di
 pole=-0.5328457,0.4180649,-0.1545088\PG=C01 [X(C6H11N1S1)]\\

11 (MeS/CHNH)



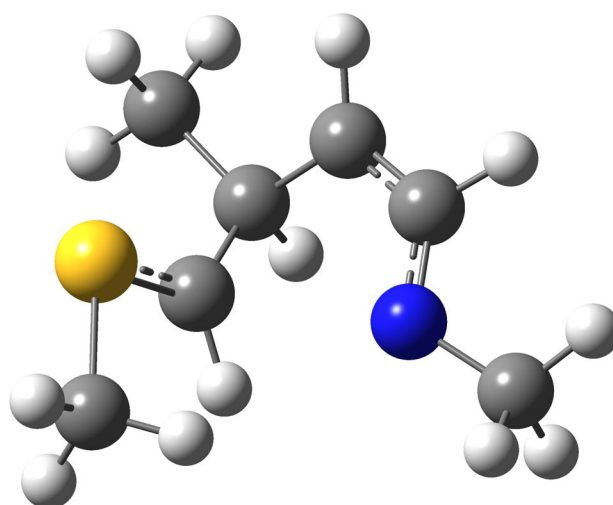
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C6H11N1S1\TSCHNEI\19-Jan-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_S_CHNH_2\0,1\C,-0.1044283683,0.11410
 04525,0.1608669948\C,0.1816469742,0.0212215027,2.7819605893\C,0.832493
 8797,-0.0250348487,1.3997029483\H,1.5315589169,0.824441946,1.333908658
 2\C,1.5947848606,-1.2916070491,1.0619670957\H,2.2433676175,-1.81704783
 15,1.748839497\H,-0.3912893689,0.9400975116,2.92875124\H,0.9554289441,
 -0.0153819784,3.5543814108\C,1.4429601113,-1.549477719,-0.2385868127\H
 ,-0.4905303516,-0.823350674,2.9458152406\H,-0.2675345227,1.1561273627,
 -0.1166569813\N,0.6346224374,-0.5953100832,-0.8854904811\H,0.074289354
 8,-0.9423967971,-1.6533368181\H,1.8929441188,-2.3397049738,-0.82642217
 23\S,-1.8124614407,-0.5919685615,0.4689878309\C,-2.6747410261,0.149920
 0851,-0.9612466136\H,-2.3066632167,-0.2316941495,-1.9157314851\H,-3.72
 61687037,-0.123731914,-0.8708113646\H,-2.5976638108,1.2388567455,-0.94
 83057331\\Version=AM64L-G03RevC.02\State=1-A\HF=-688.2610212\RMSD=5.
 842e-09\RMSF=3.935e-06\Thermal=0.\Dipole=-0.0037263,0.2186993,-0.5333498
 \PG=C01 [X(C6H11N1S1)]\\

10 (MeS/CHNMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1S1\TSCHNEI\19-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_CHNR_1\0,1\C,0.0307449961,-0.03435
66909,-0.0030921657\C,0.024064282,0.0128120295,2.6518428573\C,0.736571
1686,-0.0254694321,1.3186736096\H,0.5433271202,0.4856926577,-0.8067194
039\H,1.6810028992,0.5111759597,1.2873004896\C,0.7559886712,-1.2955163
629,0.4802071783\H,0.1153032069,-2.0991360579,0.8288512236\H,-0.253747
8434,1.037646367,2.9166064182\H,0.6756306729,-0.3690321809,3.443183290
4\C,1.9966025818,-1.7204763625,-0.2065511843\H,-0.887728573,-0.5867804
466,2.6478405324\N,2.8430366274,-0.8928493447,-0.6590515567\H,2.141706
9397,-2.8089354176,-0.3091418443\C,4.0237794961,-1.4040942836,-1.32451
10615\H,4.9179514331,-1.0390018141,-0.8101448047\H,4.0662884157,-2.503
615117,-1.3678311315\H,4.0652113992,-1.0117362226,-2.3452211494\S,-1.7
630058488,0.0303784183,-0.1037033898\C,-2.0145226345,-0.9120837948,-1.
6480392945\H,-1.6419465193,-1.9324342476,-1.5484769187\H,-3.0889662804
,-0.9415166704,-1.8317840974\H,-1.5264077285,-0.4216975216,-2.49114687
44\Version=AM64L-G03RevC.02\State=1-A\HF=-727.5641469\RMSD=6.506e-09\
RMSF=9.977e-06\Thermal=0.\Dipole=0.2875912,-0.736734,-0.2147449\PG=C01
[X(C7H13N1S1)]\
```

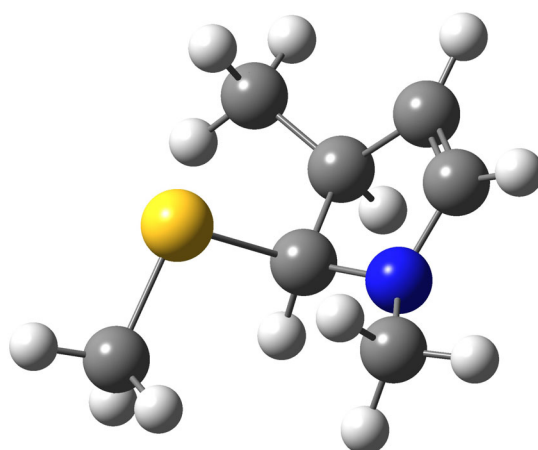
TS₁₀₋₁₁ (MeS/CHNMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1S1\TSCHNEI\19-Jan-2010\
0\# opt=(ts,noeigentest,calcfc) b3lyp/6-311g(d) scf=tight Integral=(grid
```

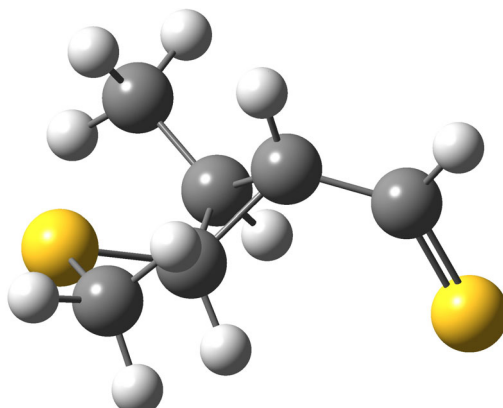
=ultrafine) freq\DA_S_CHNR_TS\0,1\C,-0.1532168144,0.1480573524,0.3848247783\C,0.2302614713,0.0034368445,2.8995197179\C,0.8236533858,0.0305253145,1.4855902928\H,1.5172186855,0.8763652708,1.4077004831\C,1.5254555377,-1.2756412773,1.1479553478\H,1.5257618318,-2.0556763806,1.9058552218\H,-0.2717755093,0.9431799171,3.1386992213\H,1.0322226621,-0.1564430172,3.624769668\C,1.9533797987,-1.5717621695,-0.1408246593\H,-0.4912845667,-0.8091448372,3.0189880683\N,1.5204479088,-0.998338983,-1.2395129459\H,2.7208204926,-2.3592069821,-0.2207099983\H,0.0600160879,0.8162536369,-0.4364071913\C,2.3632603273,-1.0792901999,-2.4163934868\H,3.0839715936,-1.9116525732,-2.3697335073\H,1.7517030218,-1.2059402154,-3.3163129612\H,2.9489887439,-0.1594735563,-2.5562533607\H,-1.5988833105,-0.7560046513,0.2144097664\C,-2.0858981362,-0.2557068955,-1.4718737966\H,-1.259140186,-0.4762241482,-2.1451024702\H,-2.9548805445,-0.8538551707,-1.7435595534\H,-2.3486592666,0.8012512402,-1.5097964121\Version=AM64L-G03RevC.02\State=1-A\HF=-727.4873426\RMSD=5.806e-09\RMSF=3.197e-06\Thermal=0.\Dipole=-0.6673883,0.5138835,-0.1806065\PG=C01 [X(C7H13N1S1)]\

11 (MeS/CHNMe)



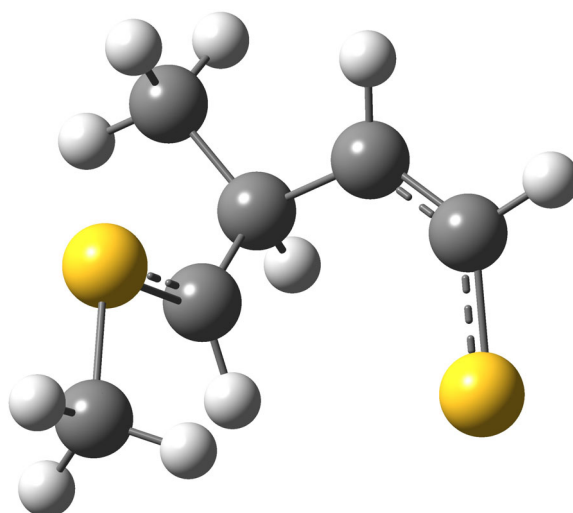
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1S1\TSCHEI\19-Jan-2010\0\# opt freq rb3lyp/6-311g(d)\DA_S_CHNR_2\0,1\C,-0.1009082206,-0.0516929703,0.1971999193\C,0.2901809157,0.0843275094,2.8087843558\C,0.883742467,-0.0366831511,1.4066771387\H,1.5274418721,0.8435624442,1.2419171231\C,1.714629298,-1.2757363626,1.1340299491\H,2.4112665507,-1.7170988593,1.8324629614\H,-0.3420591661,0.970641934,2.9051588832\H,1.0982645735,0.1696987003,3.5416341411\C,1.5520844677,-1.6144383924,-0.148247362\H,-0.3133459888,-0.7847656068,3.0739468489\H,-0.3602607804,0.9521840553,-0.1436689777\N,0.6575314528,-0.7679462408,-0.8187637351\H,2.0433055396,-2.4025971703,-0.7054829481\C,0.0275493481,-1.1916955037,-2.052982792\H,-0.7583948077,-1.9429886432,-1.8993004847\H,-0.4102726537,-0.3276878283,-2.5593562488\H,0.7871028765,-1.6102120112,-2.7162591139\H,-1.7615933819,-0.8470794003,0.6375309776\C,-2.8669713818,0.0778494624,-0.487581529\H,-2.762888949,-0.232435458,-1.5277109479\H,-3.8873354157,-0.1295614159,-0.1637560745\H,-2.6956840911,1.15324392,-0.4074516685\Version=AM64L-G03RevC.02\State=1-A\HF=-727.5761588\RMSD=9.934e-09\RMSF=2.515e-05\Thermal=0.\Dipole=0.0737864,0.3623644,-0.6537998\PG=C01 [X(C7H13N1S1)]\

10 (MeS/CHS)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10S2\TSCHNEI\07-Sep-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_CHS_1\0,1\C,-0.0156045163,-0.0392077
823,0.0068554453\C,-0.0300842543,0.0620494124,2.7654920068\H,1.0667163
718,0.0563742544,0.0064085745\C,-0.7353587356,1.2371790352,-0.51673704
74\H,-1.6975152213,1.4338066901,-0.0550247769\C,0.0449506583,2.4104832
351,-0.8844087522\H,-0.4233827649,1.0780745985,2.7216978108\H,-0.35931
23264,-0.4091673862,3.6917301715\H,1.0598985811,0.0850006845,2.7486360
876\C,-0.6601240118,-0.0664517585,-1.3281691996\H,0.0500141076,0.00292
77102,-2.1485779225\C,-1.9259986175,-0.8307372755,-1.6400156858\H,-1.6
945292037,-1.8759446763,-1.8661503255\H,-2.6316699087,-0.820738877,-0.
8077405759\H,-2.4242376007,-0.4033234477,-2.5139640546\H,-0.4313785197
,3.3627045833,-0.641646191\S,-0.6849074756,-0.9520590687,1.3943099545\
S,1.5246042447,2.4424586376,-1.5904573087\Version=AM64L-G03RevC.02\St
ate=1-A\HF=-1031.0947805\RMSD=5.580e-09\RMSF=3.443e-06\Thermal=0.\Dip
ole=-0.8094754,-0.1983574,0.5727998\PG=C01 [X(C6H10S2)]\
```

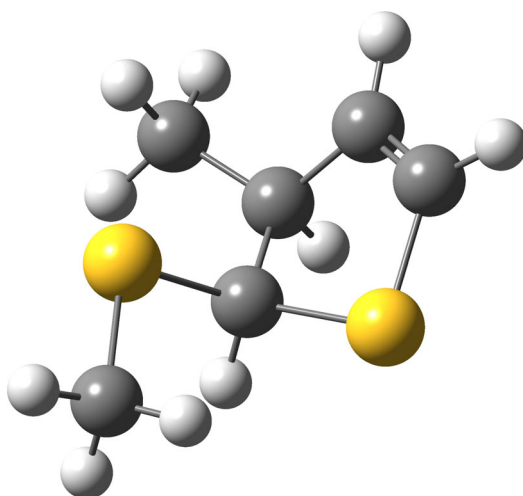
TS₁₀₋₁₁ (MeS/CHS)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10S2\TSCHNEI\08-Sep-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_S_CHS_TS\0,1\C,-0.0573765662,0.1169279095,0.0240236056\C,0.01
97786558,0.0646072007,2.3475898604\H,0.902311562,0.1770542271,2.974469
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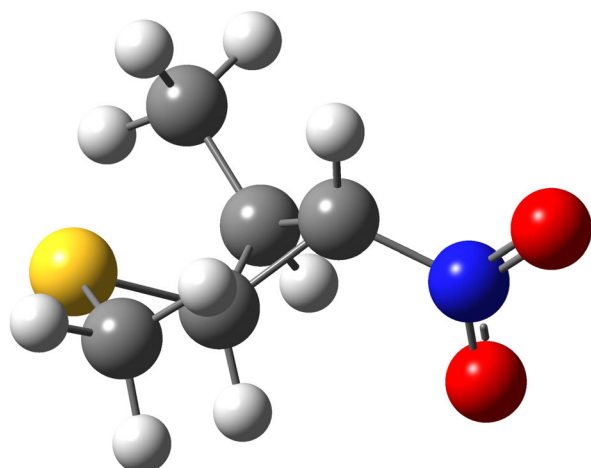
2487\C,-1.1305715493,0.723095226,2.657049486\H,-1.1665369753,1.1340756
 038,3.6684247887\C,0.1940540924,-0.8367515387,1.1167605811\H,-0.613048
 9206,-1.5774680521,1.101040053\C,1.5594148231,-1.529645058,1.108672228
 4\H,1.6879248128,-2.1457681773,0.2161403116\H,2.3824516651,-0.81073942
 22,1.1482659241\H,1.6434205519,-2.1738280417,1.9865053982\H,-1.0656414
 349,0.1971546899,-0.3626060151\S,1.0717716621,1.2137821245,-0.60334671
 09\C,0.0251655258,2.2002846394,-1.7340165756\H,-0.7948323869,2.6442790
 255,-1.1729483273\H,0.661698161,2.9854894867,-2.1393524352\H,-0.350629
 8035,1.5811518229,-2.5469293852\S,-2.5344110124,0.9727468211,1.7153792
 398\\Version=AM64L-G03RevC.02\State=1-A\HF=-1031.0459684\RMSE=7.089e
 -09\RMSF=4.685e-06\Thermal=0.\Dipole=1.9114355,-0.1070213,-1.661817\PG=C
 01 [X(C6H10S2)]\\

11 (MeS/CHS)



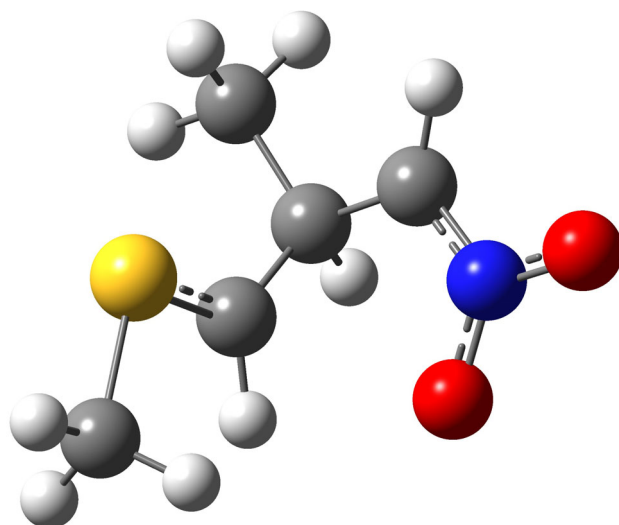
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10S2\TSCHEI\08-Sep-2010\
 0\\# opt freq rb3lyp/6-311g(d)\DA_S_CHS_2\0,1\C,-0.0504688573,-0.2473365
 7,-0.0490394799\C,0.0030761388,-0.0995997814,2.558009373\C,0.792257545
 9,-0.1096889503,1.2452493957\H,1.2987760062,0.8652072478,1.1556399146\
 C,1.8677407373,-1.1717230397,1.1578968627\H,2.3916538424,-1.5255514907
 ,2.0391889085\H,-0.7697233039,0.6720971191,2.5555177015\H,0.6794966586
 ,0.1085622569,3.3918935165\C,2.1625630141,-1.5640714002,-0.0788436136\
 H,-0.4800923627,-1.058680355,2.7538624514\H,2.930810354,-2.2662049996,
 -0.3756452847\H,-0.4398549019,0.7177750328,-0.3731939649\S,-1.47501123
 06,-1.3966191242,0.1580266055\C,-2.2615894177,-1.1771817752,-1.4708083
 708\H,-1.5928492927,-1.4935708692,-2.2718846768\H,-3.1464253469,-1.813
 8345457,-1.479275902\H,-2.5725179441,-0.1423563355,-1.6267848161\S,1.1
 625309819,-0.819502847,-1.3431974678\\Version=AM64L-G03RevC.02\State=
 1-A\HF=-1031.1156745\RMSE=4.027e-09\RMSF=3.517e-06\Thermal=0.\Dipole=
 -0.0033583,0.3448297,0.1840342\PG=C01 [X(C6H10S2)]\\

10 (MeS/NO₂)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2S1\TSCHNEI\18-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_NO2_1\0,1\C,-0.0249716374,0.55342
88563,0.3205651181\C,0.2043656983,-0.301375835,2.8358698589\C,0.784402
8118,0.0523881746,1.4846553765\H,0.4914462397,1.2559502458,-0.32532010
36\H,1.7843580559,0.4747374822,1.5046605316\C,0.5524572191,-0.85350727
59,0.298279156\H,-0.101549347,-1.7092870496,0.3814920528\H,0.102450445
2,0.5953638124,3.4530196272\H,0.8635290031,-0.9964901382,3.3619683481\
O,2.4882342939,-0.2278411875,-0.8066727308\H,-0.780790477,-0.762619725
2,2.7547304045\N,1.6709104025,-1.1222068058,-0.6178984137\O,1.69963679
11,-2.2284684985,-1.1387660768\S,-1.7996532997,0.7956255638,0.44289720
76\C,-2.2625668962,0.5135857799,-1.3027279676\H,-2.0088720325,-0.49890
90473,-1.617792399\H,-3.3429065786,0.6453334431,-1.3649117641\H,-1.780
3846536,1.2396439343,-1.9576896741\Version=AM64L-G03RevC.02\State=1-A
\HF=-799.3388645\RMSD=5.427e-09\RMSF=6.310e-06\Thermal=0.\Dipole=-0.91
43806,0.3190457,0.5950249\PG=C01 [X(C5H9N1O2S1)]\
```

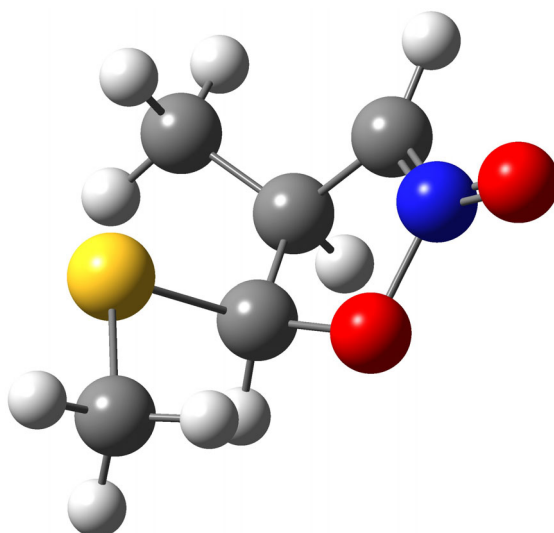
TS₁₀₋₁₁ (MeS/CHS)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O2S1\TSCHNEI\18-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
afine\DA_S_NO2_TS\0,1\C,-0.2876897265,-0.2593981535,0.3273919723\C,0
```

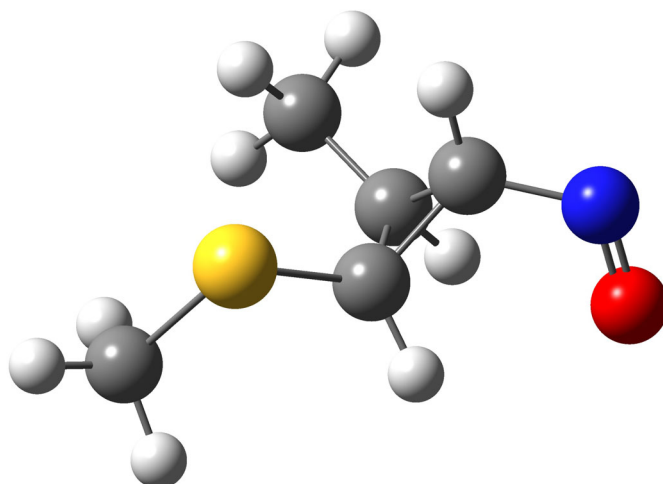
.2677381426,-0.056917807,2.813692927\C,0.7587767095,-0.0449262981,1.36
 13234768\H,1.2463086913,0.9118902699,1.1421497793\C,1.6672252589,-1.20
 57727501,1.0866840431\H,1.8999491049,-1.9641847902,1.8190749189\H,-0.4
 255888219,0.7646600153,3.0025291407\H,1.1238153538,0.0529208765,3.4824
 70517\O,1.6398943688,-0.7118719864,-1.1355405471\H,-0.2328754448,-0.99
 47645349,3.0671191048\N,2.1069503179,-1.4315445298,-0.1812997387\O,2.9
 616103918,-2.3100747944,-0.3979180208\H,-0.2739134014,0.3531012674,-0.
 5621218272\S,-1.5231503822,-1.4164230791,0.389350383\C,-2.2204587954,-
 1.2766439178,-1.2963706797\H,-1.4334896588,-1.4730528203,-2.0217700234
 \H,-2.993492641,-2.039566152,-1.3763201866\H,-2.6620421666,-0.29398455
 89,-1.4544249563\\Version=AM64L-G03RevC.02\State=1-A\HF=-799.26452\RMS
 D=4.595e-09\RMSF=6.599e-06\Thermal=0.\Dipole=-2.8018391,0.8778748,0.80
 48721\PG=C01 [X(C5H9N1O2S1)]\

11 (MeS/NO₂)



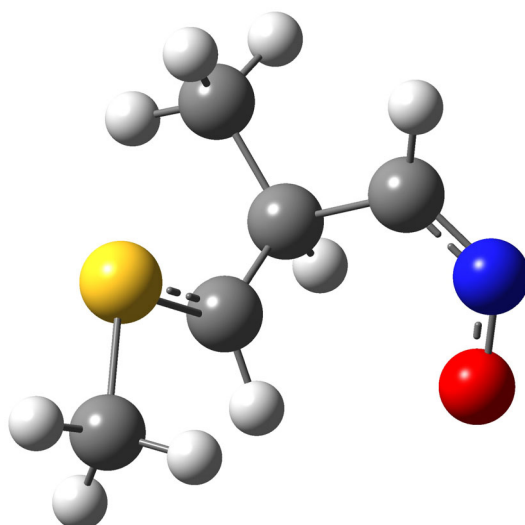
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2S1\TSCHNEI\18-Jan-2010\
 0\\# opt freq rb3lyp/6-311g(d)\\DA_S_NO2_2\\0,1\C,-0.2692236793,0.0927326235,
 0.2588342245\C,0.2730631463,-0.0948092863,2.8261506413\C,0.7866065162,0.0
 021975989,1.3886183176\H,1.4133992732,0.9040262533,1.3129580764\C,1.574859
 0193,-1.1763696487,0.9100993608\H,2.2922769057,-1.776967216,1.4469131189\H,
 -0.3406569785,0.7719438873,3.0798319149\H,1.1147221148,-0.1197689897,3.523
 1260256\O,0.3722741876,-0.45703861,-0.8831695084\H,-0.3225863349,-0.9944700
 625,2.9883508418\N,1.3732272594,-1.4347370934,-0.3488274103\O,1.8114875747,
 -2.2282949144,-1.1508868036\H,-0.5221482079,1.1216565677,0.0000519404\S,-1.8
 279599531,-0.8118781326,0.6646735116\C,-2.6687902593,-0.5856638358,-0.94091
 89108\H,-2.0508190087,-0.9798577521,-1.7454444798\H,-3.5991120297,-1.1508560
 861,-0.8911822991\H,-2.9016852377,0.4648845796,-1.1228716379\\Version=AM64
 L-G03RevC.02\State=1-A\HF=-799.3390933\RMSD=4.500e-09\RMSF=1.744e-05\Th
 ermal=0.\Dipole=-0.1844589,0.9854682,0.9833533\PG=C01 [X(C5H9N1O2S1)]\

10 (MeS/NO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1S1\TSCHNEI\26-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_S_NO_1\0,1\C,0.3604925161,0.1769556
967,-0.0246750935\H,0.6979861596,0.2962254271,1.0018151953\C,1.5151318
721,-0.1085860012,-0.9737473881\H,1.4855440988,0.2829530566,-1.9829349
674\C,0.5110847605,-1.1999379632,-0.5897123857\H,0.9435732454,-1.90025
62385,0.1224399859\C,-0.3920625263,-1.799342473,-1.6387823874\H,-1.226
1250131,-2.328675499,-1.1679274953\H,-0.8095886262,-1.037207472,-2.298
4701104\H,0.1532224073,-2.5221097493,-2.2509425955\N,2.8688371149,-0.1
79878617,-0.4589952297\O,2.9554216409,-0.5336940839,0.6967618206\C,-2.
316129391,0.7730887403,0.4023522384\H,-2.1029046785,0.7951816867,1.471
3356672\H,-3.1345236558,1.4626736658,0.193651569\H,-2.6114850746,-0.23
17118862,0.1011787391\S,-0.877926214,1.3646836463,-0.5625427714\Version
=AM64L-G03RevC.02\State=1-A\HF=-724.1019386\RMSD=5.777e-09\RMSF=7.6
81e-05\Thermal=0.\Dipole=-1.2704579,-0.5198045,-0.1737035\PG=C01 [X(C5H
9N1O1S1)]\
```

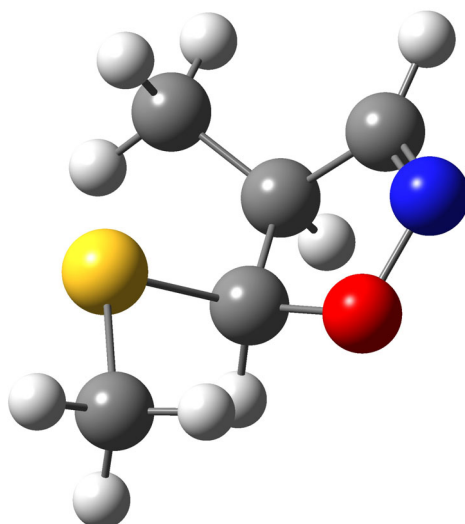
TS₁₀₋₁₁ (MeS/NO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O1S1\TSCHNEI\26-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf
=tight\DA_S_NO_TS\0,1\C,0.2098356006,-0.3679052582,-0.1330417769\C,-
```

0.0858974036,0.090672265,2.1598816469\H,0.7204268364,0.258762954,2.8636572503\O,-1.9860825933,0.8374862165,1.2396476372\C,0.0339735649,-1.092046142,1.1062216592\H,-0.960475666,-1.5527360967,1.1029805758\C,1.1315014699,-2.0654938453,1.5297469677\H,1.2357889186,-2.8784380981,0.8077472369\H,2.1028983987,-1.5711705398,1.6219510096\H,0.8899161013,-2.4987765117,2.5021384856\H,-0.6771536344,0.0337723554,-0.6093113278\N,-1.1393508651,0.8194764559,2.1665869894\C,1.218349885,1.2461652542,-2.0998246646\H,0.7536896284,2.131810649,-1.6694717147\H,2.1247564078,1.5311319318,-2.632310166\H,0.5350017927,0.7535755692,-2.7901645253\S,1.7268885748,0.0951204818,-0.7757157967\Version=AM64L-G03RevC.02\State=1-A\HF=-724.0675279\RMSD=5.998e-09\RMSF=2.480e-05\Thermal=0.\Dipole=1.5622532,-0.5338228,-1.3036606\PG=C01 [X(C5H9N1O1S1)]\

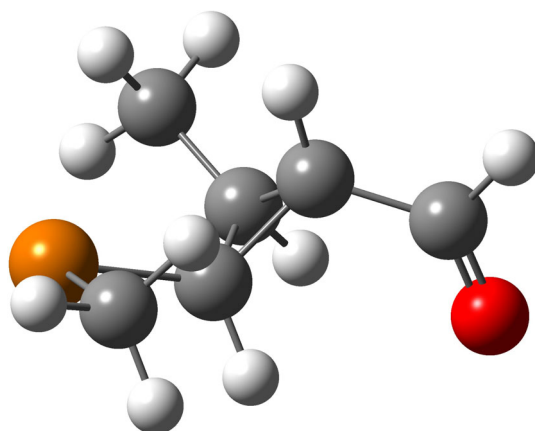
11 (MeS/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1S1\TSCHNEI\26-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_S_NO_2\0,1\C,0.0397864363,-0.079223408,0.0540156647\C,0.1062372392,-0.0720537419,2.6941154848\C,0.8495304742,0.0251459208,1.3608051111\H,1.3975460784,0.9785392921,1.3398563614\C,1.8507978874,-1.0710289749,1.0842844402\H,-0.6312780915,0.7266326106,2.7929838918\H,0.8115868276,0.023863701,3.5237163581\O,0.9298499748,-0.7438215565,-0.8615391177\H,-0.4111029289,-1.0265828136,2.8045093263\H,-0.1946281661,0.8855850836,-0.3946390517\H,2.5404000445,-1.497883154,1.8036335216\N,1.8962809333,-1.46541485,-0.1230728189\C,-2.044368375,-1.0270290808,-1.4989357317\H,-1.2686596141,-1.4812976305,-2.1122793483\H,-2.952990883,-1.6253353071,-1.5626934225\H,-2.2600559122,-0.0164943066,-1.8506843945\S,-1.5341205192,-1.0247221276,0.253833137\Version=AM64L-G03RevC.02\State=1-A\HF=-724.1479983\RMSD=4.490e-09\RMSF=3.631e-05\Thermal=0.\Dipole=-0.1709874,0.8224179,0.7008084\PG=C01 [X(C5H9N1O1S1)]\

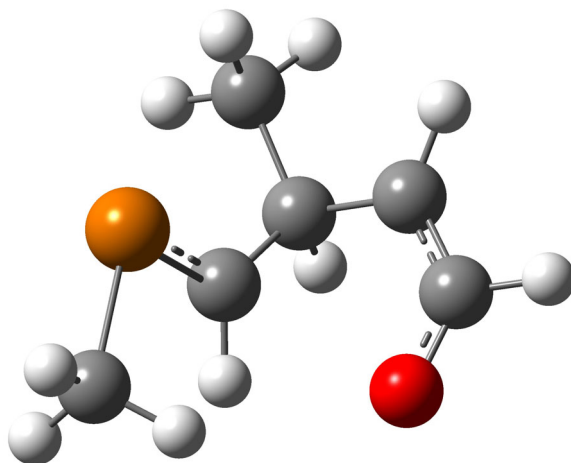
SeMe-Donor

10 (MeSe/CHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1Se1\TSCHNEI\20-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_CHO_1\0,1\C,-0.0782669503,-0.123
5273215,-0.1341047191\C,0.2027827496,0.1338052536,2.7658656053\H,0.998
9678308,-0.100010411,-0.2607821873\C,-0.781294614,1.164776862,-0.58471
63313\H,-1.6693849133,1.4570717483,-0.0341904081\C,0.0678873269,2.2605
830482,-1.1010360475\H,-0.1996639394,1.1408773051,2.6667181718\H,-0.02
98271252,-0.2561501363,3.7563651463\H,1.282168109,0.1400914855,2.62338
79484\C,-0.8738574436,-0.1323070954,-1.3930038479\H,-0.2563488159,-0.1
120632878,-2.287699244\C,-2.2022505652,-0.8357604488,-1.5529029196\H,-
2.052092525,-1.8923411888,-1.7947520959\H,-2.8059191953,-0.7840894111,
-0.6450675343\H,-2.7773115579,-0.3877125521,-2.3678376612\O,1.10101002
24,2.0941826887,-1.710799595\H,-0.2988103472,3.2884683007,-0.891431079
\Se,-0.653839399,-1.0713200417,1.4621828682\Version=AM64L-G03RevC.02\
State=1-A\HF=-2711.4640854\RMSD=3.985e-09\RMSF=4.731e-06\Thermal=0.\D
ipole=-0.687814,0.1050541,0.5035502\PG=C01 [X(C6H10O1Se1)]\
```

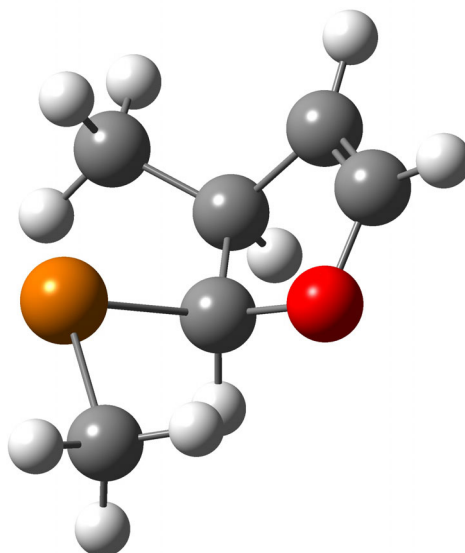
TS₁₀₋₁₁ (MeSe/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O1Se1\TSCHNEI\20-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
```

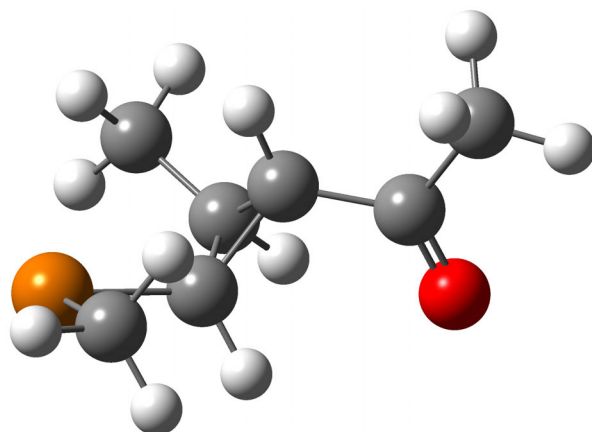
afine\\DA_Se_CHO_TS\\0,1\\C,0.0268814417,-0.0124568357,0.0299694296\\C,0.0109815448,-0.0202647297,2.3278460003\\H,0.7579422019,-0.0401129226,3.1161843505\\C,-1.02750164,0.8964513755,2.3349319736\\H,-1.2738094145,1.3185497291,3.3307140954\\O,-1.7272470798,1.2570190922,1.3554266438\\C,0.2116899269,-0.9625601619,1.1331001437\\H,-0.5797689563,-1.7201856553,1.0834886683\\C,1.5776717328,-1.6542086121,1.2071088849\\H,1.7460421207,-2.2982685316,0.3415370041\\H,2.3947136498,-0.9292494883,1.2623202743\\H,1.623845946,-2.2687267946,2.1088775031\\H,-0.9466545771,0.069188211,-0.43040283\\C,0.0361236957,2.2053022162,-1.7706634713\\H,-0.7892327442,2.5068193549,-1.130019119\\H,0.5826756335,3.0788542318,-2.1217896996\\H,-0.3108788136,1.6176529643,-2.6178818615\\Se,1.2855121302,1.1496307574,-0.6672736727\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-2711.3932264\\RMSD=5.282e-09\\RMSF=2.236e-05\\Thermal=0.\\Dipole=0.9852871,-0.248017,-1.1079053\\PG=C01 [X(C6H10O1Se1)]\\

11 (MeSe/CHO)



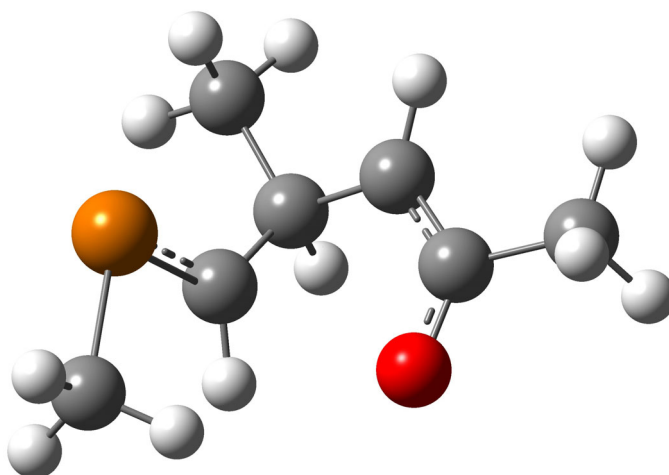
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C6H10O1Se1\\TSCHNEI\\20-Jan-2010\\0\\# opt freq b3lyp/6-311g(d)\\DA_Se_CHO_2\\0,1\\C,-0.2096917368,0.0676458601,0.2298488864\\C,0.2677714471,-0.1354334051,2.8113006104\\C,0.8189127062,0.026254299,1.3926055835\\H,1.3800628461,0.9731273861,1.3620359421\\C,1.7236440049,-1.0935472874,0.9150805837\\H,2.5026728012,-1.5542651865,1.5053332521\\H,-0.426078622,0.6683057864,3.0681332954\\H,1.0876864853,-0.1094986034,3.534370103\\C,1.4369819723,-1.3593990703,-0.3537368\\O,0.4128304302,-0.6067476163,-0.8763502558\\H,-0.2498029861,-1.0893403271,2.9369889232\\H,1.8770375605,-2.0593897794,-1.0501814306\\H,-0.4554242125,1.0718719441,-0.1082120771\\C,-2.7235331484,-0.5207230207,-1.1333771469\\H,-2.0519122859,-0.931773402,-1.8835775996\\H,-3.677464641,-1.0456518046,-1.1652722864\\H,-2.8886290296,0.54217321,-1.3080586067\\Se,-1.9583536909,-0.8237526203,0.6571375426\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-2711.4656849\\RMSD=5.472e-09\\RMSF=6.755e-06\\Thermal=0.\\Dipole=0.37009,0.2664439,-0.0068608\\PG=C01 [X(C6H10O1Se1)]\\

10 (MeSe/COMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O1Se1\TSCHNEI\29-Jan-2010\
0\# opt freq b3lyp/6-311g(d)\DA_Se_COR_1\0,1\C,0.0044372776,0.002726
7013,-0.003843003\C,0.0045705689,-0.0184365561,2.650502076\C,0.7076700
157,-0.0024985617,1.3120303924\H,0.5032224228,0.5489175782,-0.79714134
36\H,1.6439853845,0.5496178321,1.292907847\C,0.745638745,-1.259027752,
0.4438881114\H,0.1295761094,-2.0873157277,0.7786960122\H,-0.2739375969
,0.9955063922,2.9536567913\H,0.6616635993,-0.4258393144,3.4240407218\C
,2.0187171894,-1.5962528225,-0.257177545\C,2.3513196349,-3.0697113009,
-0.3892943337\H,2.4108295731,-3.5388552926,0.5983603859\H,1.5642125448
, -3.5939711179,-0.9414639078\H,3.3013409836,-3.1911065704,-0.907974628
5\O,2.7507159395,-0.731187996,-0.6970650194\H,-0.9050041418,-0.6212582
826,2.6284584957\C,-2.0700955859,-0.9464215047,-1.8403694109\H,-1.6515
545504,-1.9459158382,-1.7318544366\H,-3.1304902925,-1.0200276751,-2.08
02739492\H,-1.5566642434,-0.4037663633,-2.6324974438\Se,-1.9356868736,
0.0369021881,-0.1369139038\Version=AM64L-G03RevC.02\State=1-A\HF=-275
0.7975872\RMSE=4.976e-09\RMSE=2.568e-05\Thermal=0.\Dipole=-0.4279218,-
0.8414846,0.2069189\PG=C01 [X(C7H12O1Se1)]\

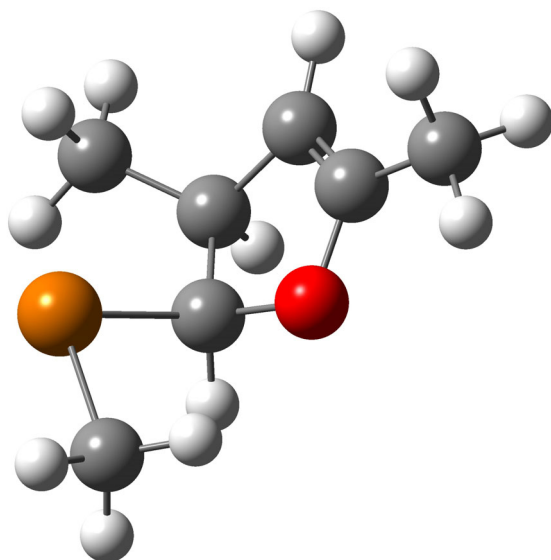
TS₁₀₋₁₁ (MeSe/COMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O1Se1\TSCHNEI\20-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
afine\DA_Se_COR_TS\0,1\C,-0.217640473,0.1616258875,0.433594989\C,0.2

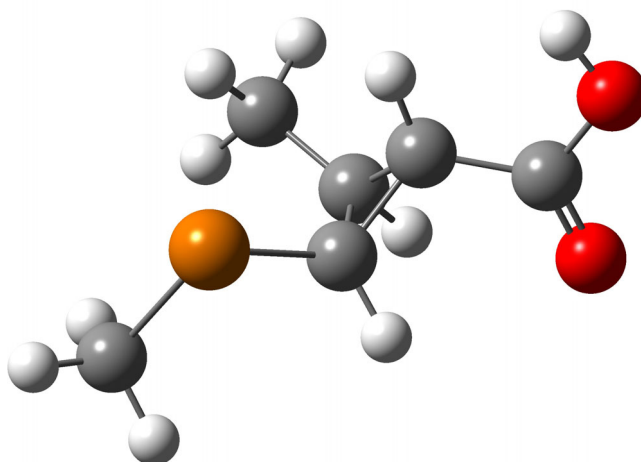
789724392,0.0248991258,2.9274225474\C,0.8009634376,0.0732134579,1.4872005425\H,1.4915420868,0.9183215379,1.3767940406\C,1.464632974,-1.2487535056,1.0977016502\H,1.5715190218,-1.9987145478,1.8748460812\H,-0.2305038067,0.9517761494,3.199004292\H,1.1181670526,-0.1217482483,3.6111568287\C,1.8287009741,-1.4874784103,-0.2258241257\C,2.827812136,-2.6037736811,-0.5110140691\H,3.0968151215,-3.1823835224,0.3744048197\H,2.4153242723,-3.2757916297,-1.2687211037\H,3.7373282187,-2.165874995,-0.9319320936\O,1.4146453383,-0.8108730936,-1.2071379714\H,-0.4157292887,-0.806418188,3.077538271\H,-0.0198978891,0.7676016008,-0.4380211654\C,-2.3177438137,-0.2134445276,-1.4693361993\H,-1.4783938941,-0.4870749994,-2.1042919444\H,-3.1997044054,-0.7916702716,-1.739603863\H,-2.5360094927,0.8502688581,-1.535825717\Se,-1.8523449547,-0.706590566,0.3830397494\\
Version=AM64L-G03RevC.02\State=1-A\HF=-2750.7223727\RMSD=9.496e-09\RMSF=6.514e-06\Thermal=0.\Dipole=-1.2316115,0.4078075,0.45419\PG=C01[X(C7H12O1Se1)]\\

11 (MeSe/COMe)



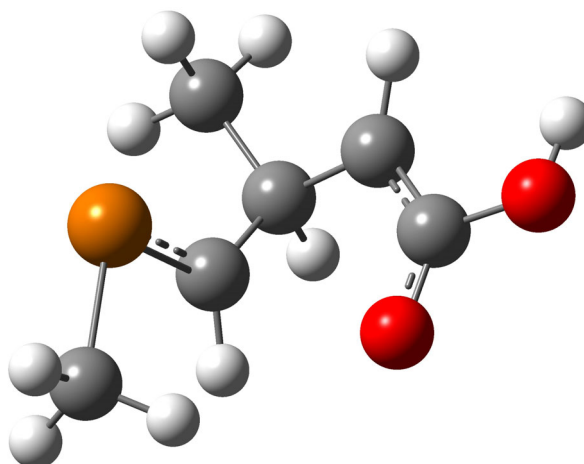
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C7H12O1Se1\TSCHNEI\20-Jan-2010\0\\# opt freq rb3lyp/6-311g(d)\\DA_Se_COR_2\\0,1\C,-0.2072269428,0.0179541618,0.3147836309\C,0.2771691596,-0.0661578028,2.8997940664\C,0.8227692017,0.0530203108,1.4748878402\H,1.3546026268,1.0152677599,1.405549385\C,1.7527979674,-1.0586377452,1.038875091\H,2.5409379724,-1.4748730246,1.6504434079\H,-0.4356386742,0.7299623091,3.1271119616\H,1.0968721303,0.0065868618,3.6200398031\C,1.4873437333,-1.3918403043,-0.2227116377\C,2.1127404243,-2.3706120522,-1.1498025621\H,1.3840552536,-3.1241862586,-1.4637350727\H,2.4715381382,-1.8700282046,-2.0545665111\H,2.9548264577,-2.8738403284,-0.6734937183\O,0.4367825221,-0.6710194504,-0.7636179274\H,-0.2174404445,-1.0267214277,3.0627116822\H,-0.4922002749,0.9999601124,-0.0569226209\C,-2.7152729019,-0.6932937808,-1.0059436172\H,-2.0332383526,-1.0935018452,-1.7527430112\H,-3.6463482438,-1.258606836,-1.0169280681\H,-2.926802416,0.3570967791,-1.2046124032\Se,-1.923018018,-0.9195135411,0.7843222228\\Version=AM64L-G03RevC.02\State=1-A\HF=-2750.7982916\RMSD=3.366e-09\RMSF=8.136e-06\Thermal=0.\Dipole=0.4392892,0.1732311,-0.1508707\PG=C01 [X(C7H12O1Se1)]\\

10 (MeSe/COOH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2Se1\TSCHNEI\23-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_COOH_1\0,1C,-0.0355173934,-0.30
37854579,-0.3448395936\C,-0.1240864971,0.1613147029,2.2731929969\C,0.6
20942996,-0.0211716693,0.972510437\H,0.4606030494,0.104205012,-1.21805
05313\H,1.526954367,0.5705637002,0.8715467276\C,0.7503185408,-1.406920
795,0.348428318\H,0.1647324936,-2.1893688139,0.8242837373\O,2.79292318
45,-1.0189986399,-0.8164879879\H,-0.3966934603,1.2111542445,2.41699454
94\H,0.4995679203,-0.1355281274,3.1210612686\O,2.4233268225,-3.0932017
296,-0.1123563059\C,2.0655794802,-1.7885172167,-0.2497554124\H,-1.0429
179401,-0.4270446451,2.3001930814\H,1.7395043106,-3.5905000051,0.35317
13758\C,-2.4647615303,1.3359104206,-0.6549523487\H,-1.9386767866,1.839
8485442,-1.4640923723\H,-3.5365339874,1.3629600455,-0.8499676201\H,-2.
2544534861,1.819819748,0.2968490812\Se,-1.9490145801,-0.5676517118,-0.
5920204168\Version=AM64L-G03RevC.02\State=1-A\HF=-2786.7276259\RMSD
=8.573e-09\RMSF=3.537e-06\Thermal=0.\Dipole=-1.2054058,0.1318327,0.97709
37\PG=C01 [X(C6H10O2Se1)]\
```

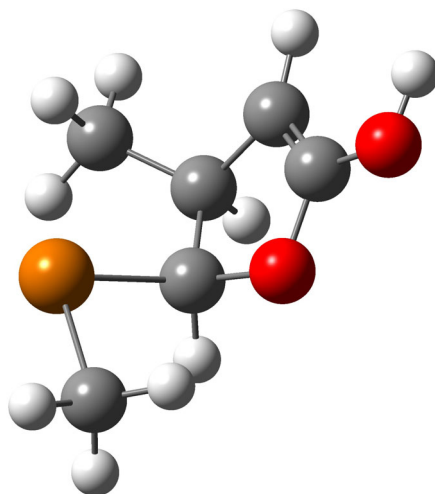
TS₁₀₋₁₁ (MeSe/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2Se1\TSCHNEI\23-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
```

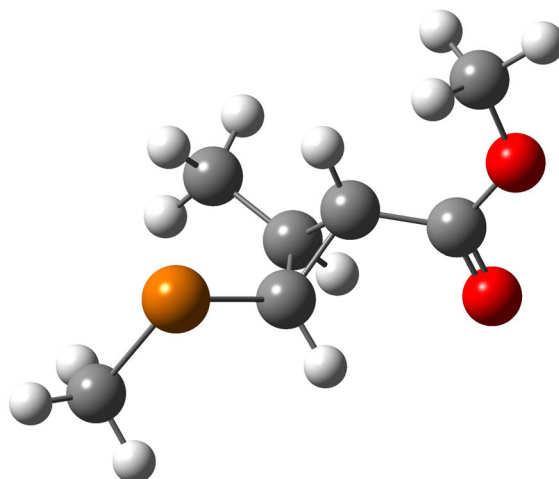
afine\\DA_Se_COOH_TS\\0,1\\C,0.0130353027,-0.0460650181,0.0228355559\\C,
0.0347856806,0.023254529,2.5659520685\\C,0.8305930214,-0.017140685,1.25
40060403\\H,1.4777396992,0.8689037652,1.207852966\\C,1.6104278767,-1.308
3117237,1.118118922\\H,1.610872398,-2.0064859617,1.9494946122\\O,1.82909
70855,-1.0854195437,-1.2160809821\\H,-0.5471115356,0.9428140025,2.65382
20536\\H,0.7301680475,-0.0271475889,3.4070302176\\O,3.0604617248,-2.6528
361188,-0.2145430607\\C,2.1307106422,-1.640427819,-0.1432278094\\H,-0.64
73444325,-0.8271422942,2.6498417567\\H,3.3453445928,-2.8823634079,0.677
7088505\\H,0.2838182072,0.5890562648,-0.8093838138\\C,-1.6964330855,-0.6
077352108,-2.195297813\\H,-0.748925699,-0.8170565422,-2.6865501283\\H,-2
.4778927821,-1.2521986059,-2.594310932\\H,-1.9831600857,0.4358863978,-2
.3055160719\\Se,-1.4884968011,-1.0734195033,-0.2911666411\\Version=AM64
L-G03RevC.02\\State=1-A\\HF=-2786.6453249\\RMSD=7.853e-09\\RMSF=6.815e-06
\\Thermal=0.\\Dipole=-1.530296,0.5827945,0.6620416\\PG=C01 [X(C6H10O2Se1)]\\

11 (MeSe/COOH)



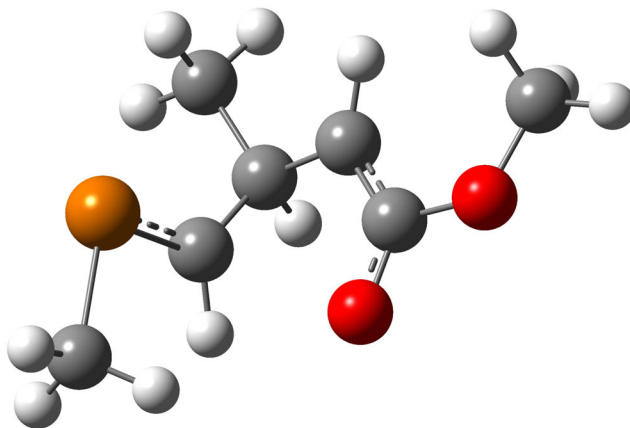
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C6H10O2Se1\\TSCHNEI\\29-Jul-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_Se_COOH_3\\0,1\\C,-0.1243697501,0.244
5595797,0.3533811256\\C,0.3169477321,0.0002236709,2.9308124701\\C,0.8866
73557,0.0159146197,1.511089751\\H,-0.1826016421,1.2748335618,0.01018690
79\\H,1.6193805163,0.8375080139,1.4614659619\\C,1.5299146916,-1.27627479
84,1.0528995329\\O,0.3680535968,-0.5299312434,-0.7562583397\\H,-0.195918
6292,0.9348099817,3.1710065122\\H,1.1271366411,-0.1276968873,3.65417654
47\\O,1.5243175836,-2.4046412922,-1.1321676612\\C,1.198061493,-1.4686411
734,-0.226993955\\H,-0.3837443123,-0.8255897267,3.0749061815\\C,-2.69976
15924,0.0846906308,-1.0112514156\\H,-2.1049716193,-0.4400648928,-1.7552
315343\\H,-3.7272080892,-0.2760590644,-1.0395173555\\H,-2.6869667776,1.1
584630418,-1.1959750722\\Se,-1.9973213104,-0.3247685079,0.7835172414\\H,
2.1612481208,-3.0112699328,-0.7375704645\\H,2.1889589239,-1.8906302706,
1.6492678482\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-2786.708002\\RMSD=
9.927e-09\\RMSF=8.424e-06\\Thermal=0.\\Dipole=0.6711951,-0.0462289,0.2588
512\\PG=C01 [X(C6H10O2Se1)]\\

10 (MeSe/COOMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2Se1\TSCHNEI\30-Jan-2010\
0\# opt freq b3lyp/6-311g(d)\DA_Se_COOR_1\0,1\C,-0.0017495834,0.0030
101141,-0.0040120994\C,-0.003059026,-0.0082683463,2.6553522651\C,0.700
4071584,-0.0040515073,1.3191437765\H,0.5057270252,0.5262961404,-0.8059
825772\H,1.6457936448,0.5310490922,1.2938079536\C,0.7098475312,-1.2632
321801,0.4543858338\H,0.0730964471,-2.0647423173,0.8051323298\O,2.7292
920797,-0.7675545539,-0.6824682699\H,-0.1864404336,1.0147525128,2.9976
245049\H,0.6091690687,-0.5038209302,3.4141688626\O,2.3187933917,-2.914
5530962,-0.3996797315\C,1.9822072637,-1.6073674017,-0.2491220843\C,1.4
838504727,-3.9760760419,0.0695358828\H,1.3574855872,-3.94217354,1.1546
377414\H,0.5074915215,-3.9694406773,-0.421339213\H,2.0082237477,-4.891
4060853,-0.1972671043\H,-0.9663846023,-0.5186709502,2.6037614304\C,-2.
3020840286,1.8473255254,0.014281209\H,-1.7685341859,2.4293234021,-0.73
54347128\H,-3.3750483759,1.9805554193,-0.1218964438\H,-2.0193072791,2.
1653915009,1.0158620334\Se,-1.9347238539,-0.0760523985,-0.229846647\
Version=AM64L-G03RevC.02\State=1-A\HF=-2826.0369774\RMSD=6.901e-09\RM
SF=3.427e-06\Thermal=0.\Dipole=-1.023944,-0.2957874,0.9477662\PG=C01 [X(
C7H12O2Se1)]\
```

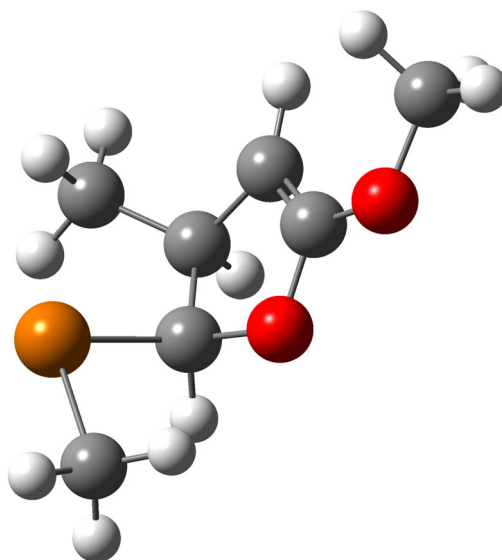
TS₁₀₋₁₁ (MeSe/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O2Se1\TSCHNEI\29-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
```

afine\\DA_Se_COOR_TS\\0,1\\C,0.0078548291,-0.0392341176,0.0222799356\\C,
0.0371804363,0.0176397914,2.5664759138\\C,0.8254967306,-0.0165514045,1.
2512080264\\H,1.4789553046,0.8643567861,1.205437401\\C,1.5996493947,-1.3
121935998,1.1016608104\\H,1.584808498,-2.0088110051,1.9302210877\\O,1.85
58782656,-1.0309004064,-1.2194675193\\H,-0.5419161983,0.9382107088,2.66
32621948\\H,0.7361618819,-0.0408142624,3.4040641891\\O,3.0734364092,-2.6
216550068,-0.2828323747\\C,2.1437741284,-1.6205888893,-0.1569243913\\C,3
.6092781237,-3.234703549,0.8817482741\\H,4.0005764152,-2.4909041725,1.5
81843489\\H,2.8616606234,-3.8519594985,1.3923793242\\H,4.4192378446,-3.8
773401139,0.5375218426\\H,-0.6475292829,-0.8310698389,2.6485159028\\H,0.
2910133561,0.5851658627,-0.8131686268\\C,-1.6869507006,-0.6065257437,-2
.2057145808\\H,-0.7332719312,-0.8258741457,-2.6802594386\\H,-2.465544138
1,-1.2527166584,-2.6075373385\\H,-1.967154896,0.4368677026,-2.333490294
8\\Se,-1.5083456705,-1.0471570574,-0.2921021083\\Version=AM64L-G03RevC.
02\\State=1-A\\HF=-2825.956522\\RMSD=5.285e-09\\RMSF=4.764e-06\\Thermal=0.
\\Dipole=-1.4265806,0.4118639,0.6047997\\PG=C01 [X(C7H12O2Se1)]\\

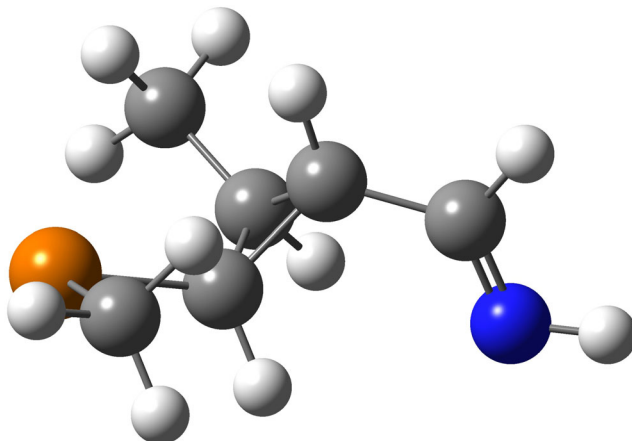
11 (MeSe/COOMe)



1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H12O2Se1\\TSCHNEI\\30-Jan-2010\\
0\\# opt freq b3lyp/6-311g(d)\\DA_Se_COOR_2\\0,1\\C,0.0000878026,0.00038
03707,0.0001251726\\C,0.0000986889,0.0001212782,2.6267390469\\C,0.806491
6463,0.000113377,1.3265324968\\H,-0.1342498683,0.9865162848,-0.43848111
69\\H,1.4218811416,0.9143497102,1.3243216627\\C,1.689254858,-1.210649407
5,1.1074005733\\H,2.3032106373,-1.6717036754,1.8649040685\\O,0.781845052
6,-0.7623315533,-0.9335066223\\H,-0.666564983,0.8638290788,2.688478657\\
H,0.6781894729,0.0436856635,3.4836542012\\O,2.2175033819,-2.4685168086,
-0.9368981428\\C,1.622654873,-1.5389366001,-0.1883206657\\C,3.1528585801
,-3.2988091986,-0.2539127578\\H,3.966717792,-2.701168855,0.1677633282\\H
,2.6599034567,-3.86067368,0.5449999864\\H,3.5457671343,-3.985529459,-1.
0000601978\\H,-0.599594844,-0.9073354251,2.7301333098\\C,-2.2438939251,-
0.6134482568,-1.7633578109\\H,-1.4665543176,-1.0999879799,-2.3480356119
\\H,-3.1986440395,-1.1094364941,-1.9338584767\\H,-2.3278070075,0.4382079
438,-2.0362874844\\Se,-1.8300927347,-0.8066489031,0.1539780291\\Version
=AM64L-G03RevC.02\\State=1-A\\HF=-2826.0234572\\RMSD=8.953e-09\\RMSF=3.2

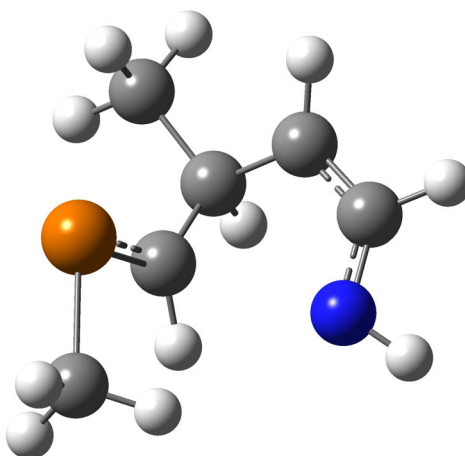
30e-06\Thermal=0.\Dipole=0.6857806,-0.0515988,0.2677369\PG=C01 [X(C7H12O2Se1)]\

10 (MeSe/CHNH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1Se1\TSCHNEI\19-Aug-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Se_CHNH_1\0,1C,0.0187609765,-0.044188109,-0.0054327287\C,0.0202452065,0.0097439114,2.6497677306\C,0.7245905659,-0.0344984298,1.3126752611\H,0.5328427161,0.4644252764,-0.8139699483\H,1.6763821838,0.4898745137,1.2787430096\C,0.7274301838,-1.3108239887,0.4768481535\H,0.0863369208,-2.1098109028,0.8346665393\H,-0.2344708853,1.0390242457,2.921285099\H,0.6665390234,-0.38939746,3.4368577987\C,1.9669038994,-1.7374353171,-0.2106140634\H,-0.9039268108,-0.5712348607,2.645861261\N,2.7886496556,-0.896263109,-0.6971591035\H,2.1184915111,-2.8245675948,-0.2695005126\H,3.5806843658,-1.3673842917,-1.1334671381\C,-2.0852712686,-1.0065416824,-1.800415257\H,-1.6770055587,-2.0055470877,-1.6542152865\H,-3.1487031085,-1.0764376297,-2.0278891809\H,-1.5719562968,-0.5036845896,-2.6185094409\Se,-1.9204111148,0.0420424667,-0.1389798958\Version=AM64L-G03RevC.02\State=1-A\HF=-2691.5756399\RMSD=5.325e-09\RMSF=6.427e-06\Thermal=0.\Dipole=0.1777987,-0.8785418,-0.1062553\PG=C01 [X(C6H11N1Se1)]\

TS₁₀₋₁₁ (MeSe/COOH)



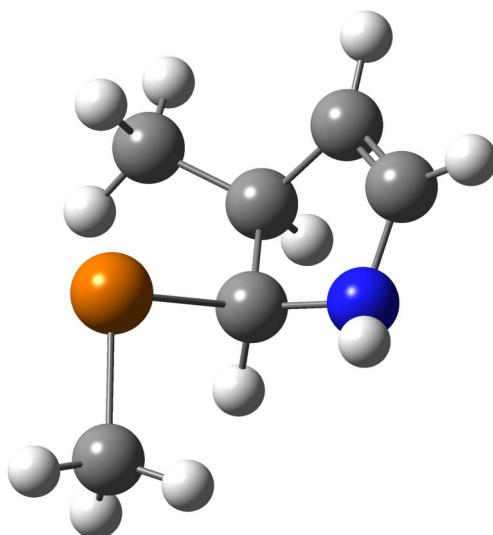
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H11N1Se1\TSCHNEI\24-Jan-2010\

```

0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
afine\DA_Se_CHNH_TS\0,1\C,0.0129277799,-0.0299557497,0.0282945643\C,
0.0351117399,0.0185220553,2.5740770578\C,0.8224569161,-0.0066520619,1.
2582193311\H,1.4772031204,0.8728730941,1.2175559558\C,1.6328167484,-1.
2895796321,1.1228538776\H,1.5830948978,-2.0032552369,1.9417456429\H,-0
.544660927,0.9382453401,2.6737213463\H,0.7311217516,-0.0468439359,3.41
43985131\C,2.2503660001,-1.6377101937,-0.0711613431\H,-0.652734296,-0.
8285355218,2.6481228917\N,1.9063298958,-1.1744084169,-1.2550991294\H,3
.0791372417,-2.3561375499,0.0182426784\H,2.6663722833,-1.2866904106,-1
.929791419\H,0.3008145912,0.5902156364,-0.8073011952\C,-1.5920499694,-
0.6766109518,-2.2366050505\H,-0.6094089417,-0.8565042411,-2.6677057316
\H,-2.3277901419,-1.3520002557,-2.6703129571\H,-1.9079356993,0.3554646
319,-2.3762313331\Se,-1.4605809721,-1.1108768931,-0.3207578546\Versio
n=AM64L-G03RevC.02\State=1-A\HF=-2691.4988617\RMSD=3.636e-09\RMSF=7.
302e-06\Thermal=0.\Dipole=-0.4929967,0.327182,-0.2435343\PG=C01 [X(C6H11
N1Se1)]\

```

11 (MeSe/CHNH)

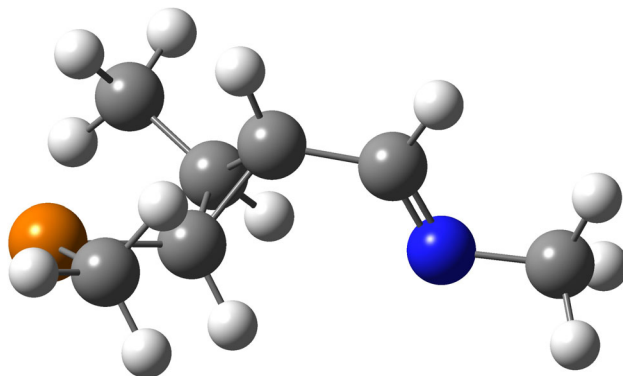


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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1Se1\TSCHNEI\24-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_CHNH_2\0,1\C,-0.0735747044,0.068
5152878,0.1644860596\C,0.2234547173,0.0319052334,2.7875694677\C,0.8617
700128,-0.0386600505,1.4012006896\H,1.5547057966,0.81554883,1.31385476
9\C,1.6364106486,-1.3026070839,1.0816479909\H,2.2862128779,-1.81664217
39,1.7759382995\H,-0.3691598195,0.9412440904,2.913436423\H,1.003860676
7,0.0336104419,3.5543149629\C,1.4953485944,-1.5701990151,-0.2189969841
\H,-0.4292290632,-0.821920238,2.9815464871\H,-0.2888408594,1.097386697
1,-0.1208688781\N,0.6770990096,-0.6290398951,-0.8706293179\H,0.1323423
187,-0.9787463113,-1.6478991696\H,1.9554798816,-2.3586111759,-0.801072
5121\C,-2.7957087919,0.2153827116,-1.0057726832\H,-2.3789741122,-0.066
5194089,-1.9727789827\H,-3.8480099525,-0.0659782816,-0.9832176906\H,-2
.7129497451,1.2923903994,-0.8610277097\Se,-1.9176208748,-0.7490014089,
0.4768620259\Version=AM64L-G03RevC.02\State=1-A\HF=-2691.5941998\RMSD
=5.868e-09\RMSF=9.427e-06\Thermal=0.\Dipole=0.0896899,0.2213374,-0.480
7455\PG=C01 [X(C6H11N1Se1)]\

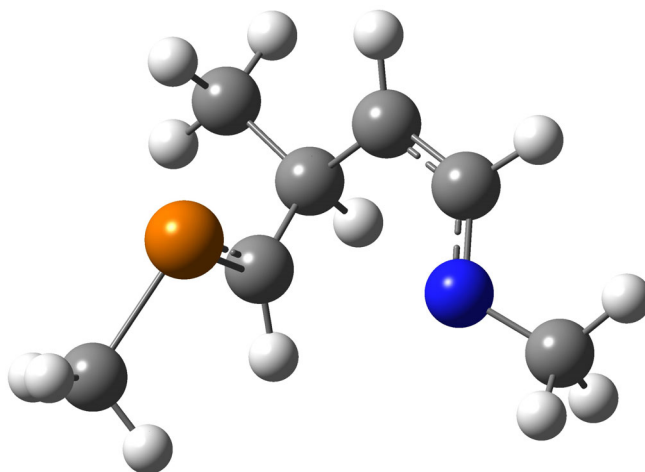
```

10 (MeSe/CHNMe)



```
11\GINC-WERZ01\Opt\RB3LYP\6-311G(d)\C7H13N1Se1\TSCHNEI\19-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_CHNR_1\0,1\C,0.0282221884,-0.087
7619096,-0.0372744077\C,0.0515524965,0.1151034429,2.6115637836\C,0.745
4665467,-0.0262947967,1.2754565689\H,0.5489839864,0.3632976498,-0.8751
346365\H,1.7105469086,0.4694072296,1.2063261894\C,0.7036702674,-1.3441
356194,0.5117372832\H,0.0397624076,-2.1006846139,0.9174533211\H,-0.177
9505963,1.1642635619,2.8229825408\H,0.6932706827,-0.2521660845,3.41774
76303\C,1.9209044436,-1.8600466857,-0.1557731902\H,-0.8854577836,-0.44
3811558,2.6467922024\N,2.7802624904,-1.0985156108,-0.6921171836\H,2.03
75683441,-2.9567093681,-0.1629033773\C,-2.1194695907,-1.0828835253,-1.
761103\H,-1.7362200666,-2.0829393187,-1.5635470705\H,-3.1867101575,-1.
1365850268,-1.9748364744\H,-1.6018113749,-0.6402446175,-2.6107205766\S
e,-1.9087833749,0.0513393902,-0.1620818218\C,3.937299819,-1.6982738413
,-1.3246108314\H,4.8482076179,-1.3142679248,-0.8553698999\H,3.95027832
63,-2.7981111023,-1.2716369751\H,3.9737893537,-1.3980768496,-2.3763108
122\Version=AM64L-G03RevC.02\State=1-A\HF=-2730.8958781\RMSE=7.433e
-09\RMSE=5.218e-06\Thermal=0.\Dipole=0.2475913,-0.7086302,-0.1220969\PG=
C01 [X(C7H13N1Se1)]\
```

TS₁₀₋₁₁ (MeSe/COOMe)



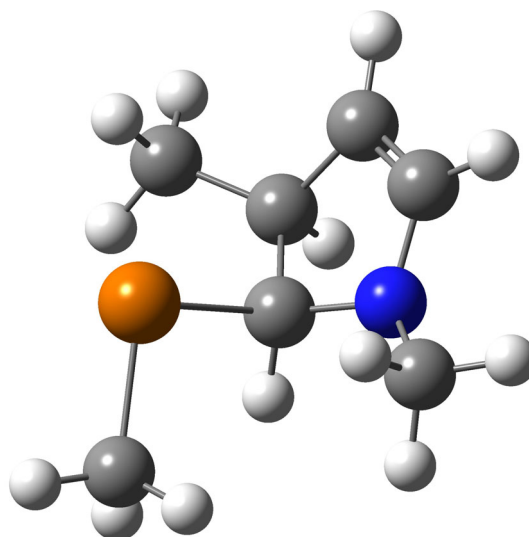
11\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1Se1\TSCHNEI\24-Jan-2010\

```

0\\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultr
afine\\DA_Se_CHNR_TS\\0,1\\C,0.100699757,-0.1090027838,-0.1961763027\\C,
-0.0124875964,0.0953862647,2.3338097482\\C,0.8493394989,-0.0734281219,1
.0744416237\\H,1.5539683931,0.7664852753,1.0159259265\\C,1.5951144282,-1
.3817894668,1.0493969746\\H,1.4807172515,-2.0776521316,1.8751211605\\H,-
0.5183496669,1.0633303986,2.341889112\\H,0.6266445217,0.0311551892,3.21
94520976\\C,2.4045670591,-1.6974676042,-0.0471345788\\H,-0.7703825016,-0
.6880733974,2.4011278502\\N,2.2805143998,-1.1489780737,-1.224858831\\H,3
.196943077,-2.4427607376,0.1260687444\\H,0.2960848095,0.6058604541,-0.9
890541876\\C,3.40056085,-1.2272897962,-2.1390781542\\H,4.131574328,-2.00
3763774,-1.862201449\\H,3.0465803993,-1.430500507,-3.1549951895\\H,3.942
8891085,-0.2727085589,-2.1754201392\\C,-2.1559685227,-0.4783657465,-1.9
455348635\\H,-1.5050730449,-0.0551437344,-2.7099537093\\H,-2.8382198834,
-1.1908804915,-2.4077488822\\H,-2.7219039557,0.3044969608,-1.4449418581
\\Se,-1.0582043983,-1.4946090317,-0.6490444054\\Version=AM64L-G03RevC.0
2\\State=1-A\\HF=-2730.8176617\\RMSD=8.268e-09\\RMSF=1.017e-06\\Thermal=0
\\Dipole=-0.5728395,0.4489198,-0.1591832\\PG=C01 [X(C7H13N1Se1)]\\

```

11 (MeSe/CHNMe)



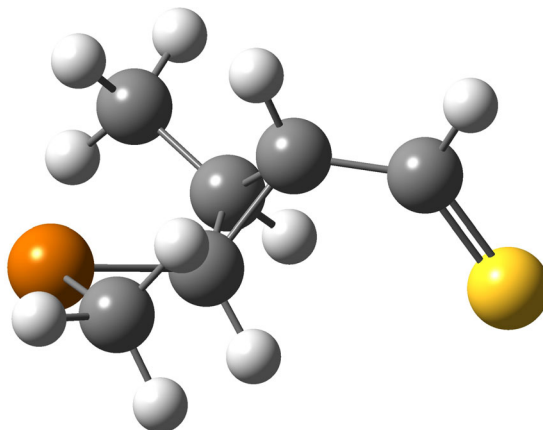
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1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H13N1Se1\\TSCHNEI\\24-Jan-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_Se_CHNR_2\\0,1\\C,-0.0704661991,-0.07
63605627,0.2111477047\\C,0.3476557773,0.1014017213,2.8173146563\\C,0.916
9180642,-0.0539052925,1.4094527184\\H,1.5701579841,0.8160986645,1.22037
60006\\C,1.734530347,-1.3032686072,1.1410873779\\H,2.4271561047,-1.75182
24316,1.8388532145\\H,-0.2840643194,0.9892533838,2.9008526818\\H,1.16727
1539,0.2055265477,3.5348904266\\C,1.5685390078,-1.6390085553,-0.1425452
635\\H,-0.2515866091,-0.7601788929,3.1153139815\\H,-0.3762484181,0.91400
11046,-0.1260233599\\N,0.6759285461,-0.7831099842,-0.8025942124\\H,2.050
1873559,-2.4295259182,-0.7042711299\\C,0.0616688431,-1.1653949485,-2.05
72158836\\H,-0.7385510326,-1.9058521574,-1.927674497\\H,-0.3566959077,-0
.2823253423,-2.5465690346\\H,0.8246094199,-1.5795081706,-2.7191201796\\C
,-2.9954671538,0.1024685836,-0.5200406223\\H,-2.8531692227,-0.183005030
3,-1.5613880392\\H,-4.031414251,-0.0821463468,-0.2372829743\\H,-2.780630
4269,1.1634190601,-0.3892545525\\Se,-1.8729447054,-0.9778682254,0.69347

```

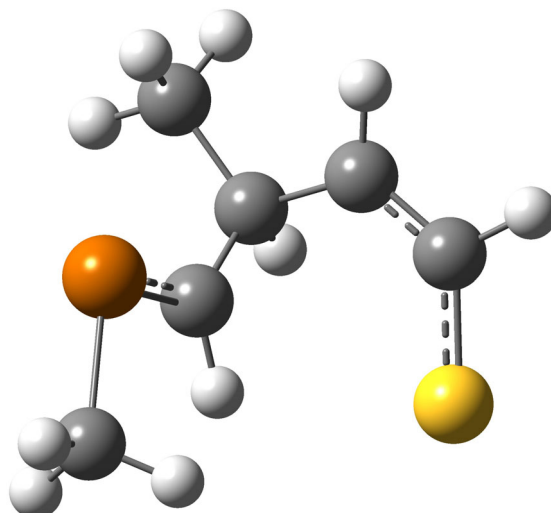
1506\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-2730.9101987\\RMSD=8.990e-09\\RMSF=4.089e-06\\Thermal=0.\\Dipole=0.2214873,0.3457425,-0.6428846\\PG=C01 [X(C7H13N1Se1)]\\

10 (MeSe/CHS)



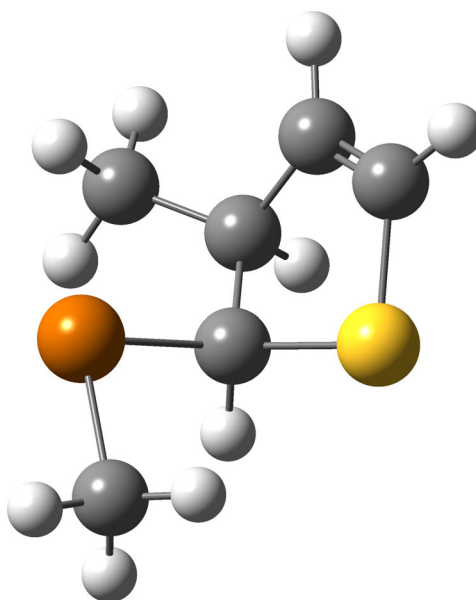
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C6H10S1Se1\\TSCHEI\\08-Sep-2010\\0\\# opt freq rb3lyp/6-311g(d)\\DA_Se_CHS_1\\0,1\\C,-0.0212867502,-0.0611683426,0.0392126435\\C,-0.0266737668,0.0708176348,2.9580834538\\H,1.0492742448,0.1173250505,0.0600277663\\C,-0.8326331667,1.1579881498,-0.4660610803\\H,-1.8167845933,1.2695268127,-0.0229400232\\C,-0.1490525357,2.3988146628,-0.807954196\\H,-0.5001799667,1.0472101771,2.869610159\\H,-0.3116117834,-0.3894993193,3.9035867115\\H,1.0567681391,0.1681548262,2.9137499385\\C,-0.6414962448,-0.1191826355,-1.3050223029\\H,0.0701073916,0.0246020244,-2.1148860655\\C,-1.840232669,-0.9715193411,-1.651804365\\H,-1.5254196055,-1.9896512864,-1.9007128481\\H,-2.5528803442,-1.0361071823,-0.8274005855\\H,-2.3625790186,-0.5634242199,-2.5209403189\\H,-0.7169017029,3.3031953699,-0.5794494825\\Se,-0.6649268076,-1.1261375294,1.5277534627\\S,1.3412930077,2.568043875,-1.4702003101\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-3034.4264668\\RMSD=6.434e-09\\RMSF=5.841e-06\\Thermal=0.\\Dipole=-0.8111578,-0.3322811,0.5317316\\PG=C01 [X(C6H10S1Se1)]\\

TS₁₀₋₁₁ (MeSe/CHS)



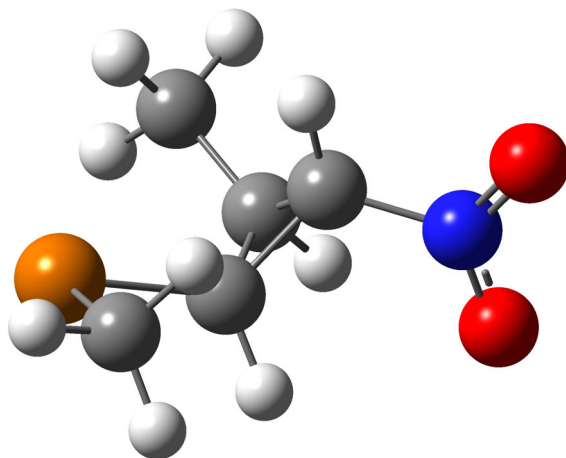
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10S1Se1\TSCHNEI\08-Sep-2010\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ult rafine\DA_Se_CHS_TS\0,1\C,-0.0712524681,0.1206756638,0.0538277089\C,0.0579836671,0.0708372514,2.3725197559\H,0.9487739864,0.2086963836,2.9827510047\C,-1.1063400831,0.691957832,2.7101738069\H,-1.1351624883,1.0903715052,3.7268698694\C,0.2341364909,-0.8237721476,1.1376561967\H,-0.5460331678,-1.5936241637,1.1400798212\C,1.6215497249,-1.4706877723,1.1024654988\H,1.7512947525,-2.0853906769,0.2093525935\H,2.4202155171,-0.7232404034,1.1207186414\H,1.7484199637,-2.1070723691,1.9810481835\H,-1.0812881845,0.1579141136,-0.3329718729\C,-0.2183465178,2.2782554644,-1.840023709\H,-1.0783775603,2.5865757899,-1.2500987209\H,0.2882415607,3.150728888,-2.2488896963\H,-0.5099941032,1.6064957802,-2.64409621\Se,1.0725629145,1.3831908957,-0.6473548871\S,-2.5316861948,0.9092908683,1.797620321\Version=AM64L-G03RevC.02\State=1-A\HF=-3034.3753136\RMSE=9.561e-09\RMSEF=7.032e-06\Thermal=0.\Dipole=1.8929986,-0.0345641,-1.6396551\PG=C01 [X(C6H10S1Se1)]\

11 (MeSe/CHS)



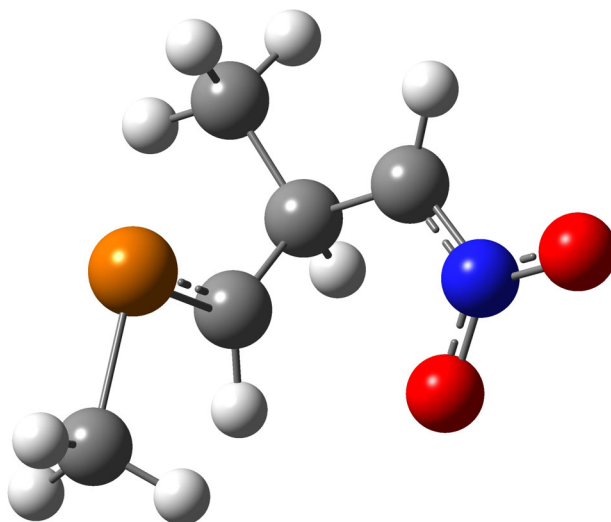
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10S1Se1\TSCHNEI\08-Sep-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Se_CHS_2\0,1\C,-0.0913202333,-0.2576100487,-0.0381864041\C,0.0118635035,-0.0842041605,2.5659785977\C,0.7722345071,-0.1095446795,1.2368926045\H,1.2809499842,0.8635667888,1.1295859551\C,1.8437738118,-1.1748243221,1.135752663\H,2.3867192763,-1.5226016171,2.0078310216\H,-0.7641518855,0.6841455189,2.5698391414\H,0.7039260728,0.1359433851,3.383807348\C,2.1119230992,-1.5741714822,-0.1051897656\H,-0.4624276638,-1.0433433082,2.7856807171\H,2.872633093,-2.2781172312,-0.4164665756\H,-0.5118451001,0.6938196147,-0.3587917772\C,-2.3808727916,-1.2968182343,-1.5891464484\H,-1.6513684979,-1.6132107316,-2.3331495277\H,-3.2565214492,-1.942875204,-1.643950109\H,-2.6844934485,-0.2644869757,-1.7617647878\Se,-1.6356672531,-1.5125560319,0.2184633115\S,1.0818000825,-0.8346990473,-1.3476931658\Version=AM64L-G03RevC.02\State=1-A\HF=-3034.4479731\RMSE=5.721e-09\RMSEF=5.565e-06\Thermal=0.\Dipole=0.0813441,0.311724,0.2130845\PG=C01 [X(C6H10S1Se1)]\

10 (MeSe/NO₂)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2Se1\TSCHNEI\24-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_NO2_1\0,1\C,0.0020000227,0.5671
125679,0.3707070424\C,0.2635894694,-0.3414646931,2.8655007083\C,0.8232
530096,0.0369397071,1.51230466\H,0.5124883555,1.2762239772,-0.27086128
3\H,1.8292655636,0.4459440189,1.5249198108\C,0.5585972502,-0.842098475
6,0.3114678265\H,-0.0990280645,-1.6954399305,0.3902879533\H,0.18385177
13,0.5414308218,3.5058203048\H,0.9220301238,-1.0571321052,3.364366322\
O,2.4813918572,-0.2165132064,-0.8201059508\H,-0.7285026038,-0.78939233
1,2.7894086025\N,1.6614904709,-1.1073165047,-0.6268794662\O,1.67554306
27,-2.2088107894,-1.1582188371\C,-2.3360945434,0.5316022534,-1.3872006
094\H,-2.0487574818,-0.4797126049,-1.669857141\H,-3.414521574,0.646554
5727,-1.4912087034\H,-1.8312671784,1.2625429334,-2.0164190646\Se,-1.91
5233389,0.8548811378,0.5123266486\Version=AM64L-G03RevC.02\State=1-A\
HF=-2802.6709347\RMSD=4.624e-09\RMSF=7.435e-06\Thermal=0.\Dipole=-0.93
76624,0.3502026,0.657709\PG=C01 [X(C5H9N1O2Se1)]\
```

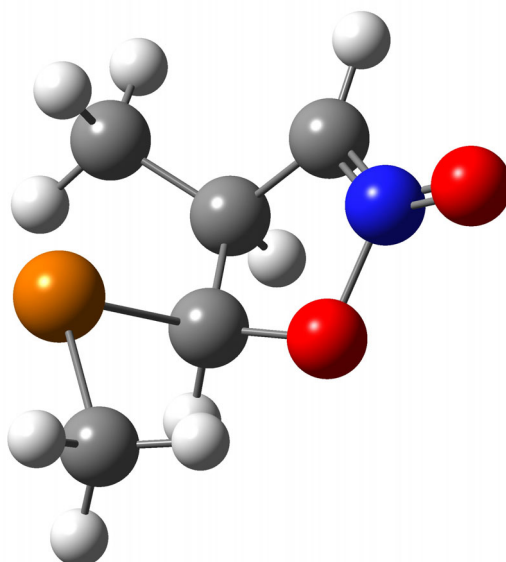
TS₁₀₋₁₁ (MeSe/ NO₂)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O2Se1\TSCHNEI\24-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ult
```

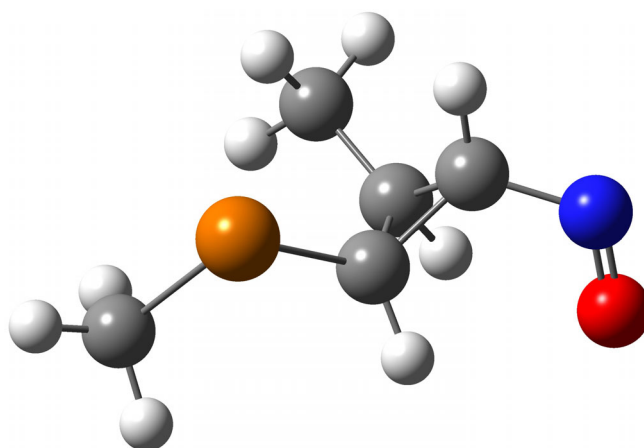
rafine\\DA_Se_NO2_TS\\0,1\\C,0.0204481108,-0.0457474373,0.0225618925\\C,
0.0317653302,0.0227180157,2.5759427865\\C,0.8282005002,-0.0093863257,1.
2661327611\\H,1.4839619265,0.8680144029,1.2113572937\\C,1.6000228678,-1.
2860831318,1.1305062852\\H,1.5771523857,-2.0812622268,1.8605486726\\H,-0.
.5614518701,0.9353862634,2.6542304454\\H,0.7246696786,-0.0134726836,3.4
192430249\\O,2.150067184,-0.7269226018,-1.0049900581\\H,-0.6424248923,-0
.8333845203,2.663375286\\N,2.2930970851,-1.5300136563,-0.0167346591\\O,3
.0630924986,-2.5052857814,-0.084126673\\H,0.2886998415,0.5982442918,-0.
8027105509\\C,-1.7244167304,-0.5914674391,-2.1871214289\\H,-0.8024407725
,-0.7695979539,-2.7357498346\\H,-2.5172555516,-1.2299339119,-2.57284226
04\\H,-2.0266665005,0.4517292321,-2.2440102273\\Se,-1.4372225474,-1.1224
596287,-0.3098592095\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-2802.5937
187\\RMSD=8.179e-09\\RMSF=2.663e-06\\Thermal=0.\\Dipole=-2.7876327,1.20042
8,0.2690578\\PG=C01 [X(C5H9N1O2Se1)]\\

11 (MeSe/NO₂)



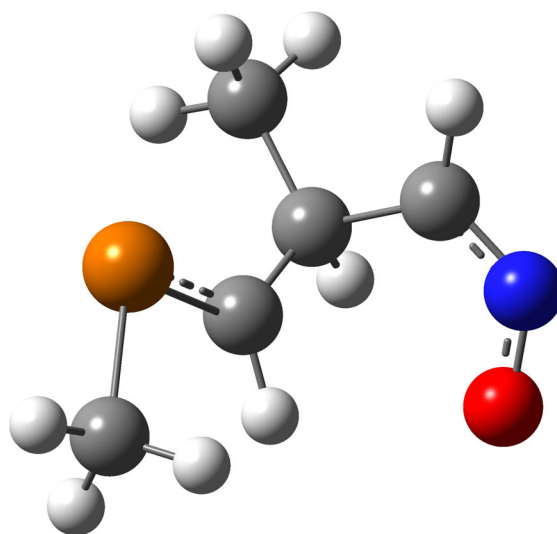
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C5H9N1O2Se1\\TSCHNEI\\24-Jan-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_Se_NO2_2\\0,1\\C,-0.2542578196,0.131
5123413,0.314335537\\C,0.3409260291,-0.1012435051,2.8646815008\\C,0.8212
364079,0.0090959893,1.4173514368\\H,1.4608876831,0.9029777588,1.3413072
259\\C,1.5816378119,-1.1726390589,0.9024022989\\H,2.3013338165,-1.793392
2595,1.4125797427\\H,-0.2644275879,0.7644755369,3.1412000546\\H,1.196623
7522,-0.1365970187,3.5437861576\\O,0.3498091054,-0.3996946481,-0.848243
9658\\H,-0.2520327431,-1.0027271835,3.0305270556\\N,1.3477393521,-1.4067
347602,-0.3556359163\\O,1.7538529047,-2.1905628866,-1.1828004164\\H,-0.5
215582046,1.1620815545,0.084931495\\C,-2.7369742869,-0.6126735552,-1.03
82586479\\H,-2.0227306014,-0.9561489619,-1.7826085818\\H,-3.6334465209,-
1.2300332922,-1.0741737722\\H,-3.0044405658,0.4293106692,-1.2094723071\\
Se,-1.9552438781,-0.8502771563,0.7543980897\\Version=AM64L-G03RevC.02\\
State=1-A\\HF=-2802.6709075\\RMSD=5.545e-09\\RMSF=7.552e-06\\Thermal=0.\\Di
pole=-0.0570318,0.9196356,1.0253561\\PG=C01 [X(C5H9N1O2Se1)]\\

10 (MeSe/NO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1Se1\TSCHNEI\26-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Se_NO_1\0,1\C,0.4157886859,0.17873
48675,-0.0471442518\H,0.7553220118,0.3062297563,0.9764840015\C,1.56158
09094,-0.1371582497,-0.9958055135\H,1.5402815936,0.2362439447,-2.01203
32727\C,0.5371823827,-1.2050285934,-0.5943680405\H,0.9598020924,-1.904
3422312,0.1252673256\C,-0.3775325067,-1.8065338222,-1.6322839346\H,-1.
216518527,-2.3177154028,-1.150103512\H,-0.7887061343,-1.0471742367,-2.
2992410179\H,0.1554528396,-2.5451696623,-2.2363969008\N,2.9153782892,-
0.2340261111,-0.4862079319\O,2.9996559399,-0.5653669541,0.6766527015\C
,-2.4191514879,0.7972077677,0.4445049248\H,-2.1727558568,0.8196472226,
1.5047181256\H,-3.2604813826,1.4634485805,0.2552605014\H,-2.6775663704
,-0.2130770825,0.1335371368\Se,-0.907183843,1.4844421425,-0.6220355504
\\Version=AM64L-G03RevC.02\State=1-A\HF=-2727.4342032\RMSD=7.902e-09\
RMSF=3.375e-05\Thermal=0.\Dipole=-1.2808733,-0.4162501,-0.1941987\PG=C0
1 [X(C5H9N1O1Se1)]\
```

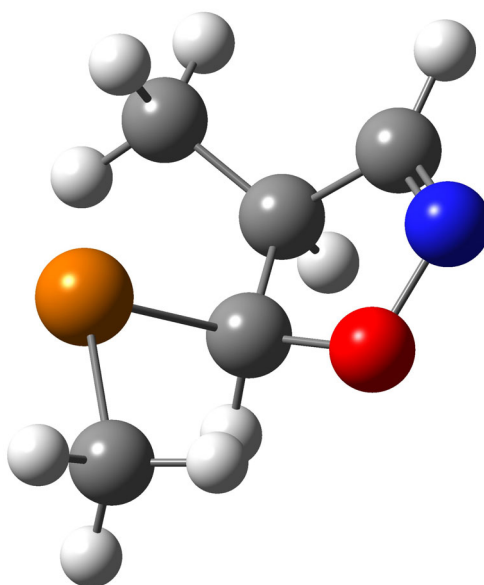
TS₁₀₋₁₁ (MeSe/NO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O1Se1\TSCHNEI\26-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine sc
f=tight\DA_Se_NO_TS\0,1\C,0.2290282758,-0.3925846425,-0.1025458922\C
,-0.1185230754,0.0656650876,2.1878160732\H,0.6737597432,0.2286635326,2
```

.9083806427\O,-1.9947466772,0.8334719704,1.231458795\C,0.0206739341,-1.1147516502,1.1296772886\H,-0.9754602733,-1.5726770104,1.1060084669\C,1.1029234906,-2.0924243287,1.5818920468\H,1.2241195221,-2.9047407881,0.8619875563\H,2.0731416106,-1.6000742787,1.7008162442\H,0.8365453886,-2.5258358322,2.5478133497\H,-0.6400683553,0.0139858991,-0.6061771411\N,-1.1675271423,0.7985740777,2.1728492088\C,1.2446488927,1.3183078605,-2.1970212206\H,0.7281788375,2.1662514658,-1.7529867405\H,2.124812633,1.659683985,-2.7393003825\H,0.5872006381,0.7708724611,-2.8690433394\Se,1.8853595737,0.1190198318,-0.7709054691\\Version=AM64L-G03RevC.02\State=1-A\HF=-2727.3975123\RMSD=6.879e-09\RMSF=1.700e-05\Thermal=0.\Dipole=1.614412,-0.5497888,-1.2101359\PG=C01 [X(C5H9N1O1Se1)]\\

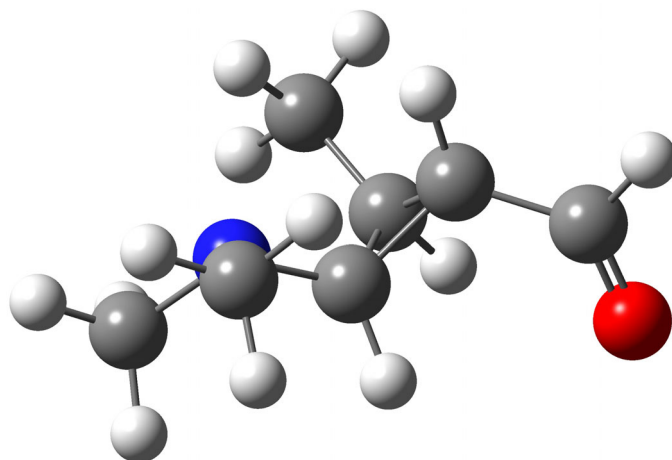
11 (MeSe/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1Se1\TSCHNEI\26-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Se_NO_2\0,1\C,-0.1296316665,-0.1958142418,0.0535612461\C,0.123312758,-0.0424361085,2.6768077238\C,0.7643773261,0.000284153,1.2891004323\H,1.2829557699,0.9651163168,1.1796534417\C,1.7747282692,-1.0834070808,0.9964222198\H,-0.640635379,0.7302954526,2.7815482829\H,0.8788606502,0.1323623279,3.4471883272\O,0.7057761736,-0.8784410407,-0.8883601756\H,-0.3403098302,-1.0097012336,2.8808973859\H,-0.4471570948,0.729305432,-0.4225574703\H,2.5272426993,-1.4548276543,1.682678768\N,1.7451920011,-1.5371287297,-0.1907489238\C,-2.3245847916,-1.3892469096,-1.4640661302\H,-1.4953872781,-1.7907474638,-2.04144799\H,-3.1720164373,-2.0719333377,-1.508637006\H,-2.6231525376,-0.4127744453,-1.8439073179\Se,-1.7885989689,-1.2679321645,0.4282075363\\Version=AM64L-G03RevC.02\State=1-A\HF=-2727.4798625\RMSD=4.036e-09\RMSF=1.931e-05\Thermal=0.\Dipole=-0.0679052,0.8330543,0.7092761\PG=C01 [X(C5H9N1O1Se1)]\\

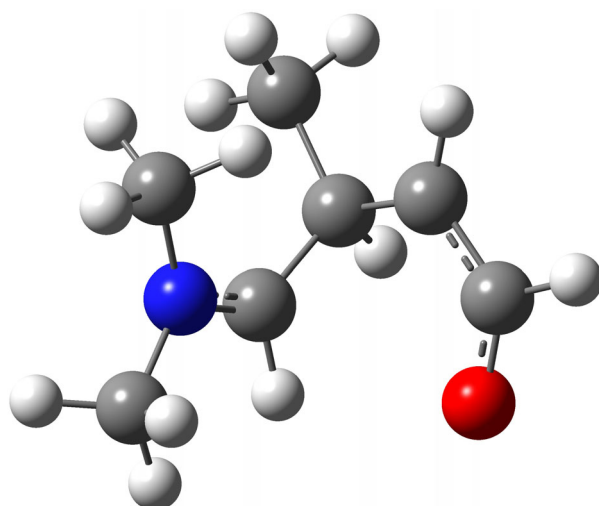
NMe₂-Donor

10 (Me₂N/CHO)



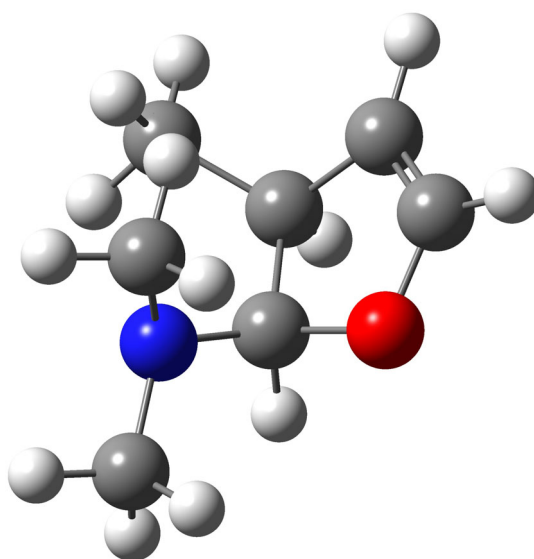
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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\12-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHO_1_1\0,1\C,-0.0059441643,-0.002
2026097,0.00406088\H,0.0170347128,0.0094163471,1.0991896223\C,1.389108
7076,-0.0157474669,-0.6275829511\H,1.486494607,0.5114556335,-1.5709782
281\C,2.5643707798,-0.0029251596,0.2663074296\C,0.4854182686,-1.255623
4078,-0.6373478971\H,0.8149252946,-2.0138237174,0.0676358123\C,-0.0503
80502,-1.7677395411,-1.9538047243\H,-0.8745697271,-2.4696254264,-1.792
4677802\H,-0.422743544,-0.9505909575,-2.5731089286\H,0.726603636,-2.29
87394871,-2.5108650399\N,-1.0161297668,0.7920960456,-0.6343440662\C,-0
.8798382854,2.2103988397,-0.3215370156\H,-1.6181940357,2.7831357462,-0
.8879397032\H,-1.0249095655,2.4315515132,0.7507997345\H,0.1133335538,2
.5607453269,-0.6083320761\C,-2.3570096593,0.3024002969,-0.3247636905\H
,-2.6106337754,0.3939305332,0.7462088522\H,-3.0953680791,0.8699784272,
-0.8964018385\H,-2.4450447988,-0.7478482557,-0.6058988704\O,2.60348116
21,-0.5355176255,1.3536700975\H,3.4527174373,0.5433271536,-0.119083289
5\\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5917841\RMSE=3.844e-09\R
MSF=1.481e-05\Thermal=0.\Dipole=-0.6207781,0.3418818,-0.7929039\PG=C01
[X(C7H13N1O1)]\
```

TS₁₀₋₁₁ (Me₂N/CHO)



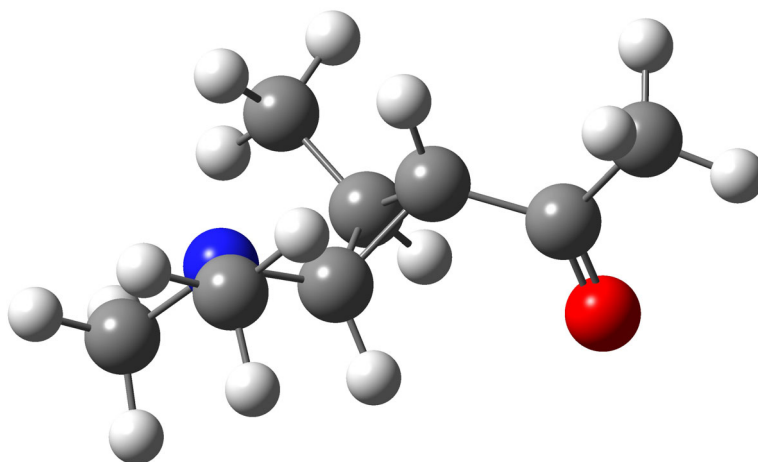
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\12-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight integral=
grid=ultrafine\DA_N_CHO_TS\0,1\C,0.1087038849,-0.156409489,-0.125981
3\C,-0.3011126296,0.2083807414,2.1445297841\H,0.3096066703,0.531666107
9,2.9817962276\C,-1.6133382786,0.6438289218,1.9677755938\H,-2.03358469
4,1.2327122387,2.8134966822\O,-2.3481803028,0.4102013982,0.9791427699\
C,0.2440392746,-0.8432219669,1.1912656658\H,-0.4592068302,-1.682664271
7,1.13580333\C,1.6126270594,-1.4019520746,1.5966653539\H,2.0308475906,
-2.0642949166,0.8332786449\H,2.3448477263,-0.6235536324,1.8164929727\H
,1.4839932604,-1.9837676092,2.512183534\H,-0.7835655913,-0.398392349,-
0.6886545958\N,0.8153073635,0.8314148359,-0.6312838357\C,0.318541768,1
.5715665684,-1.7940128481\H,-0.0381756319,2.5576155997,-1.4828110583\H
,1.1186558663,1.6937031967,-2.5266874535\H,-0.5068221139,1.0301623008,
-2.2506009346\C,1.9216819941,1.4451773381,0.0996813615\H,1.5781154358,
1.6570765186,1.1191458094\H,2.7868402536,0.7838922695,0.1342165089\H,2
.2075537648,2.3717840326,-0.3948174267\Version=AM64L-G03RevC.02\State
=1-A\HF=-404.5494287\RMSD=2.417e-09\RMSF=5.598e-06\Thermal=0.\Dipole=
2.3199293,0.4002722,-1.4983448\PG=C01 [X(C7H13N1O1)]\
```

11 (Me₂N/CHO)



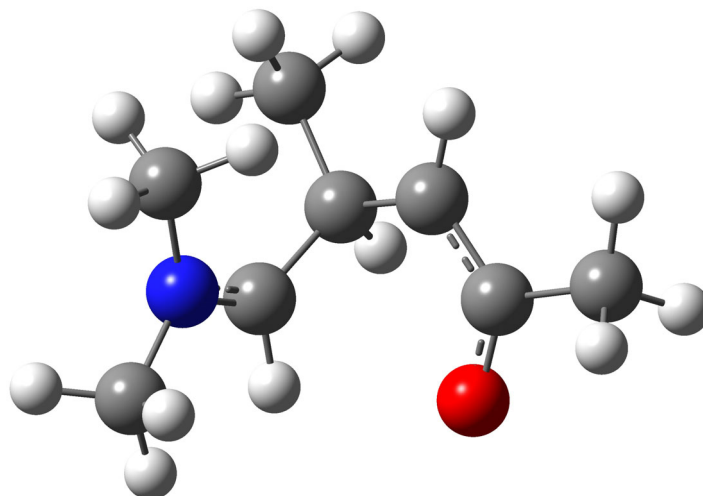
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNE\11-Jan-2010\0\# opt freq b3lyp/6-311g(d)\DA_N_CHO_2\0,1\C,-0.0185050646,-0.3102392866,0.0099417662\C,0.2004822396,0.3332620587,2.5519546504\C,0.9041876735,0.0612101314,1.2194919401\H,1.4166963628,0.9926154037,0.938930185\C,1.9173784974,-1.0631171651,1.1938200847\H,2.6617487785,-1.2503355491,1.9550437562\H,-0.5658264542,1.1037089784,2.4412530106\H,0.9275673407,0.6877134963,3.2885709333\C,1.7818941032,-1.7291835872,0.0493400888\O,0.773773951,-1.3001773159,-0.7657224568\H,-0.2815098959,-0.5535380601,2.964268864\H,2.3459394847,-2.5674926863,-0.3398682743\H,-0.1388567197,0.5427308944,-0.6565430941\N,-1.3275827886,-0.7974425766,0.3182835319\C,-1.3905903857,-2.1298530616,0.9161459293\H,-2.3812720847,-2.281068119,1.3529805809\H,-1.2121002626,-2.9285209381,0.1817743224\H,-0.6499285461,-2.2359846832,1.7057978169\C,-2.2793979221,-0.6713065356,-0.7821973469\H,-2.0645681666,-1.352684452,-1.6203615611\H,-3.2852691263,-0.8917541742,-0.4156467188\H,-2.2814460936,0.3529565548,-1.1610001227\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5955005\RMSD=7.839e-09\RMSF=4.301e-06\Thermal=0.\Dipole=-0.1409364,0.0562879,0.1910151\PG=C01 [X(C7H13N1O1)]\

10 (Me₂N/COMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNEI\12-Jan-2010\0\# opt=tight int=ultrafine freq rb3lyp/6-311g(d)\DA_N_COR_1\0,1\C,-0.147433749,0.0255978093,0.1646199033\C,0.5677136152,0.3272792243,2.6859421964\C,0.8944876559,0.2439874543,1.2129209088\H,0.0531359133,0.4948452943,-0.8042280553\H,1.7359449527,0.8444044827,0.8788787669\C,0.8187706428,-1.108566381,0.5010268309\H,0.396341822,-1.9214945718,1.0827556173\H,0.4041525499,1.3653577353,2.9920113488\H,1.3898285518,-0.0653390715,3.2914397648\C,1.8772630449,-1.4516743028,-0.4883658825\C,2.2798551245,-2.9118572306,-0.574409034\H,1.4170712673,-3.5338525094,-0.8352228001\H,3.0593941035,-3.0390437504,-1.3244834122\H,2.6439658631,-3.2665826222,0.3955453628\O,2.3931898515,-0.6040371583,-1.1911259956\H,-0.335328439,-0.2373463787,2.9221044423\N,-1.5254200512,-0.1374277648,0.5354573265\C,-2.2463699975,-0.9977502466,-0.3956271781\H,-3.2662455295,-1.1550637637,-0.0358478964\H,-2.3048966777,-0.5772091719,-1.4154929797\H,-1.7559298346,-1.9710083028,-0.4584425745\C,-2.1914846196,1.1520975052,0.6959695383\H,-2.2518098164,1.7245837529,-0.2467502262\H,-3.2092849776,0.9967246981,1.0624480797\H,-1.6565213798,1.759300976,1.4273753416\Version=AM64L-G03RevC.02\State=1-A\HF=-443.9251165\RMSD=5.234e-09\RMSF=3.353e-07\Thermal=0.\Dipole=-0.6813974,-0.4436345,0.5746322\PG=C01[X(C8H15N1O1)]\

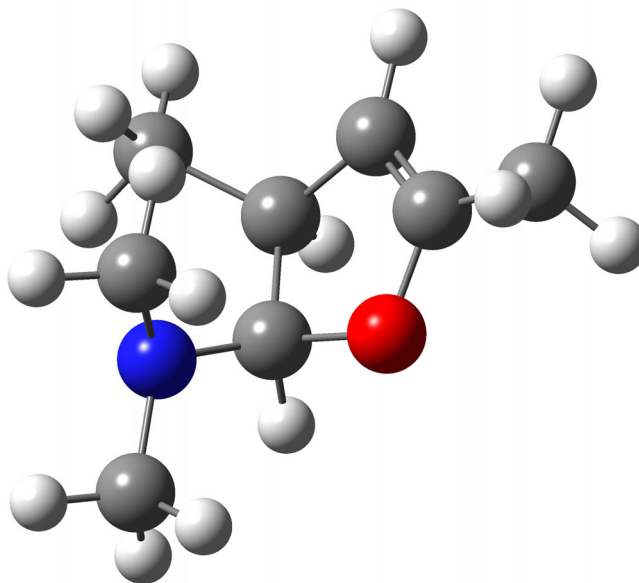
TS₁₀₋₁₁ (Me₂N/CHO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNEI\13-Jan-2010\0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\DA_N_COR_TS\0,1\C,-0.104582751,0.1400773134,0.1752545219\C,0.0687001902,-0.5253755792,2.684260916\C,0.7476670383,-0.2427596684,1.3392728656\H,1.4228911141,0.6104768558,1.4742005883\C,1.5280704338,-1.4193412015,0.7816419879\H,1.4954939633,-2.3632533451,1.3152608967\H,-0.5803380959,0.2965190311,3.0003001792\H,0.8487267251,-0.6468348264,3.4393626601\C,2.3536868517,-1.195991093,-0.3269346783\C,3.3666564475,-2.2746438078,-0.7045401607\H,3.2760727288,-3.1867495601,-0.1093734366\H,3.2556511144,-2.5257263039,-1.7635350702\H,4.3771421971,-1.8740550981,-0.5786663519\O,2.3339502935,-0.1414249023,-1.0143219274\H,-0.5172536579,-1.4458668041,2.68353517\H,0.2702277722,0.9535999232,-0.4316499776\N,-1.1561251893,-0.4699087419,-0.3268267002\C,-1.6679773126,-1.7186118149,

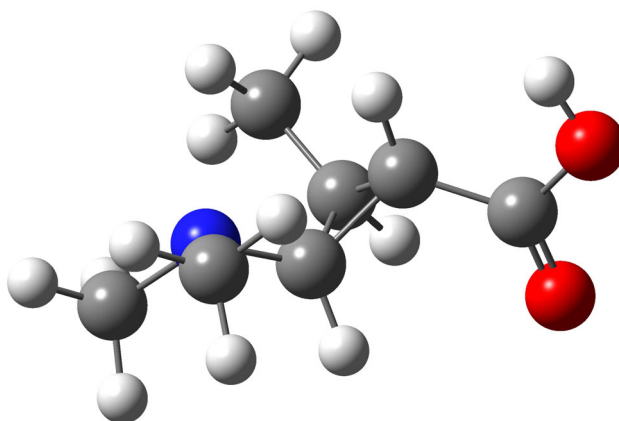
0.2334937088\H,-0.81705648,-2.3927706103,0.3875091428\H,-2.1766656393,
 -1.5469034069,1.1816023806\H,-2.3719608839,-2.1639244941,-0.4673191574
 \C,-1.659949967,-0.1004085455,-1.6518516223\H,-2.7441714639,0.02322921
 32,-1.6163823838\H,-1.2026920972,0.8326390726,-1.9731030344\H,-1.41113
 81318,-0.8811558017,-2.3763545767\\Version=AM64L-G03RevC.02\State=1-A\
 HF=-443.8787918\RMSD=3.632e-09\RMSF=5.629e-06\Thermal=0.\Dipole=-2.703
 7151,-0.0985943,0.25683\PG=C01 [X(C8H15N1O1)]\

11 (Me₂N/COMe)



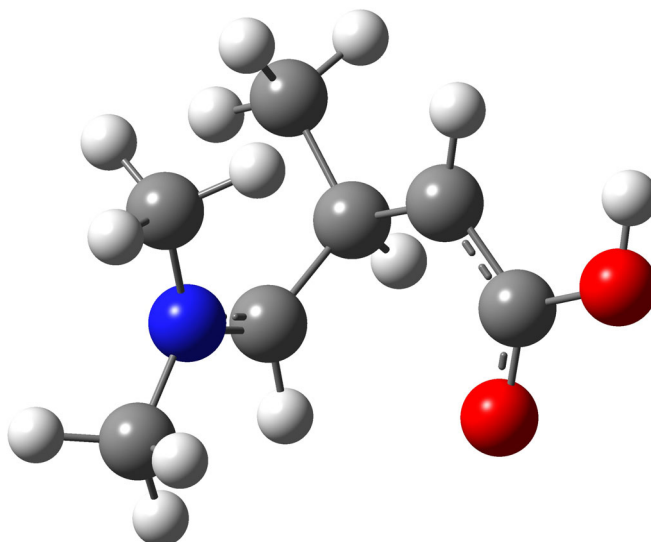
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNEI\12-Jan-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_N_COR_2\0,1\C,-0.0411264467,-0.29906
 98211,0.0007363224\C,0.1734954687,0.1586843815,2.5826351346\C,0.875160
 8805,0.0135594829,1.2294077032\H,1.3489080435,0.9838605231,1.018796438
 6\C,1.9260303567,-1.0655338105,1.1096593671\H,2.682484531,-1.278075952
 4,1.8527984201\H,-0.6175505945,0.9107653335,2.5368452954\H,0.894983896
 9,0.4779707843,3.3406397993\C,1.823751531,-1.6531009391,-0.0844639049\
 C,2.6432581267,-2.7175856061,-0.7262451006\H,3.451858941,-3.0384178713
 ,-0.0681563225\H,2.026144859,-3.5866835818,-0.9751253911\H,3.078533300
 8,-2.3554645068,-1.6630242026\O,0.7829177925,-1.1864175513,-0.85148077
 11\H,-0.2771898752,-0.7722294756,2.9278588094\H,-0.2051591755,0.599021
 4899,-0.5937540908\N,-1.32842642,-0.862631524,0.2778114921\C,-1.330264
 2246,-2.2371676605,0.7745270268\H,-2.3093960959,-2.4626510434,1.205575
 5055\H,-1.127328769,-2.9710266363,-0.0191401391\H,-0.5778973519,-2.370
 1663605,1.5490567427\C,-2.2896375666,-0.6980062656,-0.8088488946\H,-2.
 0496252473,-1.3063607211,-1.6952101563\H,-3.2837695269,-0.9876611357,-
 0.4584894302\H,-2.3371270211,0.3500801376,-1.11208852\\Version=AM64L-G
 03RevC.02\State=1-A\HF=-443.9274372\RMSD=2.493e-09\RMSF=7.997e-06\Th
 ermal=0.\Dipole=-0.0435213,-0.0629194,0.1001677\PG=C01 [X(C8H15N1O1)]\

10 (Me₂N/COOH)



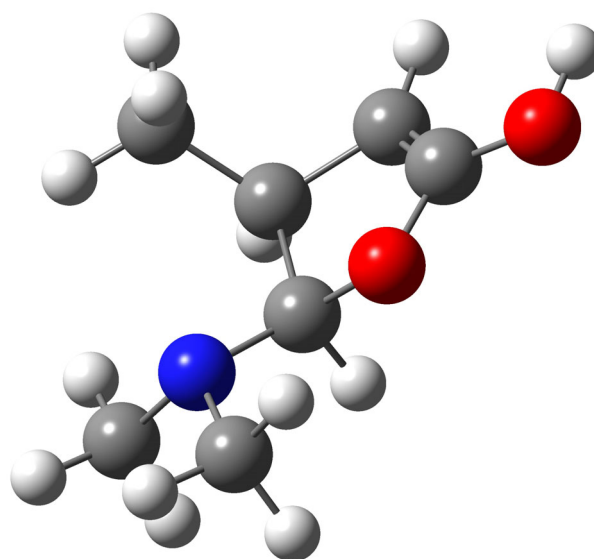
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\14-Jan-2010\0\# opt freq rb3lyp/6-311g(d) geom=connectivity\DA_N_COOH_1\0,1\C,0.067211769,0.035512687,-0.0161378323\C,-0.0589178518,-0.1217247934,2.6190417099\C,0.6939739666,-0.047848937,1.310575573\H,0.538399885,0.5999085823,-0.7883695822\H,1.6508255811,0.4641886973,1.3442327545\C,0.7053503387,-1.2608697605,0.3828638763\H,0.0366675225,-2.0678174024,0.6695510959\O,2.7836449336,-0.7991117178,-0.6845820802\H,-0.1965772431,0.8762974127,3.0459291431\H,0.4916283421,-0.7170882029,3.3530798423\O,2.2004741323,-2.9363693838,-0.5109084524\C,1.9773451209,-1.6070632405,-0.308656718\H,-1.0458646481,-0.5660046112,2.4823171046\H,1.4750548962,-3.4616703569,-0.1513953588\N,-1.4271521457,0.0173729071,-0.0924918066\C,-1.9004764411,-0.5865025905,-1.3337310291\H,-1.5020048907,-1.5983155034,-1.4315681157\H,-2.9910408858,-0.6520515994,-1.3172005106\H,-1.6049542429,-0.0155914662,-2.2314930556\C,-1.9890609373,1.351872664,0.1005552456\H,-3.0798422629,1.2906461971,0.1210760161\H,-1.6542810351,1.7627076253,1.0539209623\H,-1.7012631583,2.0579699185,-0.6980147826\Version=AM64L-G03RevC.02\State=1-A\HF=-479.8558833\RMSD=5.734e-09\RMSF=6.533e-06\Thermal=0.\Dipole=-1.5573891,-0.2335062,0.6242348\PG=C01 [X(C7H13N1O2)]\

TS₁₀₋₁₁ (Me₂N/COOH)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\15-Jan-2010\0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra fine\DA_N_COOH_TS\0,1\C,-0.235239598,0.0385121567,0.8067389563\C,0.7652235776,-0.6648862914,3.0934665025\C,0.9844398905,-0.2769748237,1.625917328\H,1.5593956007,0.657246182,1.6157183977\C,1.6856639399,-1.3335490272,0.8126638224\H,1.9453300079,-2.276359054,1.2841937133\O,1.6905590412,0.004494173,-1.1288002854\H,0.1760997112,0.0818236424,3.6330949454\H,1.7426321617,-0.737305541,3.5762304564\O,2.9209825548,-1.8626423365,-1.164761779\C,2.0599398436,-0.995733734,-0.5065742758\H,0.2793229236,-1.6352505517,3.2089344642\H,3.2362430983,-2.5240617458,-0.5374964006\H,-0.1992123926,0.9537620168,0.229634288\N,-1.2820509255,-0.7106815254,0.5498571282\C,-1.4146779376,-2.059715642,1.0926882427\H,-0.4471604975,-2.562436971,0.9611945775\H,-1.6755426506,-2.0352041776,2.1504490741\H,-2.1932337223,-2.591618797,0.5487160824\C,-2.2041186909,-0.3507023345,-0.5310733108\H,-2.0623680927,-1.0279955544,-1.3776217291\H,-3.2349701128,-0.4233934998,-0.1794663625\H,-2.0065996951,0.6665424944,-0.8611621519\Version=AM64L-G03RevC.02\State=1-A\HF=-479.8050572\RMSD=4.025e-09\RMSF=1.499e-05\Thermal=0.\Dipole=-2.5391688,-0.5318081,1.5819155\PG=C01 [X(C7H13N1O2)]\

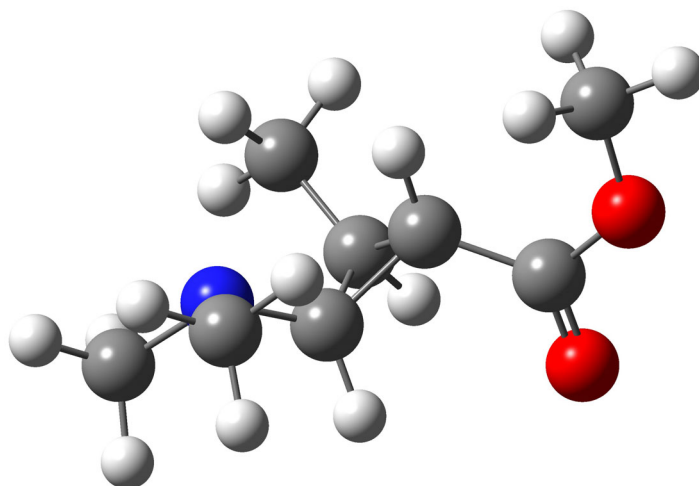
11 (Me₂N/COOH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\29-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_COOH_3\0,1\C,-0.1432764096,-0.3185291193,0.0397000264\C,0.1032270317,-0.4614868609,2.6377616679\C,0.7144094905,-0.0061893079,1.3033779202\H,0.1309688198,0.3970596274,-0.76117342\H,0.9151992475,1.0698099699,1.3407139952\C,1.954019017,-0.8059355349,0.9488394458\O,0.329346178,-1.6092993129,-0.4299521347\H,-0.7832221559,0.1137810994,2.9150894675\H,0.840304204,-0.3460134201,3.4380258592\O,2.2580882926,-2.7287692786,-0.5526163518\C,1.6001846734,-1.7104609922,0.028130289\H,-0.1846858078,-1.5132020533,2.5931880083\N,-1.5738527171,-0.3806892672,0.2303596261\C,-2.2671582918,-1.0082588888,-0.8947697585\H,-1.8999182479,-2.0210106904,-1.0409524989\H,-3.3343010531,-1.0542896044,-0.6669073167\H,-2.1406774892,-0.450261624,-1.8402738685\C,-2

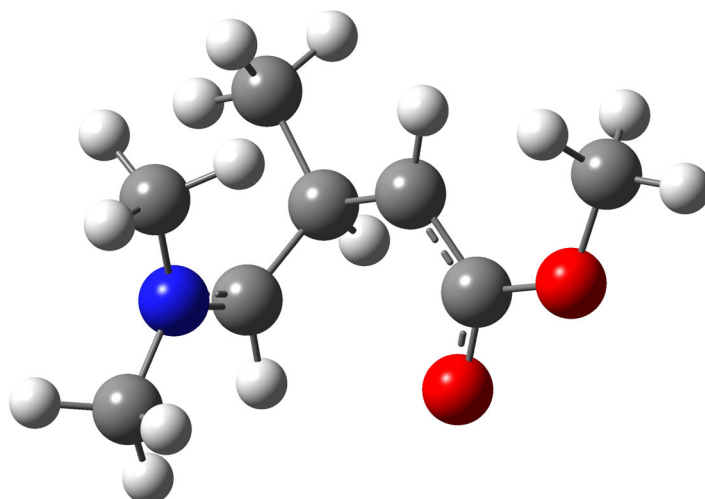
.1084934842,0.9551003187,0.4758004451\H,-1.9871021511,1.6295528572,-0.3918158104\H,-3.174599856,0.8811839611,0.6989075999\H,-1.6204374214,1.4186757985,1.3336034057\H,3.1206362922,-2.8192458859,-0.1316483063\H,2.9047924294,-0.747981155,1.4600377474\\Version=AM64L-G03RevC.02\State=1-A\HF=-479.8350027\RMSD=4.099e-09\RMSF=1.586e-05\Thermal=0.\Dipole=0.3953498,0.4448898,0.3203023\PG=C01 [X(C7H13N1O2)]\\

10 (Me₂N/COOMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O2\TSCHNEI\15-Jan-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_COOR_1\0,1\C,-0.0293822393,0.0949577575,-0.0085500681\C,0.2170884293,-0.1913718182,2.6049966668\C,0.8037019889,0.0440281009,1.2323375787\H,0.3349806725,0.7632292428,-0.7942969873\H,1.683011457,0.679695886,1.197312303\C,0.8702314133,-1.1145654181,0.2348118664\H,0.3449971363,-2.0092427915,0.5406991114\O,2.7019319209,-0.2710219605,-1.006783797\H,-0.009249959,0.7583113701,3.0993979835\H,0.9223596873,-0.7307355535,3.2440166698\O,2.5613692901,-2.4694530971,-0.9230007016\C,2.0965589336,-1.2307491661,-0.6002167852\C,1.9223775039,-3.6619103784,-0.4649267847\H,1.9109034479,-3.7224553669,0.6263687576\H,0.9039624847,-3.7510863027,-0.8523084086\H,2.5231638421,-4.4794101409,-0.8588808876\H,-0.7079755277,-0.7667964712,2.5478870937\N,-1.4490487405,-0.1124411872,0.0651218984\C,-1.978318709,-0.718582571,-1.1516174771\H,-1.4691161419,-1.6641264979,-1.3483564041\H,-3.0433686222,-0.9274093568,-1.0241768838\H,-1.8597793509,-0.0759371733,-2.0418495291\C,-2.1525691215,1.1247318596,0.3937069361\H,-2.051889261,1.8963031256,-0.389790405\H,-3.2168757717,0.9168699795,0.5287280134\H,-1.7663406342,1.5368474672,1.3268220654\\Version=AM64L-G03RevC.02\State=1-A\HF=-519.1650747\RMSD=3.696e-09\RMSF=2.617e-06\Thermal=0.\Dipole=-1.2471511,-0.7630682,0.6847041\PG=C01 [X(C8H15N1O2)]\\

TS₁₀₋₁₁ (Me₂N/COOMe)

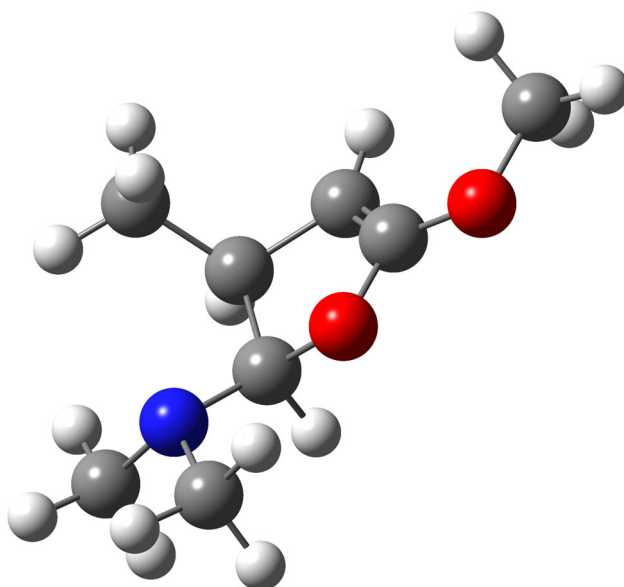


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H15N1O2\TSCHEI\16-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_N_COOR_TS\0,1\C,-0.2177158543,0.0334040244,0.7746528933\C,0.
566482005,-0.4013507181,3.2091773837\C,0.9168381289,-0.1928553309,1.73
09172227\H,1.5117410472,0.7254518656,1.6579412677\C,1.6658655927,-1.34
72598036,1.1106932498\H,1.8498035468,-2.2261929241,1.7129709306\O,1.88
63743039,-0.188785556,-0.9228757946\H,-0.0590936945,0.4050910379,3.602
3973313\H,1.4975466915,-0.4150359142,3.7805461084\O,3.0621237152,-2.06
07711462,-0.7333152952\C,2.1714331785,-1.1464684935,-0.1907284443\C,3.
5498265802,-3.1252590385,0.0622652106\H,4.0400970624,-2.7626836351,0.9
721154718\H,2.7530824671,-3.8255164267,0.3429499193\H,4.2793511497,-3.
6542106368,-0.5518749186\H,0.0627272488,-1.3507767966,3.398307038\H,-0
.1027716429,0.8617618769,0.0877199808\N,-1.264425057,-0.7199420607,0.5
316444602\C,-1.4869176935,-1.9822234469,1.2327959491\H,-0.5338486971,-
2.5262701042,1.2443549064\H,-1.8255455417,-1.8109906165,2.2541832447\H
,-2.2421078709,-2.5594074073,0.7022335325\C,-2.0873104831,-0.484213677
,-0.6581517468\H,-1.908050288,-1.2734526237,-1.3933555304\H,-3.1439826
351,-0.480592616,-0.3840758611\H,-1.8268540183,0.4733071876,-1.1031471
763\Version=AM64L-G03RevC.02\State=1-A\HF=-519.1159981\RMSD=6.007e
-09\RMSF=1.367e-05\Thermal=0.\Dipole=-2.6608944,-0.3931654,1.2520328\PG
=C01 [X(C8H15N1O2)]\

```

11 (Me₂N/COOMe)

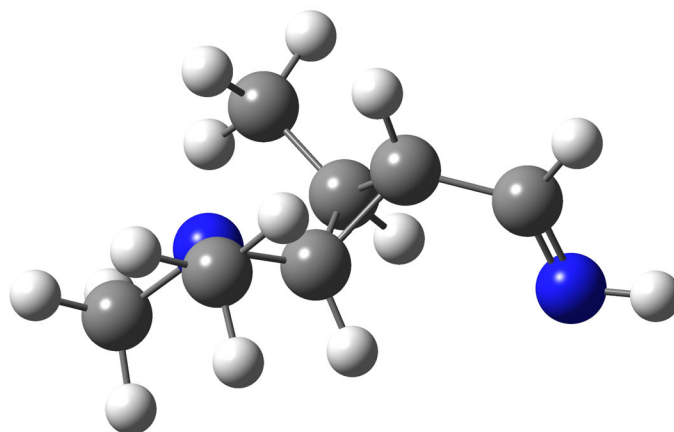


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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O2\TSCHNE\15-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_COOR_2\0,1\C,-0.1165192874,-0.4924
734438,0.0372102985\C,0.0452732561,-0.9081738343,2.6112118457\C,0.6696
650666,-0.2652698316,1.3624621554\H,0.1338880536,0.3254569121,-0.66844
88061\H,0.7908779025,0.8107143164,1.5270209594\C,1.9769539301,-0.93543
90168,0.9827289084\H,2.8948310897,-0.8661712765,1.5455756714\O,0.46220
21344,-1.6877490466,-0.5457699179\H,-0.8909221013,-0.430667561,2.90974
39386\H,0.7421660972,-0.8320261111,3.4511726663\O,2.4649901256,-2.6493
484013,-0.7101189776\C,1.7262911098,-1.7541080936,-0.0487504811\C,3.78
59084477,-2.8410049448,-0.2133937177\H,4.3646267342,-1.9147878266,-0.2
826999\H,3.7647297269,-3.1804848023,0.8265256814\H,4.2362314391,-3.604
6487953,-0.8435408013\H,-0.1621630146,-1.9657625165,2.4394170947\N,-1.
5457041421,-0.6688934385,0.1574714307\C,-2.1501833936,-1.2091830088,-1
.0602495834\H,-1.7074905481,-2.1726940561,-1.3000187542\H,-3.219569601
5,-1.3497442593,-0.8886148501\H,-2.0262169183,-0.5407349011,-1.9316217
29\C,-2.1810325072,0.5932886295,0.5225088426\H,-1.7615203364,0.9875653
378,1.4484956023\H,-2.0719064472,1.3680050131,-0.2588400475\H,-3.24761
91893,0.4262891448,0.6847506054\\Version=AM64L-G03RevC.02\State=1-A\HF
=-519.1501739\RMSD=3.193e-09\RMSF=1.157e-05\Thermal=0.\Dipole=0.443030
2,0.336858,0.2716567\PG=C01 [X(C8H15N1O2)]\

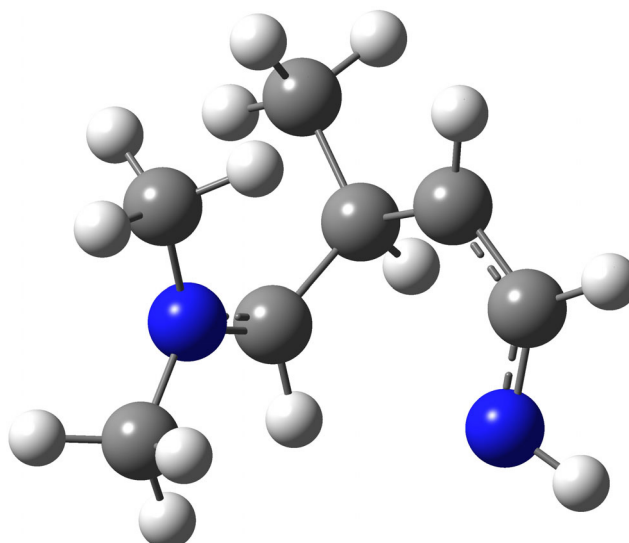
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10 (Me₂N/CHNH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H14N2\TSCHNEI\18-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHNH_1\0,1\C,0.006388724,-0.00148721
64,-0.0488022395\C,-0.0301634184,0.0191239098,2.590553065\C,0.70937587
79,0.023425032,1.2726962723\H,0.5146613347,0.5239753416,-0.8644209118\
H,1.6529886365,0.5615455173,1.2597694369\C,0.7504397149,-1.2469203719,
0.4245013367\H,0.115277634,-2.0568192475,0.768670651\H,-0.2082662263,1
.0394020511,2.9453269178\H,0.5493659572,-0.497380755,3.3615208579\C,2.
0056391138,-1.6470679521,-0.2455479973\H,-0.9982606713,-0.4758278294,2
.4983874347\N,2.8406051817,-0.7908567141,-0.6818654725\H,2.1603523641,
-2.7315631638,-0.3400781074\H,3.6399309625,-1.2504145957,-1.1177025425
\N,-1.4285357625,-0.0540390639,-0.1039368295\C,-1.906177706,-0.7594372
708,-1.2871216333\H,-1.4858324666,-1.7664644865,-1.3138520252\H,-2.995
1127578,-0.8465586894,-1.2490295105\H,-1.6372600933,-0.251403507,-2.23
08080364\C,-2.0185928011,1.2772511754,-0.0022712673\H,-1.7613355323,1.
9276269633,-0.8575782549\H,-3.1076434066,1.1949051178,0.0430671662\H,-
1.6771702791,1.7674785991,0.9104454971\\Version=AM64L-G03RevC.02\Stat
e=1-A\HF=-384.702856\RMSD=5.330e-09\RMSF=9.376e-06\Thermal=0.\Dipole
=-0.2412744,-0.4746574,-0.0405677\PG=C01 [X(C7H14N2)]\

TS₁₀₋₁₁ (Me₂N/CHNH)



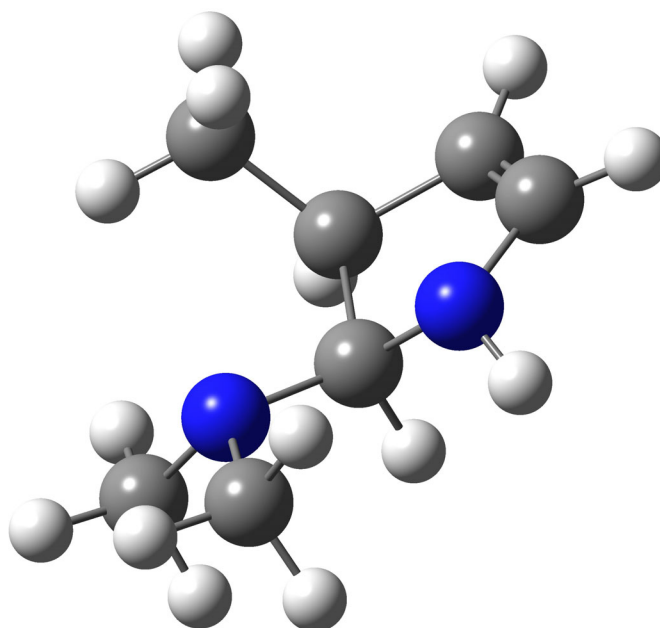
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H14N2\TSCHNEI\13-Jan-2010\

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0\\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafi
ne\\DA_N_CHNH_TS\\0,1\\C,-0.1065317541,0.0076477411,0.0405628648\\C,0.22
1670299,-0.3416539954,2.5977707072\\C,0.8250943488,-0.1724392433,1.1989
874832\\H,1.4244357739,0.7464189461,1.1976938773\\C,1.6976649265,-1.3277
286,0.7668372995\\H,1.7133222044,-2.2230799062,1.38001339\\H,-0.46520526
45,0.4712907607,2.849991254\\H,1.0367688613,-0.3371834942,3.3257652489\\
C,2.4639141974,-1.2418205678,-0.40249448\\H,-0.3083636262,-1.2882208252
,2.71960085\\N,2.2800561114,-0.3539007376,-1.3524315977\\H,3.2731782833,
-1.9864896717,-0.4783457442\\H,3.0689961401,-0.3519298978,-1.9976816653
\\H,0.1640865835,0.7909742241,-0.6552523422\\N,-1.0702076427,-0.78539627
55,-0.3950330008\\C,-1.4092908227,-2.0248160994,0.2911286407\\H,-0.48082
79676,-2.5904048276,0.4514547732\\H,-1.8802058651,-1.8281013638,1.25407
42926\\H,-2.0979328485,-2.6029554282,-0.3228164584\\C,-1.5718511939,-0.6
438302626,-1.7628725231\\H,-2.6638421981,-0.6666271837,-1.7655723198\\H,
-1.2314364152,0.2995958347,-2.1832164188\\H,-1.1927114831,-1.4581594594
,-2.3872807212\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-384.6509784\\RM
SD=3.350e-09\\RMSF=7.056e-06\\Thermal=0.\\Dipole=-1.8388559,-0.2630836,-0.
0561751\\PG=C01 [X(C7H14N2)]\\

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11 (Me₂N/CHNH)



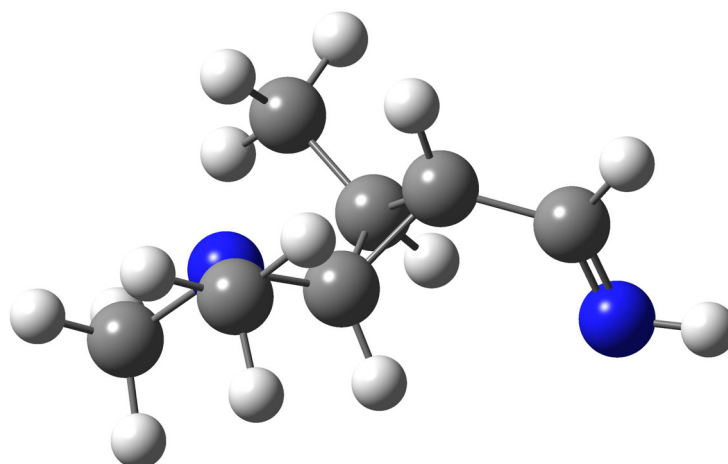
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1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H14N2\\TSCHNEI\\12-Jan-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_N_CHNH_2\\0,1\\C,-0.0909237374,-0.278844
6691,-0.0105894815\\C,0.0799741725,-0.4634298362,2.583762599\\C,0.711623
0707,0.0720245437,1.2873540062\\H,0.8297824982,1.1576470245,1.369344725
5\\C,2.0286313352,-0.6253197023,0.9994410731\\H,2.9208980671,-0.51740040
94,1.6017265303\\H,-0.8835893978,0.0026272041,2.7994096683\\H,0.74672938
27,-0.2677999165,3.4291352899\\C,1.8406077828,-1.5284039173,0.035112474
1\\H,-0.0810691573,-1.5409855801,2.5205214811\\H,0.1358783868,0.50280193
1,-0.769646266\\N,0.5206083223,-1.5461233549,-0.4578342541\\H,0.45580204
38,-1.6946640789,-1.4576860677\\H,2.5489185544,-2.2507419166,-0.3532745
649\\N,-1.5347149953,-0.3809855314,0.1766919464\\C,-2.20448003,-1.108766
0642,-0.8919766839\\H,-3.2740219607,-1.1592583976,-0.6758245505\\H,-2.08

```

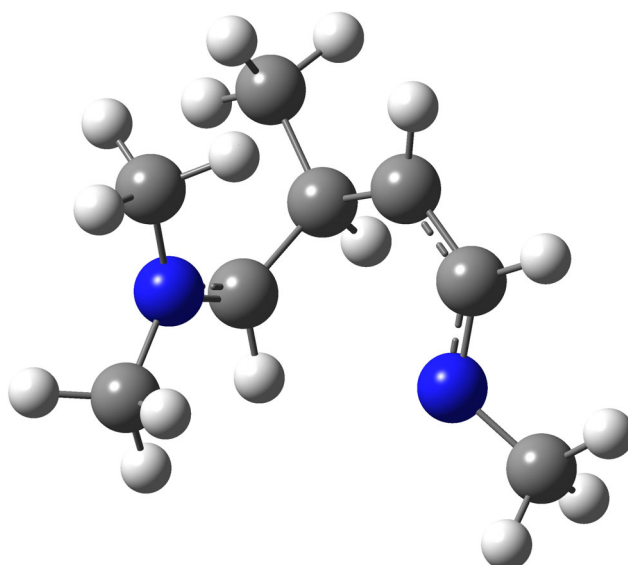
71949835,-0.6341849732,-1.8867990657\H,-1.8235012405,-2.1280089669,-0.9404801314\C,-2.1220500381,0.9410764831,0.3472943114\H,-2.0167546482,1.5775351533,-0.551893929\H,-3.187187488,0.8438638013,0.5687155241\H,-1.6553156071,1.4647690627,1.1829309245\\Version=AM64L-G03RevC.02\State=1-A\HF=-384.7176256\RMSD=9.130e-09\RMSF=5.416e-06\Thermal=0.\Dipole=-0.0183993,0.1911068,-0.5440006\PG=C01 [X(C7H14N2)]\\

10 (Me₂N/CHNMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H14N2\TSCHEI\18-Aug-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_CHNR_1\0,1\C,0.013114489,0.0923828523,0.0100713929\C,-0.0631148813,-0.1099516643,2.6409349895\C,0.6961160376,0.0030331664,1.3392088983\H,0.5347415748,0.6831641215,-0.7505765264\H,1.6409960149,0.5370663017,1.3857587555\C,0.7473218736,-1.1911932644,0.3875067509\H,0.1052224943,-2.0251363691,0.6522190132\H,-0.2443164886,0.8773374796,3.0779362483\H,0.5037259361,-0.6916570505,3.3739627461\C,2.0115209621,-1.5375916154,-0.2954597361\H,-1.0307669901,-0.5921084707,2.4930730237\N,-1.4208938926,0.049514513,-0.0706843182\C,-1.8822137361,-0.5516213693,-1.3162073751\H,-1.4634056966,-1.5540744102,-1.4220732445\H,-2.9717584215,-0.6383003533,-1.3016755908\H,-1.5983801456,0.0336600682,-2.2094511239\C,-2.0098022681,1.3692108074,0.1348574007\H,-1.6808244585,1.7793713408,1.0906177955\H,-1.7388699489,2.0888941417,-0.6585008822\H,-3.099558268,1.2867618911,0.1573792639\H,2.1641678803,-2.6105805957,-0.4810331477\N,2.8557983039,-0.6506850242,-0.6435917233\H,3.6602214486,-1.0744466161,-1.1055296858\\Version=AM64L-G03RevC.02\State=1-A\HF=-384.7028561\RMSD=8.609e-09\RMSF=5.366e-06\Thermal=0.\Dipole=-0.2425756,-0.4685752,-0.0854762\PG=C01 [X(C7H14N2)]\\

TS₁₀₋₁₁ (Me₂N/CHNMe)

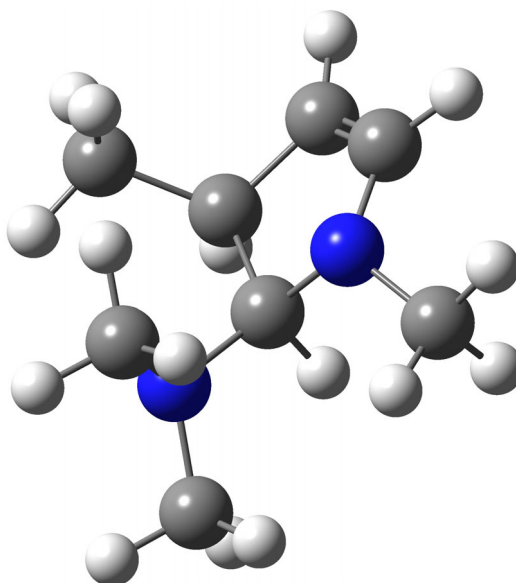


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H16N2\TSCHNEI\13-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafi
ne\DA_N_CHNR_TS\0,1\C,0.0004508369,0.3360920533,-0.1653559686\C,0.14
87168298,0.5701249936,2.4183709641\C,0.7948730299,0.1502702312,1.09285
11454\H,1.6796582571,0.7797678649,0.9368631759\C,1.2084375645,-1.29974
89474,1.0487916519\H,0.8952991129,-1.9551321818,1.8551630448\H,-0.2000
401444,1.6064367213,2.3945051538\H,0.8977790916,0.480166789,3.20911683
9\C,1.9645598947,-1.8003898144,-0.019739934\H,-0.6912633106,-0.0673366
231,2.7011720917\N,2.1369612582,-1.2052582078,-1.1701065055\H,2.454884
3924,-2.7740197413,0.1621622657\H,0.5291213564,0.7952126998,-0.9905238
887\C,3.1693431486,-1.7199638425,-2.0403748767\H,3.5421710896,-2.71377
34515,-1.7349740089\H,2.8024566913,-1.8019397702,-3.0721935896\H,4.041
0066648,-1.0495741024,-2.0752290169\N,-1.1689299113,-0.1810786194,-0.5
029047317\C,-1.5765226391,-0.2193102417,-1.9079389512\H,-0.9341860159,
0.432957642,-2.4951658161\H,-1.4872131835,-1.2378261008,-2.2974155763\
H,-2.6120389072,0.113440032,-2.0066642836\C,-1.9212299646,-1.029325916
7,0.4111466175\H,-1.2388898067,-1.7985469583,0.7997803383\H,-2.3243808
702,-0.4540679012,1.2445930019\H,-2.7469505814,-1.4964710056,-0.123066
5403\Version=AM64L-G03RevC.02\State=1-A\HF=-423.9689245\RMSE=5.262e-0
9\RMSE=5.181e-06\Thermal=0.\Dipole=-1.9635837,0.5518151,-0.1555623\PG=
C01 [X(C8H16N2)]\

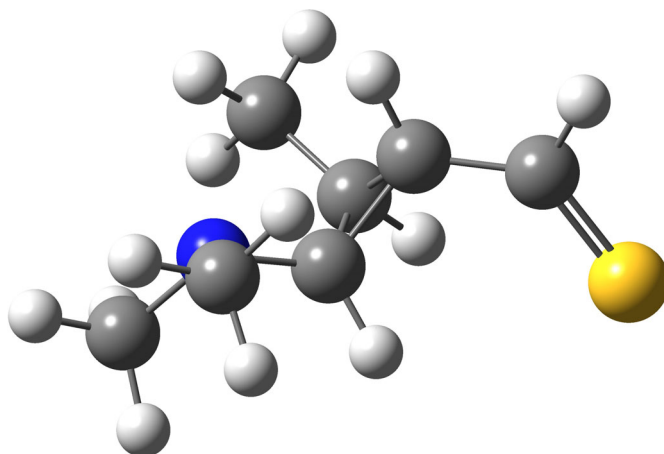
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11 (Me₂N/CHNMe)



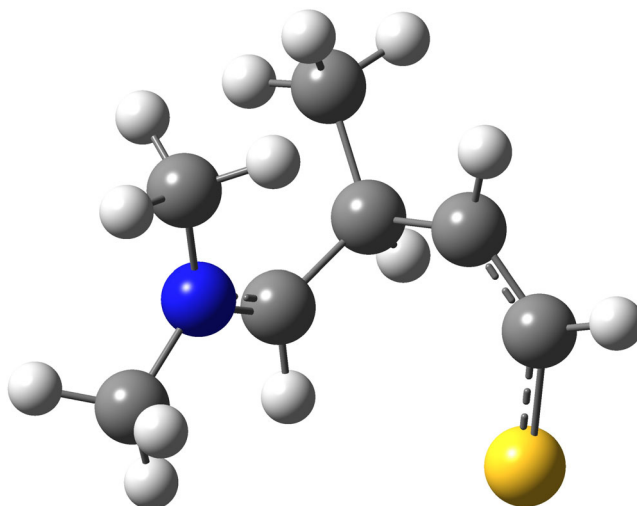
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H16N2\TSCHNEI\15-Jan-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_CHNR_2\0,1\C,-0.0173305495,-0.0471562376,0.2594732822\C,-0.0197902949,-1.2529937111,2.6102881331\C,0.7696504854,-0.4625285922,1.5565737568\H,1.1156545362,0.4577323472,2.0409980907\C,1.9143623611,-1.2577569109,0.9667511611\H,2.7474182325,-1.648994101,1.536175899\H,-0.9339281465,-0.7235546979,2.8887428046\H,0.5874216206,-1.3786560671,3.5115417899\C,1.6361544384,-1.5560308806,-0.3059094013\H,-0.2859242234,-2.2522500074,2.2577629462\H,0.3846040519,0.9322436742,-0.0420820886\N,0.4130061344,-1.0402142934,-0.7591282834\H,2.2199816473,-2.1675870915,-0.9850836406\C,0.3297972045,-0.6185305135,-2.147060012\H,0.7091898508,-1.4111641485,-2.7962561613\H,-0.7095152918,-0.4359177421,-2.4235266646\H,0.906230192,0.3003692263,-2.3500185162\N,-1.452730177,0.1247725935,0.4062352742\C,-2.2754005386,-1.0616962794,0.2169767214\H,-1.8382320345,-1.9206492625,0.7200790594\H,-3.2662678066,-0.8843933817,0.645964553\H,-2.4103861041,-1.3331280782,-0.8430136172\C,-2.0268317191,1.2960192149,-0.2379228524\H,-1.4133535689,2.1765184338,-0.0377880575\H,-2.1426767322,1.1998790096,-1.3325065006\H,-3.020118014,1.4885304055,0.1783977348\\Version=AM64L-G03RevC.02\State=1-A\HF=-424.0332082\RMSD=2.367e-09\RMSF=5.326e-06\Thermal=0.\Dipole=-0.0632189,0.1710963,-0.4212731\PG=C01 [X(C8H16N2)]\

10 (Me₂N/CHS)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1S1\TSCHNEI\20-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHS_1\0,1\C,-0.0268082058,-0.01384
49908,0.0206422209\H,-0.0004485222,0.0093137198,1.1155597703\C,1.38595
86778,-0.0373936117,-0.6020587136\H,1.4552996521,0.478206315,-1.554401
664\C,2.5769029827,0.0059857968,0.2338558129\C,0.452996406,-1.26830220
29,-0.6111128064\H,0.7768004772,-2.0278949954,0.0952231184\C,-0.060783
7127,-1.7753443726,-1.9375310389\H,-0.8914400018,-2.4727187387,-1.7898
197792\H,-0.4176150963,-0.9566006829,-2.563812128\H,0.7234803325,-2.31
16630017,-2.4785419932\N,-1.0098418764,0.799950815,-0.6290163821\C,-0.
8753332716,2.2101780869,-0.278838996\H,-1.5891097548,2.8005279343,-0.8
581490522\H,-1.0568562654,2.4070700087,0.7922353451\H,0.1299785407,2.5
589147021,-0.5217757011\C,-2.365426131,0.3110166646,-0.3846655111\H,-2
.6610826804,0.3802893256,0.6765935776\H,-3.0757686753,0.8970474801,-0.
9727203005\H,-2.4485155808,-0.7315975531,-0.6934384633\H,3.4147325648,
0.5537734061,-0.2031678228\S,2.7802523353,-0.6580511895,1.7190102047\
Version=AM64L-G03RevC.02\State=1-A\HF=-727.5539978\RMSD=3.974e-09\R
MSF=3.302e-05\Thermal=0.\Dipole=-0.9224871,0.3182203,-0.939492\PG=C01
[X(C7H13N1S1)]\

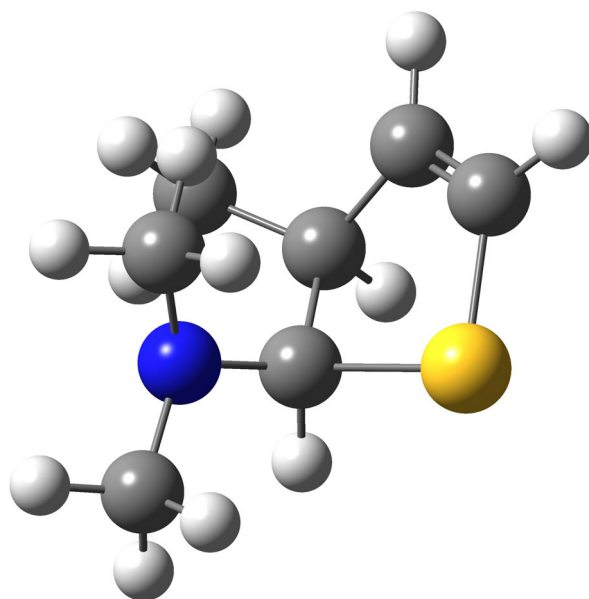
TS₁₀₋₁₁ (Me₂N/CHS)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1S1\TSCHNEI\20-Aug-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHS_1\0,1\C,-0.0268082058,-0.01384
49908,0.0206422209\H,-0.0004485222,0.0093137198,1.1155597703\C,1.38595
86778,-0.0373936117,-0.6020587136\H,1.4552996521,0.478206315,-1.554401
664\C,2.5769029827,0.0059857968,0.2338558129\C,0.452996406,-1.26830220
29,-0.6111128064\H,0.7768004772,-2.0278949954,0.0952231184\C,-0.060783
7127,-1.7753443726,-1.9375310389\H,-0.8914400018,-2.4727187387,-1.7898
197792\H,-0.4176150963,-0.9566006829,-2.563812128\H,0.7234803325,-2.31
16630017,-2.4785419932\N,-1.0098418764,0.799950815,-0.6290163821\C,-0.
8753332716,2.2101780869,-0.278838996\H,-1.5891097548,2.8005279343,-0.8
581490522\H,-1.0568562654,2.4070700087,0.7922353451\H,0.1299785407,2.5
589147021,-0.5217757011\C,-2.365426131,0.3110166646,-0.3846655111\H,-2
.6610826804,0.3802893256,0.6765935776\H,-3.0757686753,0.8970474801,-0.
9727203005\H,-2.4485155808,-0.7315975531,-0.6934384633\H,3.4147325648,
0.5537734061,-0.2031678228\S,2.7802523353,-0.6580511895,1.7190102047\
Version=AM64L-G03RevC.02\State=1-A\HF=-727.5539978\RMSD=3.974e-09\R
MSF=3.302e-05\Thermal=0.\Dipole=-0.9224871,0.3182203,-0.939492\PG=C01
[X(C7H13N1S1)]\

0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\\DA_N_CHS_TS\\0,1\\C,0.1338079531,-0.0112384659,0.0033610796\\C,0.0310479656,-0.067831511,2.3435714848\\H,0.8914532697,-0.0955865731,3.0089893423\\C,-1.0444827249,0.7253243772,2.6285523208\\H,-1.0136318042,1.2185605866,3.6024564782\\C,0.0739206199,-0.9853201279,1.1252154563\\H,-0.9157236078,-1.4478281352,1.0318505051\\C,1.1309957465,-2.0912375218,1.2157281607\\H,1.2215860753,-2.6499658645,0.2798052669\\H,2.1197334812,-1.7227034412,1.4940223513\\H,0.823818164,-2.7932520808,1.993690478\\C,0.933803925,1.7579369125,-1.4258946812\\H,1.5845600904,1.6139372598,-2.2908259583\\H,-0.1040083214,1.7604333223,-1.7500562457\\H,1.1612535209,2.7207529612,-0.9618407824\\H,-0.8326115827,0.2758319143,-0.3982243669\\S,-2.4461078953,1.0124428685,1.6835535685\\N,1.1493574778,0.677248314,-0.4565733601\\C,2.502590085,0.5707026027,0.0975385867\\H,2.4523584156,0.6732182572,1.1835161783\\H,2.9574386435,-0.3851576245,-0.1605664098\\H,3.1153289146,1.3724853012,-0.3094549249\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-727.532155\\RMSD=4.969e-09\\RMSF=1.441e-05\\Thermal=0.\\Dipole=3.4688758,-0.3327365,-2.0802235\\PG=C01 [X(C7H13N1S1)]\\

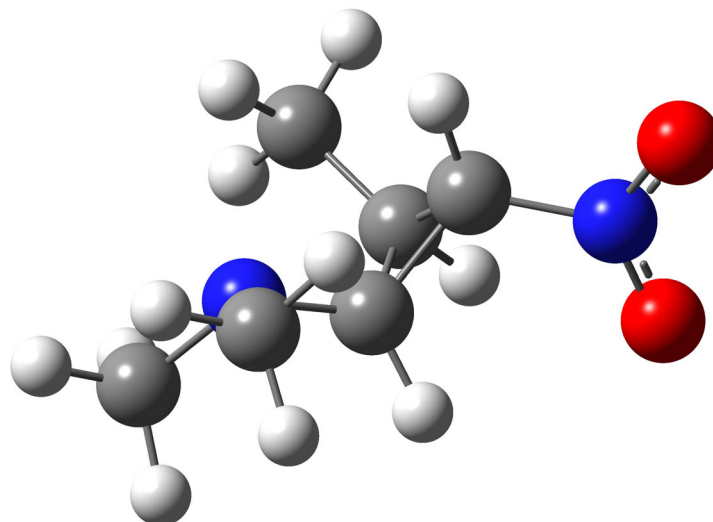
11 (Me₂N/CHS)



1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H13N1S1\\TSCHNEI\\20-Aug-2010\\0\\# opt freq b3lyp/6-311g(d)\\DA_N_CHS_2\\0,1\\C,-0.2034083874,0.3409225492,0.57411041\\C,0.3883689904,-0.9786778923,2.7278321304\\C,0.905684206,-0.2991222924,1.455695187\\H,1.5299855795,0.5509288888,1.772519096\\C,1.7755624877,-1.1506958,0.5590449025\\H,2.3981472889,-1.9453609095,0.9573079019\\H,-0.2127140351,-0.2890819176,3.3249341562\\H,1.2307866648,-1.305510507,3.3446447901\\C,1.7710720456,-0.7957999403,-0.7259613165\\H,-0.2298340129,-1.8517348563,2.5153767851\\H,2.3634822984,-1.2413809175,-1.5158125856\\H,-0.3917921839,1.3616696211,0.9033848291\\N,-1.4546792113,-0.3385351373,0.5302934946\\C,-2.5566920099,0.4803916639,0.0415113203\\H,-2.4858065638,0.6944513244,-1.037196552\\H,-3.5015118304,-0.0371628915,0.2224633221\\H,-2.5851046916,1.4301900984,0.5799083659\\C,-1.4738335231,-1.6772538459,-0.0500439647\\H,-0.6772339311,-2.2894045421,0.367879227

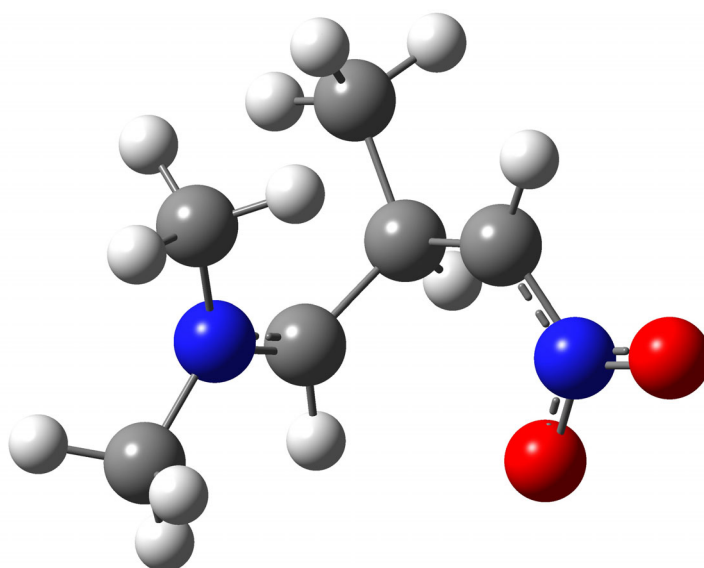
9\H,-2.4308062839,-2.1508486532,0.1818263702\H,-1.3480868284,-1.662731
6304,-1.1421440397\N,0.6823382843,0.5405043629,-1.140120234\\Version=A
M64L-G03RevC.02\State=1-A\HF=-727.5782388\RMSD=3.951e-09\RMSF=2.24
7e-05\Thermal=0.\Dipole=-0.3481583,-0.3471227,0.5033602\PG=C01 [X(C7H13
N1S1)]\\

10 (Me₂N/NO₂)



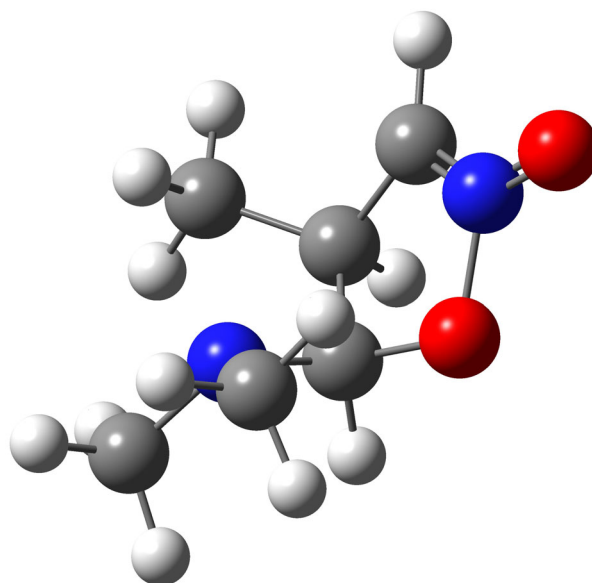
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N2O2\TSCHNEI\14-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_NO2_1\0,1\C,-0.0018103263,0.080736
1242,0.0021069891\C,0.2131821987,0.1432439261,2.645272987\C,0.82171134
53,0.1062236609,1.2619640947\H,0.460617477,0.5689228737,-0.8612989663\
H,1.7755691084,0.6102385275,1.1437338191\C,0.7243023174,-1.1701619209,
0.4544541532\H,0.1564724781,-2.0071451341,0.8331822782\H,0.1153543702,
1.174370183,2.9964323442\H,0.8435253784,-0.3903302338,3.3614930133\O,2
.6247697027,-0.7632022143,-0.801107412\H,-0.7791318374,-0.30943262,2.6
523025509\N,1.8904934812,-1.617750886,-0.3175021013\O,2.0454589517,-2.
8263471326,-0.4291005964\N,-1.4329305515,0.0565207703,0.0657786973\C,-
1.9864708546,1.4008816061,0.2098636182\H,-1.7876847632,2.0420403178,-0
.6664327434\H,-3.0685596548,1.3370353057,0.3445559671\H,-1.5634357962,
1.886773759,1.0900954099\C,-2.0208064347,-0.6522413846,-1.0677140548\H
,-3.1026652904,-0.7206077831,-0.9336712904\H,-1.8252405644,-0.15534887
81,-2.0338068908\H,-1.6218341148,-1.6668015943,-1.1206478033\\Version=
AM64L-G03RevC.02\State=1-A\HF=-495.7989854\RMSD=4.591e-09\RMSF=1.
448e-05\Thermal=0.\Dipole=-1.3230243,0.8781049,0.6385817\PG=C01 [X(C6H
12N2O2)]\\

TS₁₀₋₁₁ (Me₂N/NO₂)



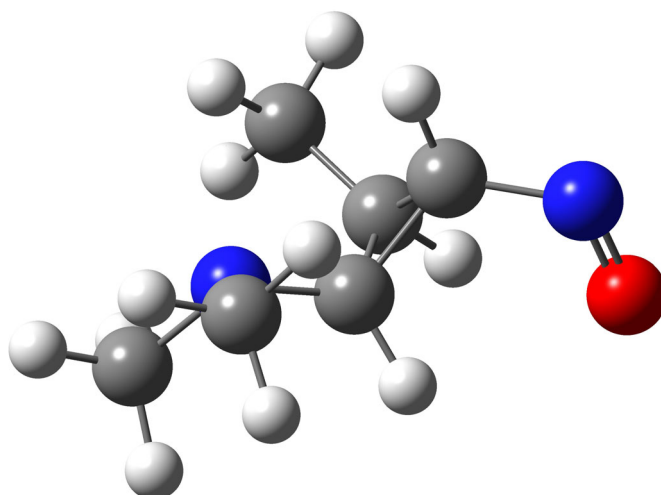
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H12N2O2\TSCHNEI\14-Jan-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight integral=
grid=ultrafine\DA_N_NO2_TS\0,1\C,-0.2233839352,0.1391926569,0.648154
6293\C,0.7901994521,-0.3328294676,2.997921539\C,0.9948405689,-0.113286
0323,1.494080078\H,1.6111487384,0.7823748716,1.3571128077\C,1.63516975
02,-1.2774184169,0.8051939799\H,1.8979806894,-2.2005117923,1.298817291
4\H,0.1948143739,0.4662150704,3.4479036627\H,1.7701484602,-0.334135783
1,3.4794750973\O,1.8698296118,0.0037763696,-1.055231984\H,0.3180592925
,-1.287672476,3.2324969152\N,2.1452389014,-1.0820118219,-0.4494445025\
O,2.8657701573,-1.9579159069,-0.9681813708\H,-0.1443454399,0.948380202
1,-0.0654457231\N,-1.3207567744,-0.5688865715,0.5441986688\C,-1.531411
0211,-1.8019140861,1.3040460647\H,-2.3660520242,-2.3492738945,0.870655
7399\H,-0.6187958581,-2.4032758795,1.2343624632\H,-1.753645184,-1.5859
599064,2.3485076783\C,-2.2767760841,-0.3050835212,-0.5368210079\H,-2.0
27624457,0.6313981515,-1.0304168505\H,-2.2360940953,-1.1146034888,-1.2
703881574\H,-3.2866649116,-0.2406890411,-0.1281461697\Version=AM64L-G
03RevC.02\State=1-A\HF=-495.7545732\RMSD=3.048e-09\RMSF=8.067e-06\Th
ermal=0.\Dipole=-3.6412758,0.4848218,1.8173627\PG=C01 [X(C6H12N2O2)]\
```

11 (Me₂N/NO₂)



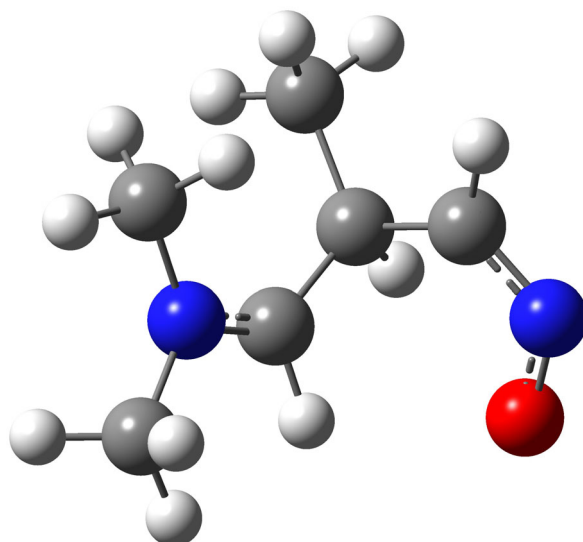
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N2O2\TSCHNEI\14-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_NO2_2\0,1\C,-0.0423851142,0.004480
0048,0.0980691424\C,0.1131617386,-0.4366682444,2.699481914\C,0.8335933
146,-0.1098668513,1.3910518702\H,1.3715330593,0.8419617689,1.512100554
9\C,1.8011618949,-1.1640397078,0.9584296653\H,2.4627863112,-1.76848491
44,1.559283737\H,-0.4967767829,0.4029974302,3.0403464272\H,0.840689047
, -0.6433335668,3.488897884\O,0.8386676638,-0.3847844125,-0.9456671891\
H,-0.5269488039,-1.3107482097,2.5791441346\N,1.8174895355,-1.330053986
8,-0.3295925795\O,2.4382287546,-2.0228362423,-1.1090073488\H,-0.300720
795,1.0520149156,-0.1164412365\N,-1.2422380153,-0.8395117076,0.1284278
572\C,-1.5389528702,-1.532899068,-1.1260846051\H,-0.7016936269,-2.1527
789217,-1.4365105683\H,-2.4010788183,-2.1818051969,-0.9569515516\H,-1.
7813939357,-0.8481118558,-1.956050542\C,-2.4010476577,-0.0779464273,0.
5812274274\H,-2.2012882241,0.4082052826,1.5367557635\H,-2.7044558753,0
.7027539209,-0.140185038\H,-3.2480802808,-0.7511537901,0.7276447325\\V
ersion=AM64L-G03RevC.02\State=1-A\HF=-495.7955919\RMSD=4.728e-09\RM
SF=1.976e-05\Thermal=0.\Dipole=-0.7900468,0.6620937,1.280749\PG=C01 [X(
C6H12N2O2)]\

10 (Me₂N/NO)



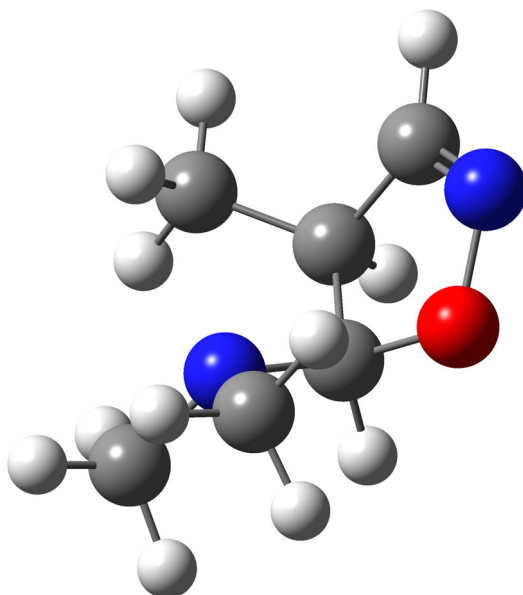
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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N2O1\TSCHNEI\26-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_NO_1\0,1\C,0.0730638569,-0.0124010
127,0.0539416057\H,0.3487004355,0.0595182385,1.1130490497\C,1.31979105
65,-0.0401633137,-0.843188455\H,1.2606176721,0.4574189273,-1.802888864
8\C,0.4554208995,-1.2847694573,-0.6148971509\H,0.9568659852,-1.9904299
755,0.0435409927\C,-0.3067100045,-1.87080986,-1.7790342118\H,-1.067935
2162,-2.5746235616,-1.4284896989\H,-0.809970734,-1.0923263293,-2.35393
49194\H,0.3639348253,-2.4181389951,-2.4464134444\N,2.6186738666,0.0663
02411,-0.240025046\O,2.7286237403,-0.4857772108,0.8389677016\N,-1.0486
275581,0.7491694658,-0.3987783254\C,-0.886292318,2.1768379857,-0.14270
59996\H,0.036809957,2.5342172496,-0.602285977\H,-1.7211450594,2.724587
1069,-0.5858708332\H,-0.8501544378,2.4188308377,0.933746708\C,-2.30761
92376,0.2411988538,0.1428125911\H,-2.3792861216,0.3555695153,1.2382925
11\H,-3.1429280609,0.7810074503,-0.3093522045\H,-2.4185231573,-0.81689
10008,-0.0967666307\Version=AM64L-G03RevC.02\State=1-A\HF=-420.563403
1\RMSD=4.147e-09\RMSF=1.269e-05\Thermal=0.\Dipole=-1.3152278,0.0125282
,-0.3901969\PG=C01 [X(C6H12N2O1)]\
```

TS₁₀₋₁₁ (Me₂N/NO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H12N2O1\TSCHNEI\27-Jun-2010\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_N_NO_TS\0,1\C,-0.0927152693,0.1075159427,-0.1052175329\C,0.221964301,-0.0121385683,2.2003529919\H,1.1772877091,-0.0380931252,2.7135552704\O,-1.8266756146,0.829189456,2.0045852338\C,-0.0171104617,-0.9073075561,0.9517455667\H,-1.048739442,-1.2599643073,1.0757501298\C,0.9507860707,-2.089013915,0.873712887\H,0.8721782916,-2.6261048231,-0.0757453717\H,1.9938665674,-1.8036818716,1.0227056119\H,0.6993552415,-2.7900798736,1.6719829925\H,-1.0647933618,0.5855013291,-0.1669709045\N,-0.7556202429,0.7001664285,2.6834804752\N,0.8628732121,0.6703466842,-0.8286933525\C,0.575305805,1.8830256542,-1.5971349066\H,1.046830793,2.751556697,-1.1265501401\H,0.9578911681,1.7798319011,-2.614899944\H,-0.4990825603,2.0476373946,-1.6369480304\C,2.2775957091,0.3179095177,-0.7065127667\H,2.6429387471,0.5673479162,0.2941270659\H,2.4330457316,-0.7430401988,-0.8913417561\H,2.8478699211,0.8840722048,-1.4407575796\Version=AM64L-G03RevC.02\State=1-A\HF=-420.5438353\RMSD=3.906e-09\RMSF=7.933e-06\Thermal=0\Dipole=2.1939716,-0.2946108,-2.7027806\PG=C01 [X(C6H12N2O1)]\

11 (Me₂N/NO)

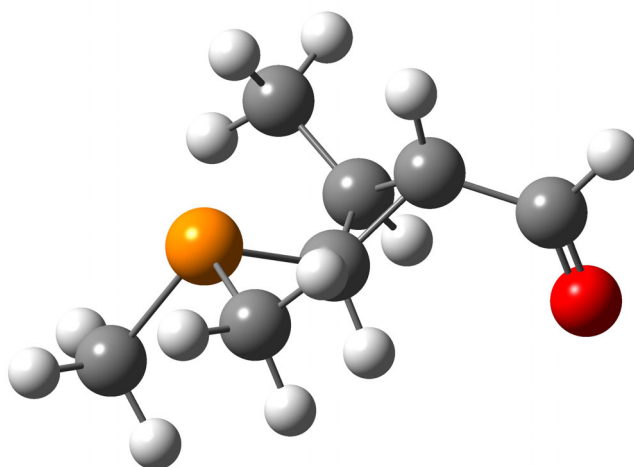


1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N2O1\TSCHNEI\26-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_NO_2\0,1\C,-0.0008225425,-0.0267204164,0.028608003\C,0.0225461373,-0.4205527824,2.6545132857\C,0.777944772,-0.0467892532,1.3770639445\H,1.2572783772,0.9317174465,1.5175907123\C,1.8579115057,-1.0293922736,1.0003737252\H,-0.6425902896,0.381123258,2.9822237381\H,0.7287533662,-0.6012958247,3.4694524779\O,0.9490071078,-0.5522802489,-0.9175697347\H,-0.5700970995,-1.3225134075,2.5019468681\H,-0.2134987258,0.9974193812,-0.3123111359\H,2.5546193196,-1.4989487637,1.6860244699\N,1.9447516305,-1.2903381051,-0.238985069\N,-1.220899673,-0.8407699267,0.03740866\C,-2.3696085031,-0.0330758326,0.432896658\H,-3.2447599105,-0.6746871504,0.5542748809\H,-2.1900783422,0.4615927792,1.3878872303\H,-2.6164349017,0.746419401,-0.3113636234\C,-1.4950543109,-1.5341972296,-1.2221045905\H,-2.3944805549,-2.1390328116,-1.08607

02428\H,-1.6682958014,-0.8471937411,-2.0683555604\H,-0.6724631974,-2.1
936059083,-1.4842879361\\Version=AM64L-G03RevC.02\State=1-A\HF=-420.60
43435\RMSD=2.847e-09\RMSF=8.381e-06\Thermal=0.\Dipole=-0.5864224,0.524
5337,1.0263384\PG=C01 [X(C6H12N2O1)]\\

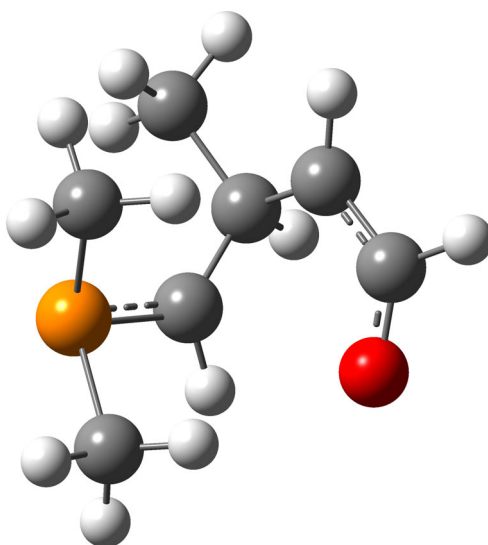
PMe₂-Donor

10 (Me₂P/CHO)



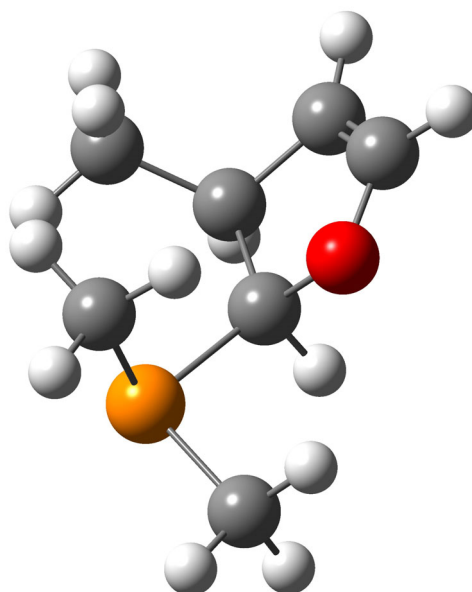
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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13O1P1\TSCHNEI\02-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_CHO_1\0,1\C,0.0788799997,-0.056182
8491,-0.1941170265\H,0.0162187818,0.0091993196,0.891132511\C,1.5318023
671,-0.1086656605,-0.6906275478\H,1.7448164444,0.3422631635,-1.6555263
11\C,2.6137280579,-0.0267131735,0.3170384333\C,0.6407191876,-1.3483213
956,-0.7003253809\H,0.8940338164,-2.0493842506,0.090865395\C,0.2422384
851,-1.9867666726,-2.0120631957\H,-0.6576997418,-2.597405717,-1.888196
4018\H,0.0343087734,-1.2438551919,-2.7841482443\H,1.0370723947,-2.6426
756968,-2.3785202947\C,-0.9457227456,2.5639490262,-0.210911684\H,-1.72
39865441,3.2634003794,-0.5257122546\H,-1.0058188844,2.4401296178,0.874
252597\H,0.0193845275,3.0115944089,-0.4575453357\C,-2.7094162065,0.340
1865682,-0.3284981986\H,-2.6550112144,0.3462372531,0.7641139104\H,-3.5
501546324,0.9657326049,-0.6384598027\H,-2.9157485238,-0.6791987561,-0.
6613827042\O,2.5246368977,-0.4328417979,1.4537822696\H,3.5582169142,0.
4409112558,-0.0360129191\P,-1.1472154845,0.9591942642,-1.1318567638\\V
ersion=AM64L-G03RevC.02\State=1-A\HF=-691.2244387\RMSD=8.626e-09\RM
SF=6.181e-06\Thermal=0.\Dipole=-0.4066385,0.1502704,-0.5729067\PG=C01
[X(C7H13O1P1)]\
```

TS₁₀₋₁₁ (Me₂P/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13O1P1\TSCHNEI\02-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_CHO_TS\0,1\C,-0.0971584826,-0.2897001263,0.0152623489\C,0
.058577357,-0.0788543674,2.2875260237\H,0.8199990947,-0.1484081894,3.0
587296452\C,-0.8987126089,0.9297573306,2.2849970737\H,-1.05738101,1.44
48377133,3.254543185\O,-1.621900318,1.2584008685,1.3164105624\C,0.0001
543111,-1.1545066883,1.2060251095\H,-0.9145753572,-1.7512910365,1.2956
219908\C,1.2059586818,-2.1006206533,1.2803130946\H,1.1745724984,-2.841
4831067,0.478972023\H,2.1555279969,-1.5660599583,1.2143295052\H,1.1901
511015,-2.6281407538,2.237323724\H,-1.0631936312,-0.2445832968,-0.4781
570914\C,0.2289124535,2.088171516,-1.4573582821\H,-0.209802399,2.61405
55777,-0.6102756358\H,0.9190302108,2.7408022999,-1.9953275568\H,-0.569
2254397,1.8024771203,-2.1441391618\C,2.4012795279,1.2287108772,0.26621
71186\H,1.914274859,1.6814266124,1.1333314866\H,3.0623822789,0.4320106
23,0.6063176737\H,3.0123459396,1.9697756191,-0.2547934564\P,1.13872544
07,0.5686276295,-0.9079222014\\Version=AM64L-G03RevC.02\State=1-A\HF=-
691.1507742\RMSD=8.216e-09\RMSF=2.842e-05\Thermal=0.\Dipole=1.1360483,
-0.2542522,-0.4216372\PG=C01 [X(C7H13O1P1)]\\
```

11 (Me₂P/CHO)

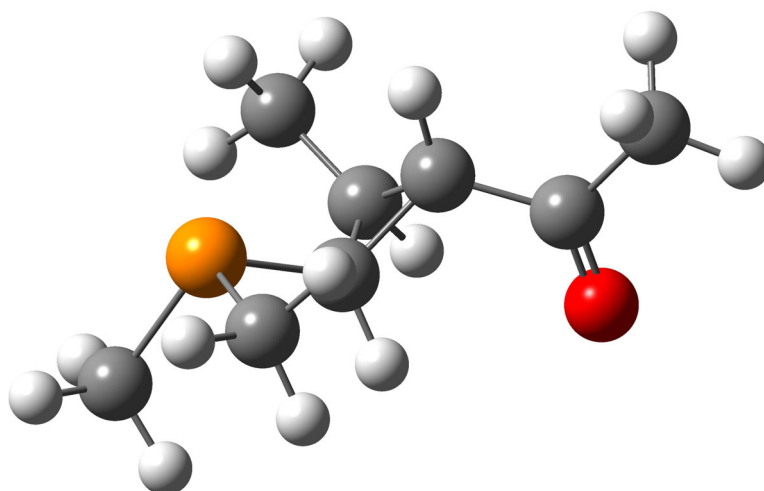


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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13O1P1\TSCHNEI\02-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_CHO_2\0,1\C,0.0394348602,0.0335150
408,0.1388109139\C,0.3358783454,-0.4472255112,2.7234971069\C,0.9203886
988,0.127274202,1.4232641031\H,1.1540720127,1.1830553682,1.5963717199\
C,2.1362291536,-0.6530692804,0.9572148016\H,3.0675360452,-0.7303847898
,1.5007435201\H,-0.5785839532,0.0748646976,3.0196196335\H,1.0568466601
,-0.3368576466,3.5387169539\C,1.8182955705,-1.3297719887,-0.1430453873
\O,0.559117169,-1.0983277923,-0.6269539678\H,0.1150091751,-1.512275450
5,2.6258171056\H,2.3908617648,-2.0480082208,-0.7155547073\H,0.25066517
06,0.9213395463,-0.4708244574\C,-2.1472239615,-1.805911083,0.651538333
5\H,-3.1894291393,-2.0267221258,0.4083283825\H,-1.4987700387,-2.454993
7688,0.060975767\H,-2.0043615304,-2.0222294564,1.7105080712\C,-2.23331
35115,0.005316154,-1.5206395874\H,-1.6826414613,-0.7589394789,-2.07260
31119\H,-3.3049323871,-0.1619981827,-1.6520581361\H,-1.9999864916,0.98
43282335,-1.9456398168\P,-1.8310052358,-0.0062842315,0.2981315122\Ver
sion=AM64L-G03RevC.02\State=1-A\HF=-691.2213266\RMSD=9.967e-09\RMS
F=1.006e-05\Thermal=0.\Dipole=0.2580502,-0.1305411,0.0247089\PG=C01 [X
(C7H13O1P1)]\

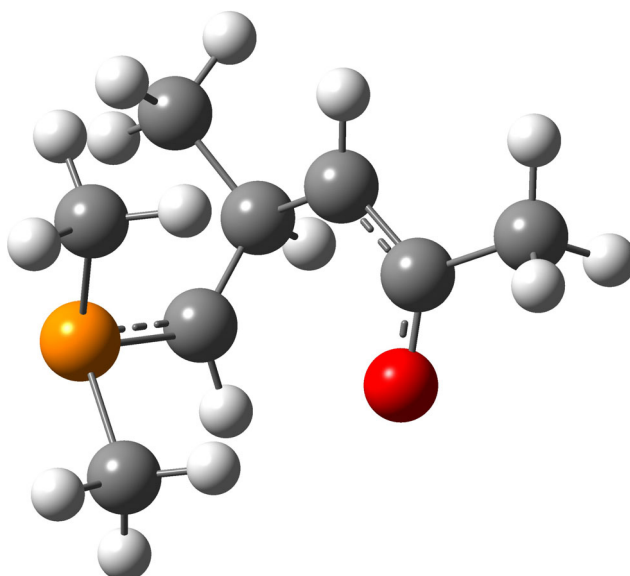
```

10 (Me₂P/COMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15O1P1\TSCHNEI\01-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_COR_1\0,1\C,-0.0200184197,-0.11252
17921,0.1813919346\C,0.2677051488,-0.0800327844,2.823633515\C,0.827683
0924,-0.081567347,1.4187100054\H,0.4126104473,0.4130232065,-0.66828374
94\H,1.7507425137,0.4781416451,1.2924856101\C,0.7923531989,-1.35060160
74,0.5781289136\H,0.2376956662,-2.1853631238,0.9970536809\H,0.01827185
25,0.9371142297,3.1420624119\H,1.0015003498,-0.4755501643,3.5321385845
\C,1.9924373224,-1.689261999,-0.2435365248\C,2.3438906521,-3.160385605
1,-0.3513369035\H,1.5164026203,-3.7191356995,-0.801163566\H,3.23954526
68,-3.2858128096,-0.9583004183\H,2.5112894898,-3.58862609,0.6424591651
\O,2.6550627832,-0.8307475792,-0.7912326306\H,-0.6386310808,-0.6828326
503,2.9046230321\C,-2.1545116074,-0.7704835361,-1.5321621311\H,-3.2235
015268,-0.7311112317,-1.7555067169\H,-1.6213042637,-0.1649071392,-2.27
09510827\H,-1.8341325628,-1.8093100076,-1.637226662\C,-2.2459804845,1.
6120531869,0.0100683888\H,-1.6974887206,2.0680407176,-0.8195430744\H,-
3.3164907839,1.7416242405,-0.1672149789\H,-1.996098204,2.1474057926,0.
9285066285\P,-1.8645279292,-0.1992980563,0.2155843327\\Version=AM64L-G
03RevC.02\State=1-A\HF=-730.5580205\RMSD=6.834e-09\RMSF=1.508e-05\Th
ermal=0.\Dipole=-0.4875924,-0.3324938,0.2605639\PG=C01 [X(C8H15O1P1)]\
```

TS₁₀₋₁₁ (Me₂P/COMe)

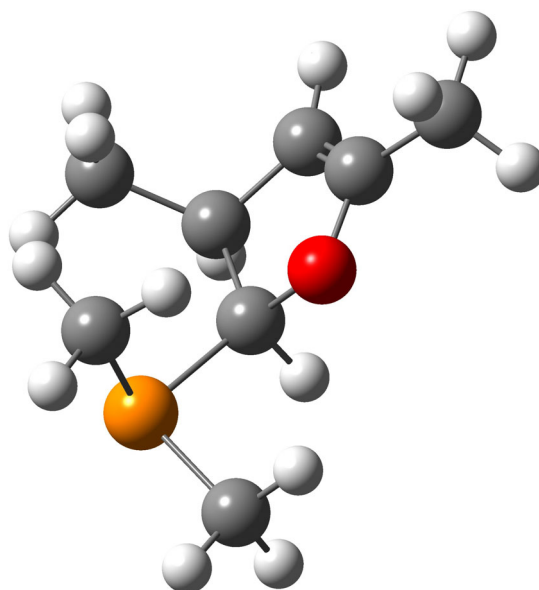


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H15O1P1\TSCHNEI\01-Jun-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_COR_TS\0,1\C,0.094370113,0.2553862277,0.1888222035\C,0.12
33636219,0.1834562822,2.7517429612\C,0.8956595691,0.2013891081,1.42638
74911\H,1.5914798356,1.0481997239,1.4419269162\C,1.6313683397,-1.10917
51404,1.1808291339\H,1.6524845113,-1.8456416446,1.9776745556\H,-0.43011
68694,1.1132117877,2.8979807727\H,0.8301267799,0.0701141753,3.57778947
16\C,2.3203743295,-1.2811541262,-0.0245448137\C,3.4558543405,-2.297443
0836,-0.0811165381\H,3.5189561268,-2.9241191426,0.8103175694\H,3.33802
31517,-2.93358136,-0.9620461594\H,4.4027524876,-1.7622409601,-0.197008
4991\O,2.0922150827,-0.5949638524,-1.0538356414\H,-0.5836027327,-0.646
7116191,2.8068985309\H,0.3907056719,0.9872501263,-0.5558869527\C,-1.44
04327571,-2.232612674,0.4552117009\H,-0.4711806373,-2.7138396513,0.303
7977252\H,-1.6583513775,-2.203356875,1.5225868885\H,-2.2309253116,-2.8
094549367,-0.0311421705\C,-1.1985519668,-0.8222258522,-2.0685554998\H,
-2.0707011464,-1.352671431,-2.4554325821\H,-1.1312547982,0.1370509394,
-2.5838924883\H,-0.2900493024,-1.3894077082,-2.2674801378\P,-1.4267240
973,-0.5274004916,-0.2517847559\\Version=AM64L-G03RevC.02\State=1-A\HF
=-730.4799293\RMSD=4.239e-09\RMSF=1.549e-05\Thermal=0.\Dipole=-0.92350
88,-0.2973171,0.4940855\PG=C01 [X(C8H15O1P1)]\\

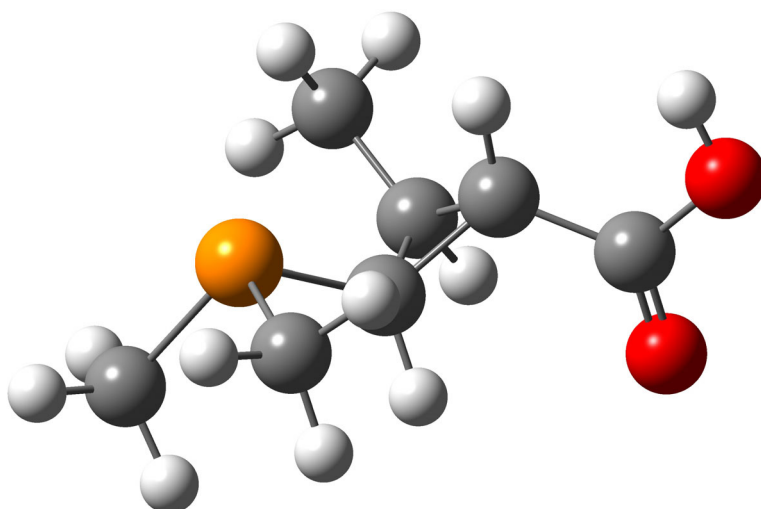
```

11 (Me₂P/COMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15O1P1\TSCHNE\01-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_COR_2\0,1\C,0.048857494,-0.0113405
073,0.134377394\C,0.3296998517,-0.4558730142,2.7268550628\C,0.9269354
385,0.0866896051,1.4179544903\H,1.17634313,1.1415251054,1.5764586934\C
,2.1257008742,-0.7206619278,0.963975074\H,3.0552701768,-0.7990287286,1
.5112745672\H,-0.5798628572,0.0819999921,3.0100740732\H,1.0494349341,-
0.3379028583,3.5421226374\C,1.8104379399,-1.4230382765,-0.1257142215\C
,2.5739061071,-2.4394562944,-0.8996715024\H,3.5589257257,-2.6038309591
, -0.4613497197\H,2.0367431957,-3.3930869459,-0.9171308844\H,2.69976107
36,-2.1223395798,-1.9394082804\O,0.5431730557,-1.1676991967,-0.6028203
818\H,0.0976963946,-1.520574741,2.6502010056\H,0.282272912,0.861404467
2,-0.4894510501\C,-2.1901933509,-1.7896093338,0.6331075247\H,-3.245985
7812,-1.9740069649,0.4196678993\H,-1.5808295839,-2.4554213905,0.019935
2827\H,-2.023365761,-2.0191996206,1.6859304887\C,-2.2170642031,0.02943
30693,-1.5347378672\H,-1.6854676136,-0.7480873154,-2.0870933994\H,-3.2
922599293,-0.1065863282,-1.6728837582\H,-1.9534291581,1.0029846241,-1.
9546816452\P,-1.8228519945,0.00079356,0.2859639346\\Version=AM64L-G03
RevC.02\State=1-A\HF=-730.553474\RMSD=9.003e-09\RMSF=3.321e-06\Therm
al=0.\Dipole=0.3451673,-0.2413316,-0.0874985\PG=C01 [X(C8H15O1P1)]\

10 (Me₂P/COOH)

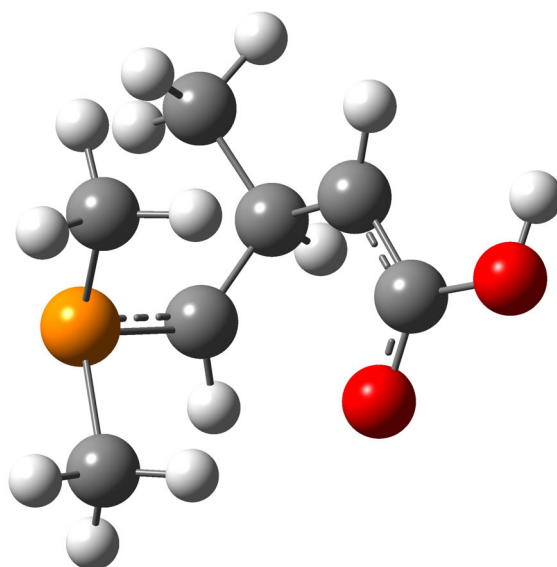


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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13O2P1\TSCHNE\01-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_COOH_1\0,1\C,-0.0126878827,-0.1216
871246,0.1746177382\C,0.2701337661,-0.0640128861,2.8188515797\C,0.8330
311425,-0.0716400042,1.4149505232\H,0.4147065595,0.4011253031,-0.67856
60664\H,1.7504336084,0.4959944249,1.2875112038\C,0.8097356892,-1.34532
82018,0.5866358814\H,0.2518843242,-2.1757468804,1.0137078738\O,2.69532
09763,-0.8503520744,-0.7873977993\H,0.011985364,0.9535862552,3.1274926
769\H,1.0065131763,-0.4467867649,3.5314321361\O,2.3245013219,-2.992089
134,-0.3299088043\C,2.01360689,-1.6700254656,-0.2336905182\H,-0.631579
3506,-0.6733398429,2.9037301435\H,1.6955463809,-3.5284930388,0.1683986
974\C,-2.1374687132,-0.7801476229,-1.5512134331\H,-1.8012410184,-1.812
0706743,-1.6733205078\H,-3.2070429638,-0.7539943423,-1.7733670779\H,-1
.6144256594,-0.1553862352,-2.2810071042\C,-2.2578579409,1.578966166,0.
0283458365\H,-3.3298687575,1.6992698709,-0.1458088197\H,-2.0130442025,
2.1023370761,0.9549414153\H,-1.7156673889,2.0538064871,-0.7946122244\P
,-1.8577743259,-0.2304764066,0.204430111\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-766.4886809\RMSD=3.031e-09\RMSF=1.721e-05\Thermal=0.\Dipole
=-1.1696235,-0.1530179,0.6771666\PG=C01 [X(C7H13O2P1)]\

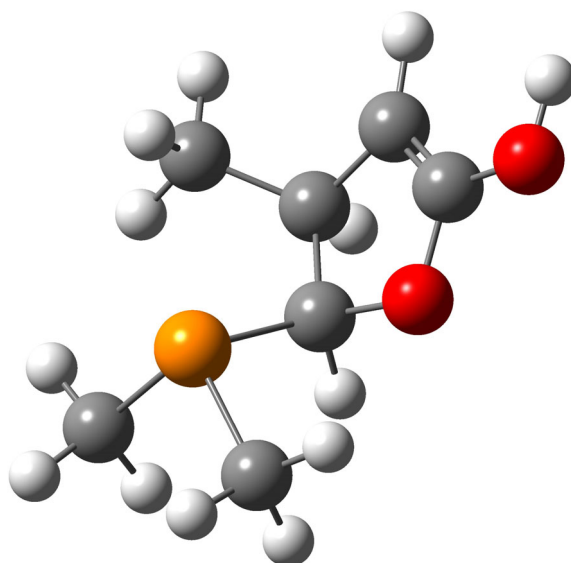
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TS₁₀₋₁₁ (Me₂P/COOH)



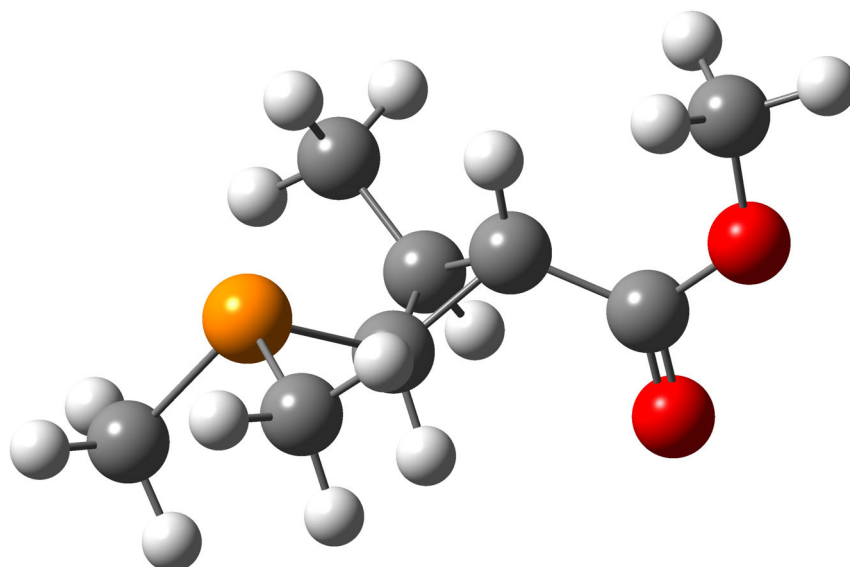
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13O2P1\TSCHNEI\02-Jun-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_COOH_TS\0,1\C,-0.1599576938,-0.0119421406,0.0474787671\C,
0.0597799309,-0.1555364144,2.5915735568\C,0.7493574185,-0.0852619227,1
.2202315388\H,1.3940778306,0.8032513181,1.2157873726\C,1.5237487791,-1
.3419394864,0.9051481475\H,1.6976683236,-2.0781457049,1.6837820363\O,1
.6294579878,-0.8073231865,-1.3783641439\H,-0.5151183414,0.7501978224,2
.7934540371\H,0.8219655288,-0.2583577102,3.3683370043\O,3.0245417334,-
2.3837224408,-0.6396683641\C,2.0213006625,-1.4732384185,-0.4027257232\
H,-0.6110935196,-1.0132131682,2.6712927918\H,3.3675577054,-2.703752273
4,0.2029000514\H,-0.0016176457,0.8046579441,-0.6516331409\P,-1.6545823
557,-0.8697480339,-0.3098363511\C,-1.5192991855,-2.6036078041,0.301404
8677\H,-0.540380401,-3.0181383104,0.0508948509\H,-1.6504409417,-2.6365
547091,1.3825775418\H,-2.3142045986,-3.2010791809,-0.1516775345\C,-1.5
967190075,-1.0334654084,-2.1541873085\H,-2.4600966376,-1.6121695974,-2
.4872938166\H,-1.6588405803,-0.042695617,-2.6065937013\H,-0.6698570201
,-1.5082230006,-2.4728188862\Version=AM64L-G03RevC.02\State=1-A\HF=-7
66.4029691\RMSD=8.053e-09\RMSF=2.115e-06\Thermal=0.\Dipole=-1.1163721,
-0.2345194,1.0569307\PG=C01 [X(C7H13O2P1)]\
```

11 (Me₂P/COOH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13O2P1\TSCHNEI\29-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_COOH_3\0,1\C,0.0289572393,0.084517
5176,0.0164628898\C,-0.0789398673,-0.464056943,2.5978040745\C,0.779350
6234,-0.0985422484,1.3808298804\H,-0.0263282965,1.1367764702,-0.274271
7974\H,1.2850991737,0.8498682952,1.6175025424\C,1.7986674144,-1.150899
5154,1.0039612771\O,0.8654579204,-0.5646157219,-0.9908143336\H,-0.7707
037448,0.3388612723,2.8665903032\H,0.5659679225,-0.6327008736,3.464914
334\O,2.4977653183,-2.0734637032,-1.1614033115\C,1.7767089763,-1.31006
53624,-0.3221572607\H,-0.6516842965,-1.3785958655,2.4291173183\H,3.160
2998179,-2.5533593576,-0.6517139807\H,2.4641427924,-1.6434451949,1.698
9661785\P,-1.6900523114,-0.6995499101,-0.1768302515\C,-2.7353260049,0.
6547326934,0.5693832676\H,-3.7691128287,0.5107027239,0.2454877457\H,-2
.7264690941,0.6040488429,1.6585828442\H,-2.4185755955,1.6559428103,0.2
592739667\C,-1.9340545494,-0.2696324167,-1.9707950156\H,-1.2327368115,
-0.8420780279,-2.5774442731\H,-2.9483196668,-0.5463210556,-2.268611580
2\H,-1.7874075614,0.7951520023,-2.1782206093\Version=AM64L-G03RevC.02
\State=1-A\HF=-766.460923\RMSD=2.537e-09\RMSF=2.402e-06\Thermal=0.\Dip
ole=0.2691156,0.2801529,0.6079191\PG=C01 [X(C7H13O2P1)]\

10 (Me₂P/COOMe)

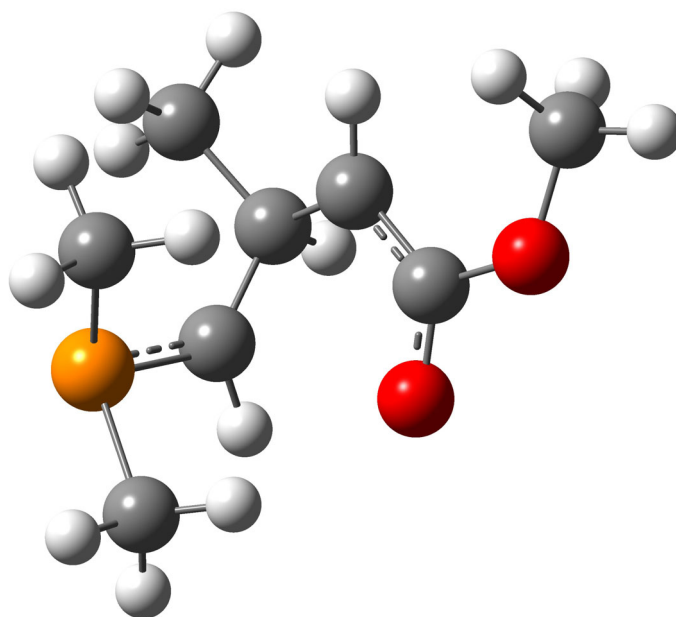


```

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15O2P1\TSCHNEI\02-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_COOR_1\0,1\C,-0.0432269373,0.03649
02836,0.0033275672\C,-0.043147653,0.0878370814,2.6631721017\C,0.664518
6258,0.0406563921,1.3269044041\H,0.5044400801,0.5314729867,-0.79579887
84\H,1.6217266806,0.5530913396,1.2989665716\C,0.6541253112,-1.23581413
17,0.4977299679\H,0.0020762924,-2.0197679989,0.8610106312\O,2.67280266
59,-0.8067976789,-0.671267539\H,-0.2745493724,1.1202557839,2.943149391
4\H,0.5908522135,-0.3310076777,3.4502275565\O,2.2554233399,-2.93345895
16,-0.2728965488\C,1.9224714363,-1.6170390011,-0.189327169\H,-0.981837
3424,-0.4694833557,2.6534602123\C,-1.9995983828,-0.4887878497,-1.94901
411\H,-1.7224221062,-1.5410653929,-2.0423374734\H,-3.03259576,-0.38864
17355,-2.2910069761\H,-1.3550057698,0.0998390547,-2.6082549106\C,-2.15
58070724,1.8675259473,-0.3689066546\H,-3.1907800479,2.0508269808,-0.66
78799348\H,-1.9933664629,2.3716999576,0.5859972894\H,-1.4930832489,2.3
140338815,-1.1159240988\P,-1.8827912326,0.0367889472,-0.1670903002\C,1
.4407958279,-3.963009854,0.2914049265\H,1.3287980184,-3.8450142923,1.3
721132167\H,0.4567559933,-4.0067399207,-0.1824558762\H,1.9717807875,-4
.8912738107,0.0897409747\Version=AM64L-G03RevC.02\State=1-A\HF=-805.7
977635\RMSD=3.871e-09\RMSF=5.712e-06\Thermal=0.\Dipole=-1.0798422,-0.4
076633,0.5373172\PG=C01 [X(C8H15O2P1)]\

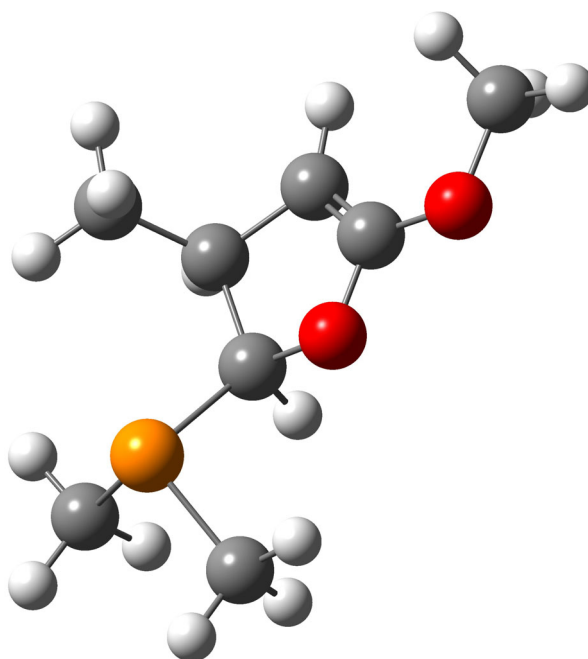
```

TS₁₀₋₁₁ (Me₂P/COOMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H15O2P1\TSCHNEI\02-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_COOR_TS\0,1\C,-0.1818832384,0.008714541,0.0584619876\C,-0
.0751911801,-0.0432230223,2.6152127475\C,0.6695531754,-0.0262124898,1.
272862359\H,1.3267313082,0.8523635344,1.262320665\C,1.4421846163,-1.30
28616239,1.0310917458\H,1.5410088854,-2.0169343264,1.838310188\O,1.698
3862739,-0.8033517447,-1.2457606554\H,-0.6486608796,0.8740570212,2.762
3379915\H,0.6532652526,-0.1266199731,3.4259881376\O,3.0259969172,-2.37
97239647,-0.4424701107\C,2.0237556583,-1.4666045737,-0.2404244534\H,-0
.7583835643,-0.8910849476,2.696715156\H,0.0263232852,0.7879867347,-0.6
690245308\P,-1.669254655,-0.8458026452,-0.3409636973\C,-1.589820346,-2
.5535647636,0.3492348111\H,-0.6077088612,-2.9929273028,0.1604142333\H,
-1.769431272,-2.5385521672,1.4238704645\H,-2.373383923,-3.1585545403,-
0.1135447387\C,-1.5103499574,-1.0950304043,-2.1703286066\H,-2.36313974
72,-1.6764784048,-2.5254041155\H,-1.5311323548,-0.1251935019,-2.669474
7506\H,-0.5752569003,-1.596036472,-2.4167984764\C,3.6076521696,-3.0444
999009,0.6714977224\H,2.9034427181,-3.7436980621,1.135983988\H,4.45309
18846,-3.6071589684,0.2768958026\H,3.9589495262,-2.333176341,1.4243188
969\Version=AM64L-G03RevC.02\State=1-A\HF=-805.7142402\RMSE=6.894e-
09\RMSEF=3.139e-06\Thermal=0.\Dipole=-1.0411151,-0.3406805,0.9404283\PG=
C01 [X(C8H15O2P1)]\
```

11 (Me₂P/COOMe)

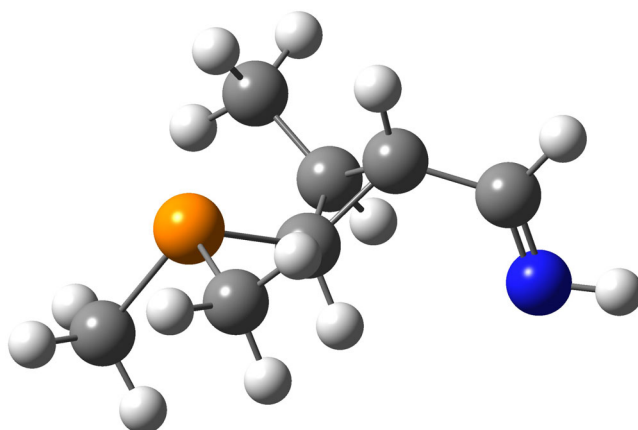


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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15O2P1\TSCHNEI\30-Jul-2010\
0\# opt freq b3lyp/6-311g(d)\DA_P_COOR_2\0,1\C,-0.0289590086,-0.02908
01296,0.002936791\C,-0.027922123,-0.0207103167,2.6340713906\C,0.786194
6258,0.000892747,1.3297759636\H,0.5392986268,0.5112046078,-0.765952984
9\H,1.4125162857,0.9000799489,1.3272413282\C,1.6035435747,-1.263849571
2,1.1467527866\O,-0.0485787354,-1.4240651887,-0.4194708762\H,-0.619899
5578,0.8897705239,2.7706967382\H,0.6468271589,-0.1051609299,3.49113351
22\O,1.2452440772,-3.2322865198,-0.279177806\C,1.0141524572,-2.0065223
548,0.1983074208\H,-0.7102160036,-0.8728525296,2.6611427527\C,-2.15067
06031,0.3600279893,-1.8072700312\H,-2.161887622,-0.7042001892,-2.04602
99695\H,-3.136318229,0.7695939511,-2.0411436798\H,-1.4069934961,0.8520
446222,-2.4416934094\C,-1.4609533511,2.403546646,0.038126577\H,-0.7081
758846,2.7066389581,-0.6963790912\H,-2.3862268133,2.943075854,-0.17736
43103\H,-1.1271744692,2.7142454176,1.0303924219\P,-1.8103634429,0.5714
649219,0.0094287516\H,2.4308272794,-1.5573725843,1.7743427529\C,2.2976
740068,-3.9510671166,0.3566190553\H,2.3391684609,-4.92060674,-0.134616
8443\H,3.2526799912,-3.431408469,0.2320285927\H,2.090002278,-4.0815485
016,1.4229073273\Version=AM64L-G03RevC.02\State=1-A\HF=-805.7782908\R
MSD=6.031e-09\RMSF=1.218e-05\Thermal=0.\Dipole=0.7808548,0.2131821,0.1
615724\PG=C01 [X(C8H15O2P1)]\

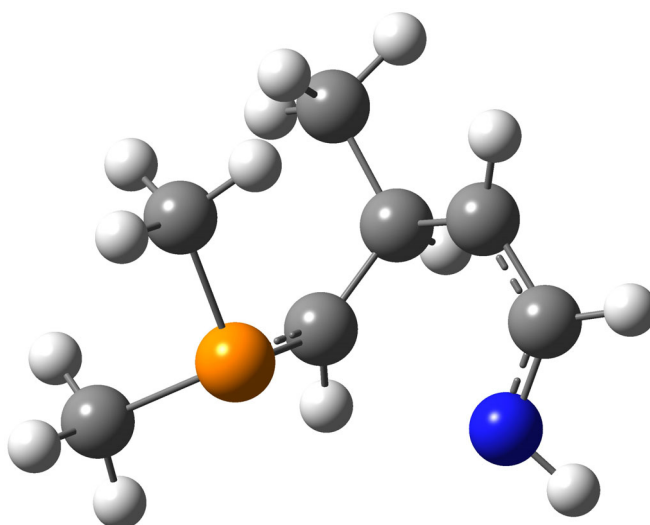
```

10 (Me₂P/CHNH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H14N1P1\TSCHNEI\30-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_P_CHNH_1_1\0,1\C,0.0124954274,-0.1212095072,0.1522279423\C,0.2232958045,-0.0240567188,2.8023944163\C,0.8248938999,-0.0378354834,1.4147067271\H,0.4527240102,0.401159493,-0.6954427953\H,1.7323274636,0.5500143912,1.3031107037\C,0.8552087155,-1.320007427,0.5957671979\H,0.3154290503,-2.1613743845,1.0210864381\H,-0.0772497869,0.9889944207,3.0890454229\H,0.9505644989,-0.3725862979,3.5419007335\C,2.0720791778,-1.6732095286,-0.1716475482\H,-0.6598424853,-0.6620626785,2.8727333912\N,2.7416674779,-0.8041485159,-0.8153681103\H,2.3543620125,-2.7350436921,-0.1333705359\C,-2.0510811848,-0.8487446123,-1.61724158\H,-1.6912404707,-1.875534451,-1.7119596946\H,-3.1142880479,-0.8461240859,-1.869996822\H,-1.5177446202,-0.225175723,-2.3407319282\C,-2.2678249102,1.5290897933,-0.0787095262\H,-1.7122341446,2.0057887146,-0.8918038281\H,-3.3369320071,1.6212558239,-0.2861356723\H,-2.0625549791,2.0711790363,0.8468753911\H,-1.8267735362,-0.2679122934,0.1374856563\H,3.5516648051,-1.227757006,-1.2673176226\\Version=AM64L-G03RevC.02\State=1-A\HF=-671.3356129\RMSD=5.748e-09\RMSF=1.315e-05\Thermal=0.\Dipole=0.1565348,-0.3539637,-0.0670338\PG=C01 [X(C7H14N1P1)]\

TS₁₀₋₁₁ (Me₂P/CHNH)



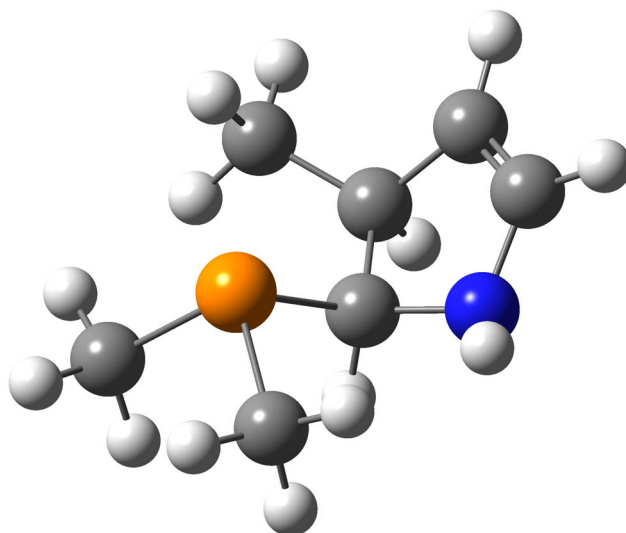
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H14N1P1\TSCHNEI\02-Feb-2010\

```

0\\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\\DA_P_CHNH_TS\\0,1\\C,0.0265438015,0.0634043068,0.0007381196\\C,-0.
0280019176,0.2105995381,2.568572287\\C,0.7888066654,0.0996843305,1.2723
761258\\H,1.4570820898,0.9689276828,1.2279864938\\C,1.6123552995,-1.1658
05744,1.210978864\\H,1.5904128762,-1.8659241825,2.0410434251\\H,-0.62030
76403,1.1280354157,2.5893938973\\H,0.662781241,0.2306371772,3.417066176
\\C,2.3803024529,-1.3935857375,0.0749938947\\H,-0.7003797439,-0.63540907
92,2.710167728\\N,2.102314107,-0.8437305362,-1.0861030691\\H,3.258491436
3,-2.0441172212,0.1905236782\\H,2.9246137549,-0.7959313814,-1.692683388
6\\H,0.2453780538,0.8419133989,-0.7248071433\\P,-1.0466838507,-1.1889973
826,-0.706933296\\C,-1.8921410541,-2.0348800316,0.7169348509\\H,-2.42145
40064,-1.3534226169,1.3850979765\\H,-2.6132465108,-2.7397702092,0.29678
89856\\H,-1.1643484191,-2.6118106664,1.2891961894\\C,-2.4168477848,-0.08
74910688,-1.3397018724\\H,-2.020740102,0.5774369153,-2.110065859\\H,-3.1
775268116,-0.7150927801,-1.8095543677\\H,-2.8875598898,0.5155992519,-0.
559935883\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-671.2487975\\RMSD=7.2
46e-09\\RMSF=6.784e-06\\Thermal=0.\\Dipole=-0.5363864,0.2845965,0.4245279
\\PG=C01 [X(C7H14N1P1)]\\

```

11 (Me₂P/CHNH)



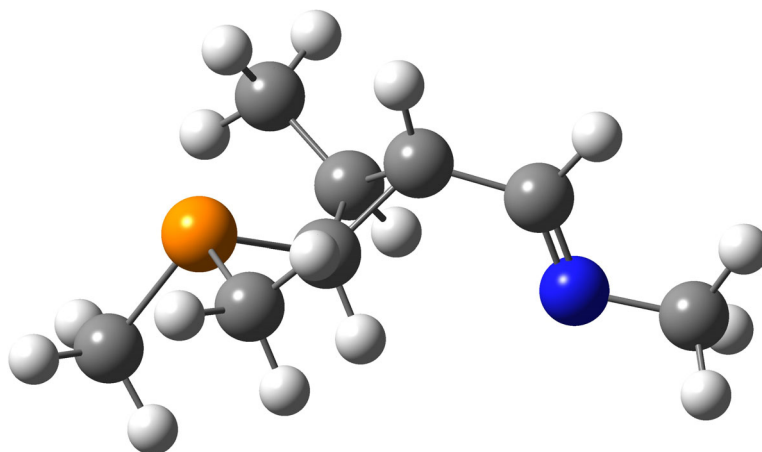
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1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H14N1P1\\TSCHNEI\\29-Jan-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_P_CHNH_2\\0,1\\C,0.112271989,-0.181974
3079,0.0162510911\\C,0.320765446,0.3218956287,2.6093314835\\C,1.01644545
34,0.0332495519,1.2774633245\\H,1.6623740532,0.8979769859,1.0530062743\\
C,1.8776672466,-1.21622245,1.2561090485\\H,2.5392386065,-1.5159648009,2
.0571318548\\H,-0.2440238938,1.2578062887,2.5818349288\\H,1.0676956056,0
.4217250226,3.4021628432\\C,1.7982030838,-1.7741939962,0.0465458601\\H,-
0.3560975879,-0.4856812459,2.8990352245\\H,-0.0686442827,0.7632705811,-
0.5060553134\\N,0.9510244828,-1.0648786997,-0.820717516\\H,0.4708560953,
-1.6106665859,-1.5229793465\\H,2.3353709348,-2.6344059622,-0.3343632037
\\C,-2.1481123878,-1.1714533355,-1.416931737\\H,-3.2227020331,-1.3692356
342,-1.4213566615\\H,-1.9614707643,-0.2806734535,-2.0259999992\\H,-1.673
9973931,-2.0324645765,-1.8938253137\\C,-2.5899724667,0.5373370476,0.756
0873783\\H,-2.3606887107,1.3789246181,0.094130986\\H,-3.6517553693,0.300
1294865,0.6529506971\\H,-2.4254372987,0.8501220133,1.7872313414\\P,-1.59

```

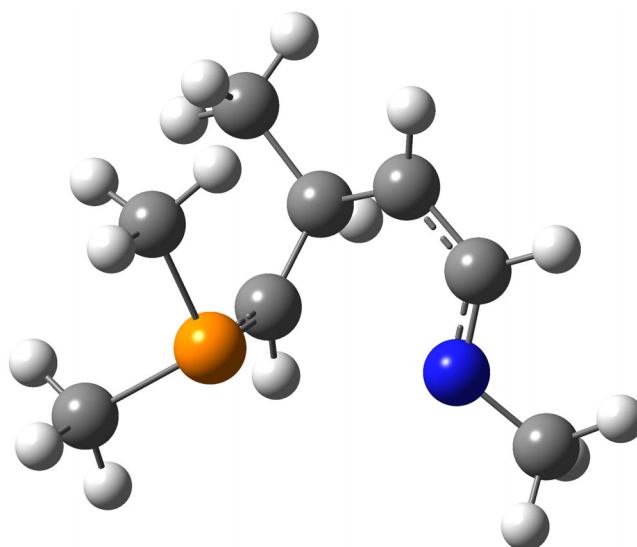
03567178,-0.9871925972,0.3583912194\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-671.3447797\\RMSD=2.044e-09\\RMSF=4.304e-06\\Thermal=0.\\Dipole=-0.2430452,0.188469,-0.3588126\\PG=C01 [X(C7H14N1P1)]\\

10 (Me₂P/CHNMe)



1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C8H16N1P1\\TSCHEI\\30-Jul-2010\\0\\# opt freq rb3lyp/6-311g(d)\\DA_P_CHNR_1\\0,1\\C,0.019230938,-0.0555324233,0.0074686893\\C,-0.019005696,-0.0729404414,2.6692266233\\C,0.7108433345,-0.0929330729,1.3444725213\\H,0.5817618815,0.4578278584,-0.7704756825\\H,1.6712164964,0.4160537993,1.3441995304\\C,0.7088908757,-1.3390950716,0.4742443397\\H,0.0575216429,-2.1419649903,0.8079920514\\H,-0.2512536217,0.9527606981,2.9739164135\\H,0.5975942369,-0.5177705502,3.456202551\\C,1.9558044056,-1.7854325159,-0.1915146637\\H,-0.9598762436,-0.6249934768,2.6271004183\\N,2.7717728229,-0.9807435207,-0.7310945209\\H,2.141521153,-2.8725304095,-0.1813323716\\C,-1.9200967084,-0.547838705,-1.9713171743\\H,-1.644928399,-1.6005051907,-2.0660508142\\H,-2.949608753,-0.4422109937,-2.3224115521\\H,-1.2668594251,0.0420168991,-2.6212357418\\C,-2.0774242262,1.7997873458,-0.3796668216\\H,-1.4070558663,2.2465084045,-1.1200576712\\H,-3.1095210601,1.9919017299,-0.6836813876\\H,-1.9170574217,2.2974162177,0.5791451336\\P,-1.8153147134,-0.0342628656,-0.1847060318\\C,3.9724669243,-1.5167974937,-1.3391083751\\H,4.0065707682,-1.2274573188,-2.3939327038\\H,4.8516120735,-1.0730838089,-0.8617702358\\H,4.0513922878,-2.6131116838,-1.2716947111\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-710.6558024\\RMSD=7.913e-09\\RMSF=2.140e-05\\Thermal=0.\\Dipole=0.209579,-0.1860034,-0.1340952\\PG=C01 [X(C8H16N1P1)]\\

TS₁₀₋₁₁ (Me₂P/CHNH)

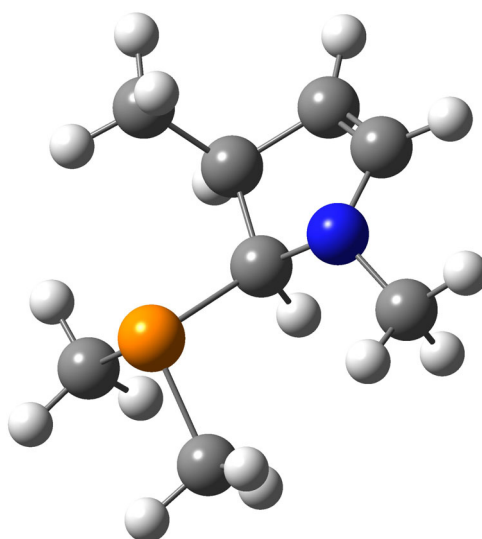


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H16N1P1\TSCHNEI\31-May-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_CHNR_TS\0,1\C,0.019375716,0.0183165766,0.0225433825\C,-0.
009023135,-0.0148515272,2.5928318402\C,0.7988515949,-0.0213323478,1.28
57252611\H,1.4458564287,0.8649783072,1.2970858427\C,1.6504284369,-1.25
72947388,1.1340369828\H,1.6540079624,-2.012222656,1.9151543665\H,-0.61
80812907,0.8875303112,2.6803373275\H,0.6876233091,-0.0402891797,3.4365
578061\C,2.4060835159,-1.4093661006,-0.0231704744\H,-0.6647858236,-0.8
812781186,2.6796125126\N,2.1330865751,-0.7890196649,-1.145129544\H,3.2
870645812,-2.0666924089,0.0316783534\H,0.2007348571,0.8591699716,-0.64
19990312\P,-1.0162559281,-1.2124255808,-0.7701588243\C,-1.78792426,-2.
2188129479,0.5889934125\H,-2.3384282272,-1.6240295144,1.3199249054\H,-
2.479620159,-2.9243488164,0.1231192317\H,-1.0189200896,-2.7999013444,1
.099807761\C,-2.4496828816,-0.1257199801,-1.2767731556\H,-2.1024802886
,0.6243072333,-1.9905627702\H,-3.1913376581,-0.7442241135,-1.787403144
9\H,-2.928742727,0.3816859519,-0.4363811797\C,3.2044922429,-0.58102942
5,-2.0972339638\H,4.0268382092,-1.3038179669,-1.9753506108\H,2.8227204
491,-0.6593064979,-3.1193833248\H,3.6433692256,0.4209091435,-1.9906231
798\Version=AM64L-G03RevC.02\State=1-A\HF=-710.5677851\RMSD=7.823e
-09\RMSF=1.069e-05\Thermal=0.\Dipole=-0.5961351,0.2760948,0.3877755\PG
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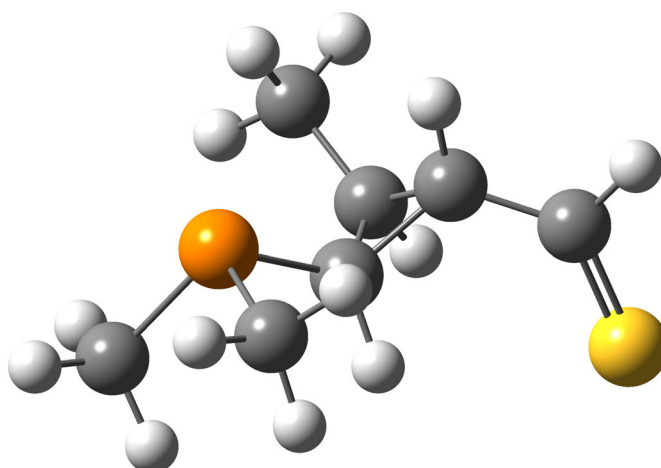
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11 (Me₂P/CHNMe)



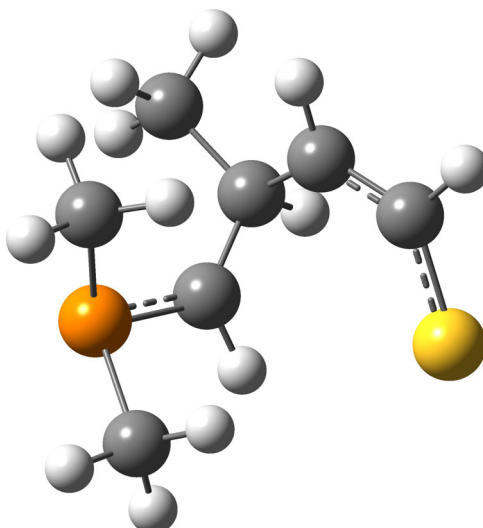
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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H16N1P1\TSCHEI\31-May-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_CHNR_2\0,1\C,0.0500215139,-0.26124
27811,0.309220662\C,0.4141482985,-1.3365596984,2.685617399\C,0.6019313
513,-0.1135273151,1.7664299253\H,0.1377075296,0.7565518034,2.241604818
1\C,2.0772041386,0.0944169764,1.4797211157\H,2.8090105812,0.3775964617
,2.2244811086\H,-0.633378721,-1.5237430368,2.9365935953\H,0.950917718,
-1.1759284863,3.6252544057\C,2.3423711591,-0.3562229767,0.2514441168\H
,0.8149607044,-2.2400266461,2.2219455681\H,-0.1589672217,0.7585548482,
-0.0659448073\N,1.204403076,-0.7980605248,-0.446118097\H,3.3089509247,
-0.4496449558,-0.2298789351\C,-2.1566124195,-0.7812833737,-1.521216631
2\H,-3.2330189821,-0.9690030579,-1.5570524016\H,-1.9849696085,0.274204
8211,-1.7549426395\H,-1.7001490082,-1.3943287051,-2.2986085631\C,-2.64
03866386,-0.1070850255,1.142156017\H,-2.5387941658,0.9352147243,0.8231
933871\H,-3.6811851834,-0.4079466832,1.0009450921\H,-2.4256196344,-0.1
662465837,2.210085105\P,-1.5439780594,-1.2697636871,0.1744990791\C,1.2
124325455,-0.6099339686,-1.8875673138\H,2.187404683,-0.9029316963,-2.2
818703904\H,0.4658539569,-1.2422491756,-2.3663943804\H,1.0225368319,0.
4366062179,-2.1806958078\\Version=AM64L-G03RevC.02\State=1-A\HF=-710.6
615158\RMSD=5.038e-09\RMSF=5.065e-06\Thermal=0.\Dipole=-0.0531464,0.52
54223,-0.3468117\PG=C01 [X(C8H16N1P1)]\
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10 (Me₂P/CHS)



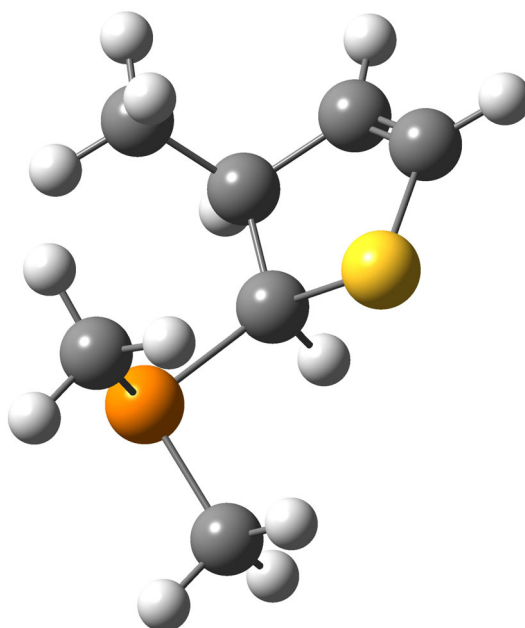
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13P1S1\TSCHNE\07-Sep-2010\0\# opt freq rb3lyp/6-311g(d)\DA_P_CHS_1\0,1\C,-0.0123764194,-0.0087302944,0.0142511317\H,-0.0171238141,-0.0027363983,1.10335847\C,1.4222207051,-0.0128435399,-0.5578838636\H,1.5474708743,0.4848440564,-1.5152474429\C,2.581339925,0.0517017275,0.3281043708\C,0.5230665273,-1.2594425916,-0.5932920267\H,0.8289344606,-2.0049239243,0.1365514076\C,0.0726677304,-1.8172147606,-1.9241424718\H,-0.8186161565,-2.4401303757,-1.7969757808\H,-0.1735730581,-1.0301723228,-2.6390336529\H,0.8530786861,-2.44458596,-2.3634677793\C,-1.0567789249,2.5968631128,0.2264288545\H,-1.8449383222,3.3135889569,-0.016650526\H,-1.0863819646,2.396873543,1.3013989421\H,-0.0997282415,3.0643348104,-0.0144400221\C,-2.8044443215,0.3637450736,0.0090669733\H,-2.7119929958,0.292022407,1.0965711664\H,-3.6625953249,0.9981534218,-0.2260070366\H,-3.0108718403,-0.6315739935,-0.389860235\H,3.4503489869,0.5513480261,-0.1054087482\P,-1.2803540686,1.0626126239,-0.801921697\S,2.7132354788,-0.5345638155,1.8518155091\\Version=AM64L-G03RevC.02\State=1-A\HF=-1014.1860966\RMSD=5.554e-09\RMSF=7.379e-05\Thermal=0.\Dipole=-0.7178732,0.14826,-0.6629937\PG=C01 [X(C7H13P1S1)]\

TS₁₀₋₁₁ (Me₂P/CHS)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13P1S1\TSCHNEI\07-Sep-2010\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_P_CHS_TS\0,1\C,-0.0382965577,0.0617142822,0.0166924163\C,0.0086602963,0.0378152614,2.3058381145\H,0.8641481846,0.1961677149,2.9599335525\C,-1.1976270907,0.6094713479,2.6164370429\H,-1.2750023392,0.9876257196,3.6389557245\C,0.2333626901,-0.8894668234,1.11154263\H,-0.5396591653,-1.663983079,1.1063364272\C,1.6148928306,-1.5510224368,1.1413269263\H,1.7648426205,-2.1830435181,0.2635974988\H,2.4262602454,-0.8205493297,1.1740449622\H,1.6981871738,-2.1764669997,2.0336350555\H,-0.9915065463,-0.0470783829,-0.4916226634\C,-0.1982405351,2.5983783218,-1.2456654777\H,-0.6994509314,3.0370557433,-0.3826205965\H,0.3457594976,3.3714153463,-1.7912433209\H,-0.9521812695,2.1802562153,-1.9138860134\C,2.0363069889,2.0796097725,0.5396333237\H,1.4276366608,2.3829271707,1.3943393109\H,2.8224444583,1.4061245619,0.8795414078\H,2.5153800517,2.9552363257,0.0961454318\P,0.9875074032,1.2677366125,-0.7453745979\S,-2.5954385837,0.7573124695,1.6643771839\Version=AM64L-G03RevC.02\State=1-A\HF=-1014.1309454\RMSD=2.809e-09\RMSF=8.408e-06\Thermal=0\Dipole=2.1006742,0.2805991,-0.8083808\PG=C01 [X(C7H13P1S1)]\

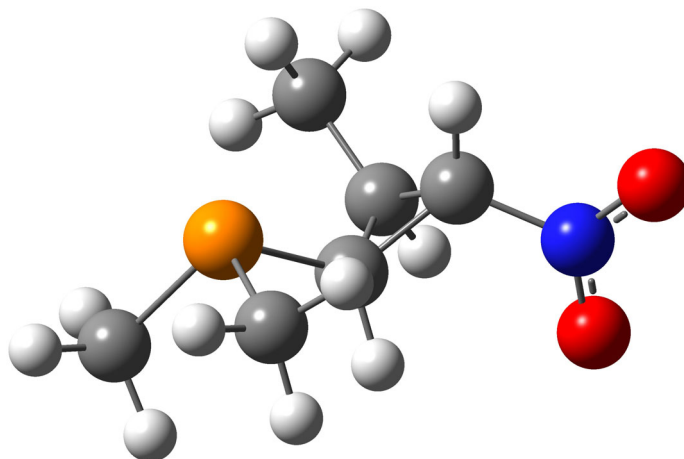
11 (Me₂P/CHS)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13P1S1\TSCHNEI\07-Sep-2010\0\# opt freq rb3lyp/6-311g(d)\DA_P_CHS_2\0,1\C,-0.1454113257,0.0649533945,0.1198794123\C,0.4380901729,0.2106208738,2.6705905902\C,0.9343127489,-0.0344383848,1.2350524054\H,1.6996863789,0.7170127335,1.0101278128\C,1.4984444797,-1.4353436202,1.112121624\H,2.4475661288,-1.7039929256,1.5646085151\H,0.0570208246,1.2281481896,2.7943278695\H,1.2602486005,0.0802032741,3.3794832262\C,0.6957224588,-2.323735623,0.5279745249\H,-0.348465731,-0.4967404931,2.9433799487\H,0.8794385598,-3.3854650372,0.4181168942\H,0.3910866764,0.2577278696,-0.8147966722\C,-2.7404002194,0.8380535669,1.29710996\H,-3.5746931447,1.541523396,1.2323424902\H,-3.0887373335,-0.1506429723,0.9912981162\H,-2.4322885854,0.7905159598,2.3419614734\C,-2.1625154193,1.3387278215,-1.4331043384\H,-2.5903976143,0

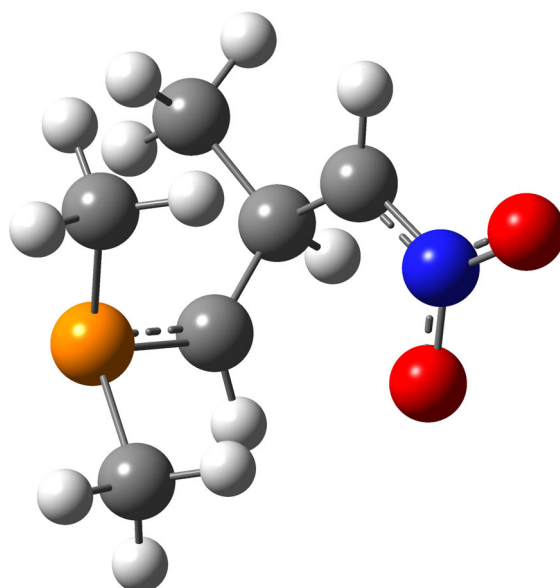
.3509498756,-1.6226797573\H,-2.9596808047,2.0819822646,-1.5096681812\H
 ,-1.4337400143,1.5591430499,-2.2162758662\P,-1.3576619263,1.4897528182,
 0.23876184\S,-0.8275378842,-1.6655682829,-0.1019523928\\Version=AM64L-G
 03RevC.02\State=1-A\HF=-1014.2051243\RMSD=7.171e-09\RMSF=5.171e-06\
 Thermal=0.\Dipole=0.1670083,0.0419617,0.1230532\PG=C01 [X(C7H13P1S1)]\\

10 (Me₂P/NO₂)



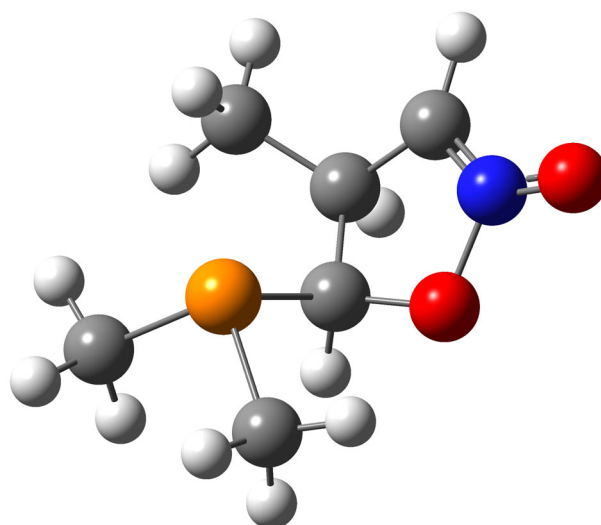
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N1O2P1\TSCHNEI\03-Jun-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_P_NO2_1\0,1\C,-0.0091663506,-0.120
 4483208,0.1853879772\C,0.2733427999,-0.0629704851,2.8413916335\C,0.835
 6709322,-0.0648227715,1.4371815913\H,0.4294088351,0.4027899342,-0.6612
 929333\H,1.7520707865,0.5023191885,1.3040211661\C,0.8020795189,-1.3272
 785532,0.6152042538\H,0.3178871453,-2.2171735171,0.9924846682\H,0.0081
 223419,0.9532044233,3.1473071612\H,1.0133577098,-0.440864457,3.5519221
 692\O,2.6415576632,-0.7789199429,-0.6902076727\H,-0.6235909969,-0.6787
 643682,2.9262838805\N,1.9918031068,-1.6838717405,-0.1807319247\O,2.248
 2899917,-2.8757780651,-0.2734833171\C,-2.2559567949,1.5649843757,0.003
 0597281\H,-1.7119275228,2.0335434692,-0.8221344369\H,-3.3274452326,1.6
 810834175,-0.176579809\H,-2.017139374,2.0971855189,0.9261572226\C,-2.1
 103705795,-0.8126362341,-1.5541775759\H,-3.1778803841,-0.8002574951,-1
 .7868380274\H,-1.5873702397,-0.1900846656,-2.2859170755\H,-1.763020281
 3,-1.8425519701,-1.6601434254\P,-1.8579633145,-0.2424018599,0.19763024
 \\Version=AM64L-G03RevC.02\State=1-A\HF=-782.4316448\RMSD=2.440e-09\
 RMSF=3.614e-05\Thermal=0.\Dipole=-1.1331844,0.8985514,0.4726042\PG=C01
 [X(C6H12N1O2P1)]\\

TS₁₀₋₁₁ (Me₂P/NO₂)



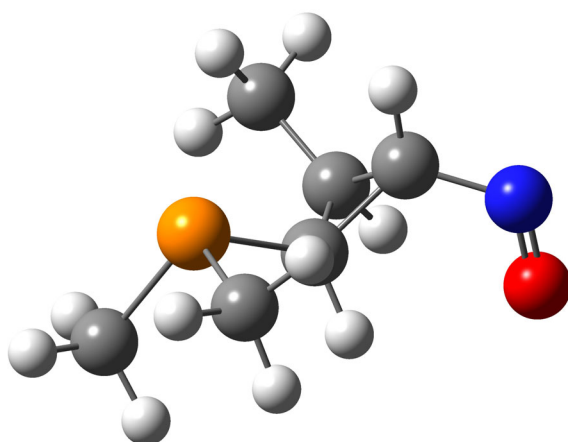
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H12N1O2P1\TSCHNEI\03-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_NO2_TS\0,1\C,-0.066651586,0.2610659116,0.2275170785\C,0
.2333241005,0.1789586276,2.7804849607\C,0.8677834575,0.1705542421,1.38
37897397\H,1.5821603206,0.9991543626,1.3155770534\C,1.5199086754,-1.13
79495146,1.0741918363\H,1.6316323033,-1.9456949698,1.7820037567\H,-0.2
752267359,1.125462881,2.9710362486\H,1.0160399526,0.0511711887,3.53197
80137\O,1.9036901266,-0.4455988953,-1.0577741802\H,-0.4886929898,-0.62
89751312,2.9129725329\N,2.1299849969,-1.3039899964,-0.1384144221\O,2.8
986104008,-2.2644753637,-0.322563608\H,0.1421049625,1.0290349475,-0.51
07090576\P,-1.5980953055,-0.5300361706,-0.0952170205\C,-1.5877954554,-
2.2278824078,0.6176482878\H,-0.6639819185,-2.7484708824,0.3556294444\H
,-1.6789821703,-2.1878313535,1.7025570763\H,-2.4488354984,-2.777091113
5,0.2300019912\C,-1.5587277238,-0.798294463,-1.9271654121\H,-2.4850060
168,-1.2862130922,-2.2347806507\H,-1.4988749059,0.1659665853,-2.433374
0867\H,-0.7002332363,-1.4027568248,-2.2193402635\\Version=AM64L-G03Re
vC.02\State=1-A\HF=-782.3516301\RMSD=7.183e-09\RMSF=1.740e-05\Therm
al=0.\Dipole=-2.3334245,0.5223879,0.8870347\PG=C01 [X(C6H12N1O2P1)]\\
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11 (Me₂P/NO₂)



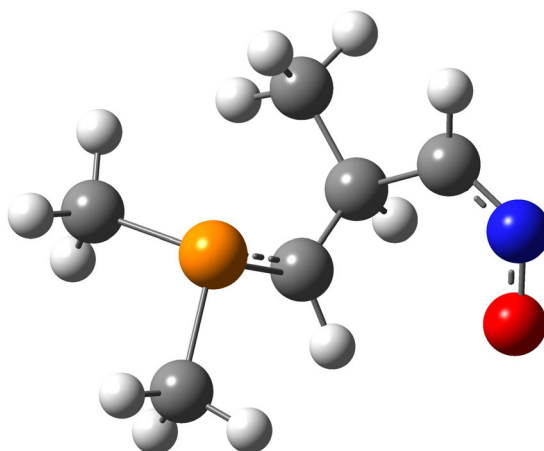
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N1O2P1\TSCHNEI\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_NO2_2\0,1\C,0.1128696089,-0.2751
747015,0.0529743287\C,0.1831714519,0.2326369162,2.6370688784\C,0.95036
36814,0.0070294231,1.3322121053\H,1.5619073879,0.903535574,1.144971545
9\C,1.843391631,-1.1922523485,1.3357906278\H,2.4782325594,-1.564327423
4,2.1246531933\H,-0.4387311702,1.1285885116,2.5766383997\H,0.882253950
3,0.3811886123,3.4641329489\O,0.9651437455,-1.1053308779,-0.758794447\
H,-0.4526344967,-0.6191368893,2.8868428347\N,1.8808022584,-1.793002823
4,0.1817354197\O,2.4940539846,-2.7331987453,-0.2781005975\H,-0.0533210
82,0.6403548142,-0.5226106786\C,-1.8980446266,-1.4538361788,-1.5245951
4\H,-1.1680854849,-2.145250013,-1.9451061167\H,-2.8897290507,-1.900232
6469,-1.6286406579\H,-1.8714138667,-0.5236529427,-2.1007999035\C,-2.66
62232006,0.2435971817,0.6035183598\H,-2.6055319344,0.5668199342,1.6434
336956\H,-2.4592423685,1.1007447363,-0.0455505454\H,-3.6953636734,-0.0
7649405,0.4231683577\P,-1.5344353767,-1.2043609882,0.2813576474\Versi
on=AM64L-G03RevC.02\State=1-A\HF=-782.4236992\RMSD=6.971e-09\RMSF
=8.660e-06\Thermal=0.\Dipole=-0.7327048,1.4465306,0.8252122\PG=C01 [X(C
6H12N1O2P1)]\

10 (Me₂P/NO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N1O1P1\TSCHNEI\27-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_P_NO_1\0,1C,0.1053843971,-0.09131
47573,-0.1487129078\H,0.2908712418,0.0268361339,0.9190308976\C,1.42495
5946,-0.1565616724,-0.9267314966\H,1.4786519794,0.2603030972,-1.925282
3897\C,0.5685394364,-1.4006934911,-0.6994332221\H,1.0133424534,-2.0494
684862,0.0524047886\C,-0.0710645752,-2.1074105714,-1.8717802327\H,-0.9
082641328,-2.726914205,-1.5349937961\H,-0.4566475364,-1.4065110431,-2.
614075897\H,0.6490998508,-2.7652582417,-2.3653921142\N,2.6803312827,-0
.0227540494,-0.2219084624\O,2.6710976871,-0.419075024,0.9248727811\C,-
0.9187647319,2.5246944549,-0.0597549053\H,-0.0228330504,2.9552621362,-
0.5117848452\H,-1.745676333,3.2149883494,-0.2428941941\H,-0.762189964,
2.4459875533,1.0198058986\C,-2.6506193796,0.2950540338,0.2803015801\H,
-2.3725252506,0.3499226569,1.3367310134\H,-3.5445741694,0.9036437206,0
.1235563749\H,-2.9089184741,-0.7384249016,0.0403216587\P,-1.2968830144
,0.8860194717,-0.8545594679\\Version=AM64L-G03RevC.02\State=1-A\HF=-70
7.1955906\RMSD=5.363e-09\RMSF=6.056e-06\Thermal=0.\Dipole=-1.0583566,-
0.1036615,-0.2046958\PG=C01 [X(C6H12N1O1P1)]\\
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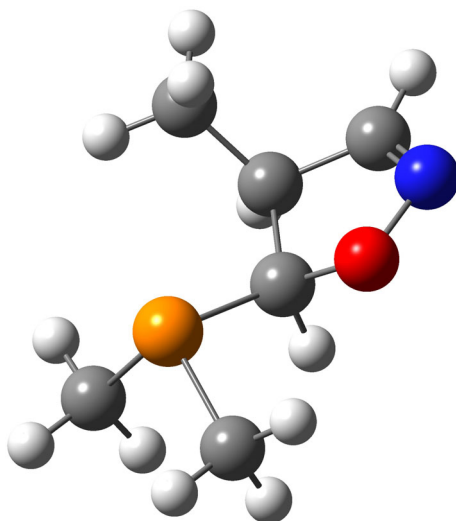
TS₁₀₋₁₁ (Me₂P/NO)



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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H12N1O1P1\TSCHNEI\27-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_P_NO_TS\0,1C,-0.0145902429,0.1214736483,0.1608116623\C,-
0.1543102167,-0.1724144673,2.5168244539\H,0.6812653316,-0.2490892919,3
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.2008556655\O,-2.0688092167,0.9047467352,2.016813614\C,-0.0836301736,-
0.9604860527,1.1149391487\H,-1.0499408385,-1.4701244809,1.0437351412\C
,1.0753473958,-1.9550034408,1.2008783027\H,1.164515426,-2.5315226617,0
.2783969139\H,2.0298736447,-1.4533385657,1.3826257055\H,0.9078898441,-
2.6536406793,2.0235274455\H,-0.9726014075,0.5478850216,-0.120461461\N,
-1.1870166923,0.514300724,2.8005066516\C,0.6842298059,2.2725834959,-1.
4908876826\H,-0.0142295862,2.9329287205,-0.9735718495\H,1.469524374,2.
8950263531,-1.9246486208\H,0.155271114,1.7607579121,-2.2987288964\C,2.
3889696339,-0.0270014955,-1.4183022534\H,2.864510325,-0.8337986447,-0.
8613388969\H,1.7590817684,-0.4548905287,-2.2008616605\H,3.1798294678,0
.5661052808,-1.8837519195\P,1.4398691161,1.1001766518,-0.2661346481\\
Version=AM64L-G03RevC.02\State=1-A\HF=-707.1468768\RMSD=6.262e-09\RM
SF=1.867e-05\Thermal=0.\Dipole=1.3235394,-0.7079787,-1.2413734\PG=C01 [X
(C6H12N1O1P1)]\\

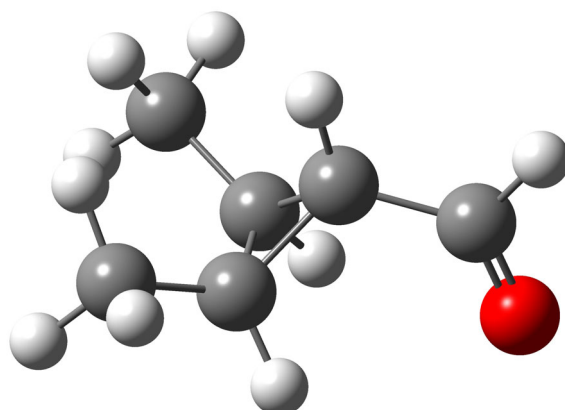
11 (Me₂P/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H12N1O1P1\TSCHNEI\27-Jun-2010\
0\\# opt freq rb3lyp/6-311g(d)\DA_P_NO_2\\0,1\C,-0.2384156101,-0.4780
850626,0.2110599927\C,0.4989230153,-0.8585026426,2.7149883499\C,0.6163
296239,-0.0373066304,1.4189069071\H,0.4342736556,1.0172351796,1.644917
1695\C,1.9765155038,-0.2386167347,0.7861946125\H,-0.4789486917,-0.7284
633562,3.1847654078\H,1.2558025178,-0.5375813453,3.4363456442\O,0.6590
802561,-1.2991779279,-0.5877035322\H,0.6405403552,-1.9235892692,2.5248
808632\H,-0.4799704457,0.4058702171,-0.3965063992\H,2.9223730549,0.097
0354915,1.1965494401\N,1.9829482202,-0.9589701858,-0.2630487942\C,-2.9
277320223,-0.1013518713,1.0084813727\H,-3.9549214804,-0.4734397773,1.0
240440942\H,-2.6939221635,0.2446998476,2.0178397556\H,-2.8825577327,0.
7518901978,0.3247621129\C,-2.3089710402,-1.6903513088,-1.2612813146\H,
-3.2865962271,-2.1766698711,-1.2997103865\H,-2.3697916801,-0.737136811
6,-1.7950890598\H,-1.59083016,-2.3311055034,-1.7741643837\P,-1.7911206
597,-1.4949938459,0.5138993882\\Version=AM64L-G03RevC.02\State=1-A\HF=
-707.2350376\RMSD=7.068e-09\RMSF=7.359e-06\Thermal=0.\Dipole=-0.603167
2,1.0199583,0.7777145\PG=C01 [X(C6H12N1O1P1)]\\

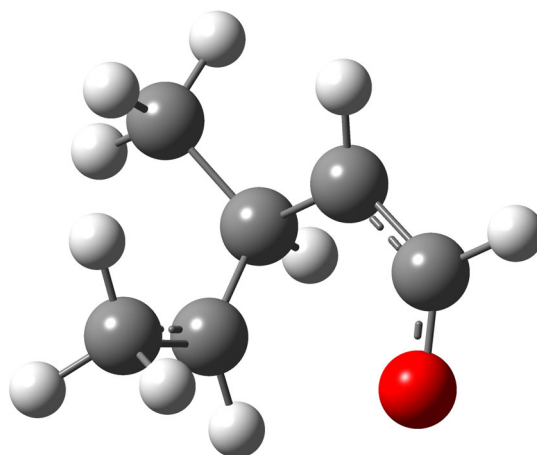
Me-Donor

10 (Me/CHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1\TSCHNEI\09-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHO_1\0,1C,-0.0434397804,-0.017158
1572,-0.0621094503\H,-0.0148544416,-0.0214089224,1.0242625381\C,1.3626
908731,0.0037788137,-0.6764801984\H,1.4758804357,0.529031203,-1.620593
9046\C,2.5260258809,0.0463347469,0.2328918251\C,0.4915697324,-1.259395
8799,-0.6887380221\H,0.8381626431,-2.0016475177,0.0253827781\C,-0.0105
942084,-1.8266745182,-1.9970798128\H,-0.9005295589,-2.4435314286,-1.83
68204848\H,-0.2744332076,-1.0497163393,-2.7176149932\H,0.7500575508,-2
.4600422038,-2.4621509597\O,2.5662941034,-0.4863378544,1.3200148744\H,
3.4049677538,0.6155915536,-0.1410001525\C,-1.1500441608,0.819968773,-0
.6623887783\H,-2.1315450503,0.4158368224,-0.3948716824\H,-1.1041799496
,1.8473621592,-0.2903205647\H,-1.0987027154,0.8642391718,-1.7522871374
\\Version=AM64L-G03RevC.02\State=1-A\HF=-309.9224252\RMSD=3.715e-09\
RMSF=1.292e-05\Thermal=0.\Dipole=-0.5515957,0.2611771,-0.9859529\PG=C
01 [X(C6H10O1)]\
```

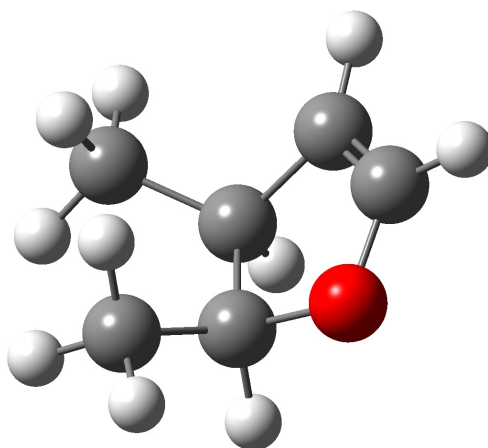
TS₁₀₋₁₁ (Me/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O1\TSCHNEI\09-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) geom=connectivity
int=ultrafine scf=tight\DA_Me_CHO_TS\0,1C,0.085705371,-0.0888880255,-
```

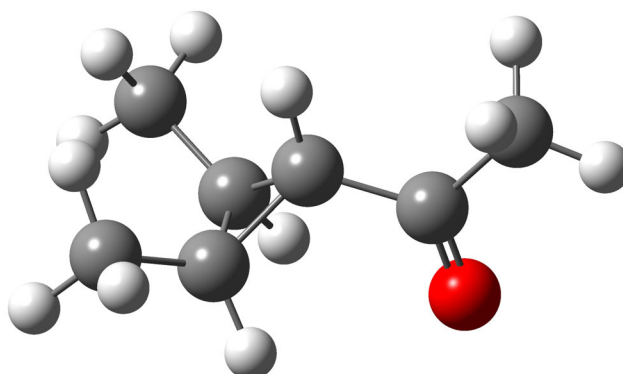
0.0156771795\C,0.0704237692,0.039108339,2.2128627459\H,0.8345414683,0.0719993165,2.9842112742\C,-0.9678549038,0.9623798435,2.1581787104\H,-1.2471348876,1.4411254459,3.1169731682\O,-1.6275738154,1.2499029588,1.1345306354\C,0.1903771387,-1.0135725392,1.1079966082\H,-0.6566414885,-1.7060452407,1.1145236642\C,1.5001959219,-1.8011505267,1.2433243001\H,1.6022353396,-2.5372277701,0.4432888643\H,2.3756502184,-1.1487786934,1.2249232401\H,1.5009395586,-2.3305623154,2.1992386658\H,-0.8239920184,-0.0973618883,-0.6030001597\C,1.110176397,0.8849069959,-0.453349731\H,1.3720866961,0.6910536311,-1.5033828657\H,0.6818700314,1.8938561866,-0.4343913744\H,2.0140247959,0.8792866508,0.1544627057\\Version=AM64L-G03RevC.02\State=1-A\HF=-309.8452821\RMSD=7.591e-09\RMSF=8.652e-06\Thermal=0.\Dipole=1.1356511,-0.6664248,-0.4045311\PG=C01 [X(C6H10O1)]\\

11 (Me/CHO)



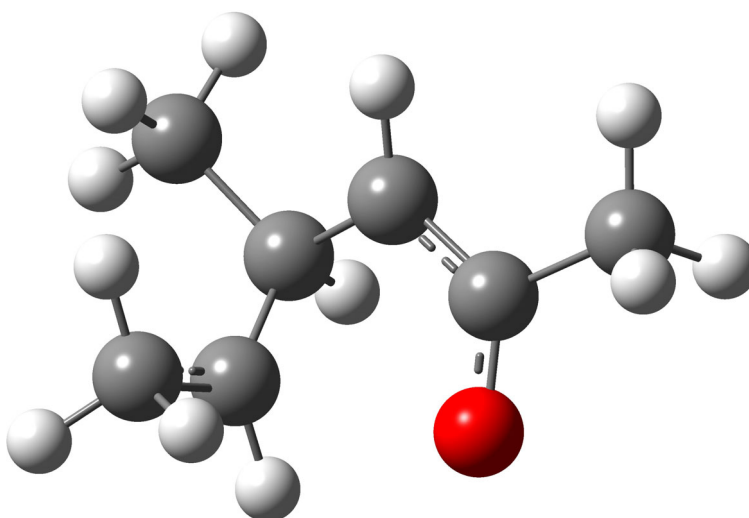
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O1\TSCHNEI\04-Jan-2011\0\# opt freq rb3lyp/6-311g(d) iop(1/7=600)\DA_Me_CHO_2\0,1\C,-0.0392439327,0.1266761986,0.1017814701\C,0.133203985,-0.0452078836,2.3632871068\C,1.3719484481,-0.3164025997,1.9634804304\C,1.3924479953,-0.4046624876,0.4504952699\H,-0.2720918101,0.0580368423,3.3615839047\H,2.2230074631,-0.494306421,2.6059620209\H,1.4506917623,-1.4611553016,0.1521940947\H,-0.5654019773,-0.57100314,-0.5529868038\O,-0.7822734106,0.1242711379,1.36619908\C,2.5662633699,0.320498867,-0.2181287165\H,3.5110923886,-0.129968866,0.0985349024\H,2.5227729924,0.2462537902,-1.3088286071\H,2.6008960964,1.3783024631,0.0510150416\C,-0.1258302794,1.5338431814,-0.472216206\H,0.3531697324,1.5964011863,-1.4528000923\H,-1.1743528954,1.8162436598,-0.5875352955\H,0.3475655822,2.2618957305,0.19065507\\Version=AM64L-G03RevC.02\State=1-A\HF=-309.92448\RMSD=3.756e-09\RMSF=1.220e-05\Thermal=0.\Dipole=0.3837202,-0.0202384,-0.2319065\PG=C01 [X(C6H10O1)]\\

10 (Me/COMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O1\TSCHNEI\09-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_COR_1\0,1C,-0.0427094894,-0.010994
6425,-0.0596535791\H,-0.007507492,-0.0272305895,1.0263485816\C,1.35431
79382,0.0333845039,-0.6832083425\H,1.4425163847,0.5635535925,-1.627356
1087\C,2.5322652954,0.0882564913,0.2267014901\C,0.5090076335,-1.242418
0317,-0.6996092058\H,0.8685634912,-1.9825682019,0.0101830976\C,0.00335
93772,-1.8124501861,-2.0056230286\H,-0.8714715526,-2.4493187213,-1.840
1443715\H,-0.2853816074,-1.0378162721,-2.719436273\H,0.7716111324,-2.4
271966876,-2.4836702071\O,2.53328594,-0.4720006529,1.3057536676\C,-1.1
711108725,0.8089706152,-0.6433123103\H,-2.1427706207,0.3880046545,-0.3
658731257\H,-1.1386545329,1.8359153167,-0.2678333858\H,-1.1348854144,0
.8591274702,-1.7337855174\C,3.7317757598,0.8789763068,-0.2609400836\H,
4.1017599699,0.4700468685,-1.2071248659\H,3.4522021265,1.9201332885,-0
.4537843432\H,4.5259576157,0.847746652,0.4838977002\Version=AM64L-G0
3RevC.02\State=1-A\HF=-349.2557215\RMSE=2.664e-09\RMSE=2.101e-06\Th
ermal=0\Dipole=-0.2974288,0.3882901,-1.0036988\PG=C01 [X(C7H12O1)]\
```

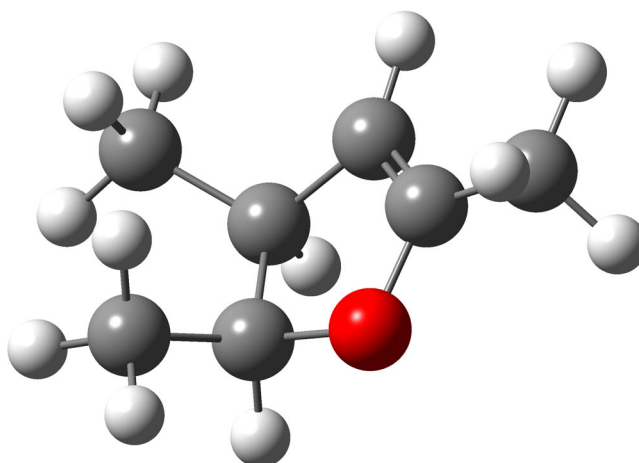
TS₁₀₋₁₁ (Me/COMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O1\TSCHNEI\09-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=ti
ght\DA_Me_COR_TS\0,1C,0.0509241521,-0.1138773315,0.0283785414\C,0.1
563503569,0.0320775509,2.2460486708\H,0.9714183124,0.0972137116,2.9601
```

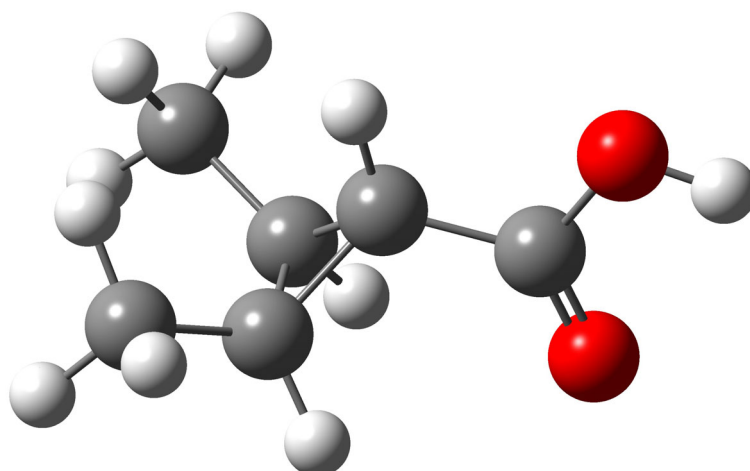
148522\O,-0.9382562752,0.9025959799,2.2658380304\O,-1.656954914,1.1113
605764,1.2560105886\C,0.2469392384,-1.0269061037,1.1498507218\H,-0.576
8127825,-1.7451024616,1.2057178509\C,1.5856706873,-1.7727359387,1.2144
790812\H,1.6650060668,-2.5126582701,0.4152561836\H,2.4378879191,-1.093
8181073,1.1405500571\H,1.6583858542,-2.2929089604,2.1728774471\H,-0.88
26067928,-0.1626406911,-0.5175766239\C,1.0169822826,0.8926888765,-0.46
50099466\H,1.2357352273,0.6981347288,-1.5248961437\H,0.5540366797,1.88
5937665,-0.4342527252\H,1.9477890096,0.9259632077,0.0998012959\C,-1.31
57009895,1.5846478716,3.5735270782\H,-2.284070675,1.1993448516,3.90532
76183\H,-0.5874141105,1.4241341639,4.3700906904\H,-1.4374070031,2.6577
484398,3.4058278645\\Version=AM64L-G03RevC.02\State=1-A\HF=-349.174823
6\RMSD=8.082e-09\RMSF=2.114e-05\Thermal=0.\Dipole=1.0349195,-0.5204168
,-0.3403551\PG=C01 [X(C7H12O1)]\

11 (Me/COMe)



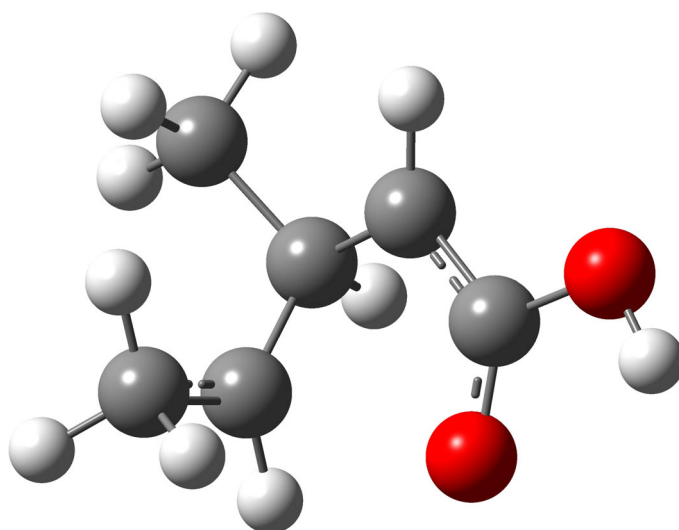
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O1\TSCHNEI\09-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_COR_2\0,1\C,-0.01295453,-0.03291809
04,0.0340343047\C,0.0515325479,-0.0044656189,2.6632117582\C,0.83426825
99,0.0409820638,1.3459172482\H,1.3982573767,0.9854836145,1.3385288353\
C,1.7903601791,-1.1111819664,1.1288782504\H,2.4794488501,-1.4870756551
,1.8728935599\H,-0.6467616517,0.8334563357,2.751175037\H,0.7418219638,
0.0611183781,3.5089215474\C,1.7019824076,-1.5371386978,-0.1317895945\O
,0.7566710779,-0.8778548569,-0.8786513931\H,-0.5133001284,-0.932631685
,2.7739382698\H,-0.0782234538,0.9452260152,-0.4474089105\C,-1.40491962
35,-0.6379273877,0.1559711992\H,-2.0592450277,-0.0172489872,0.77381976
28\H,-1.8535258662,-0.7224800703,-0.8361301211\H,-1.3640377401,-1.6382
067532,0.5937951956\C,2.4564437414,-2.5862542353,-0.8703433806\H,1.776
9785548,-3.3506725491,-1.2597893702\H,2.9756304827,-2.1508232611,-1.72
99697799\H,3.1932630997,-3.0657760875,-0.2249657075\\Version=AM64L-G
03RevC.02\State=1-A\HF=-349.2566619\RMSD=2.074e-09\RMSF=6.589e-06\
Thermal=0.\Dipole=-0.0116856,0.0533998,0.3024698\PG=C01 [X(C7H12O1)]\

10 (Me/COOH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\09-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_COOH_1\0,1\C,-0.0231748194,-0.01177
53382,-0.0604277802\H,0.0012113556,-0.0233191821,1.0255288448\C,1.3707
785832,-0.0028446531,-0.6847958021\H,1.4902594535,0.5226138828,-1.6251
862858\C,2.5384581803,0.034471943,0.2191524632\C,0.5053628927,-1.26143
58167,-0.6915637645\H,0.8403935276,-2.0074785198,0.0234202741\C,-0.004
7362448,-1.8281652108,-1.9973799167\H,-0.8913421044,-2.4483163304,-1.8
323923584\H,-0.2759014044,-1.051405887,-2.7155020407\H,0.7553374094,-2
.4576222181,-2.4688895901\O,2.6080926365,-0.4862015194,1.308523172\C,-
1.1293771276,0.8308456285,-0.6543939404\H,-2.1114545949,0.4362420858,-
0.3756575979\H,-1.0708912042,1.8597369058,-0.2880499622\H,-1.088448925
4,0.8704203626,-1.744965372\O,3.5702285222,0.7386150302,-0.3112002986\
H,4.2872078084,0.7125227148,0.3408301703\Version=AM64L-G03RevC.02\S
tate=1-A\HF=-385.196589\RMSE=1.966e-09\RMSE=4.409e-06\Thermal=0.\Dip
ole=-0.2614397,0.1627784,-0.5413319\PG=C01 [X(C6H10O2)]\
```

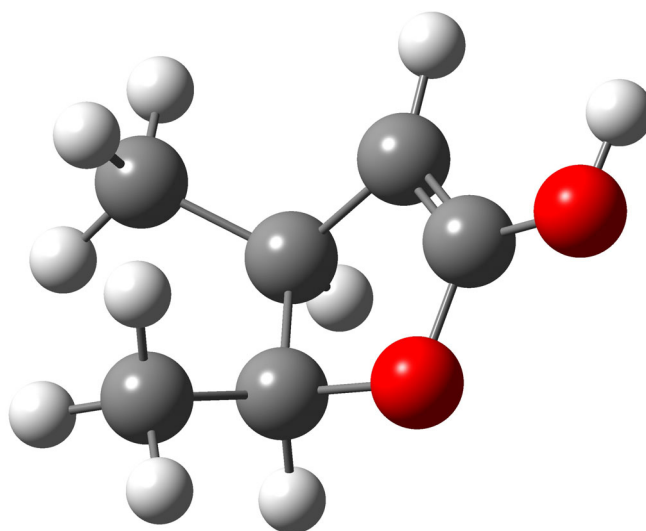
TS₁₀₋₁₁ (Me/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\09-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=ti
ght\DA_Me_COOH_TS\0,1\C,0.0517536409,-0.1061355816,0.0360449109\C,0.
```

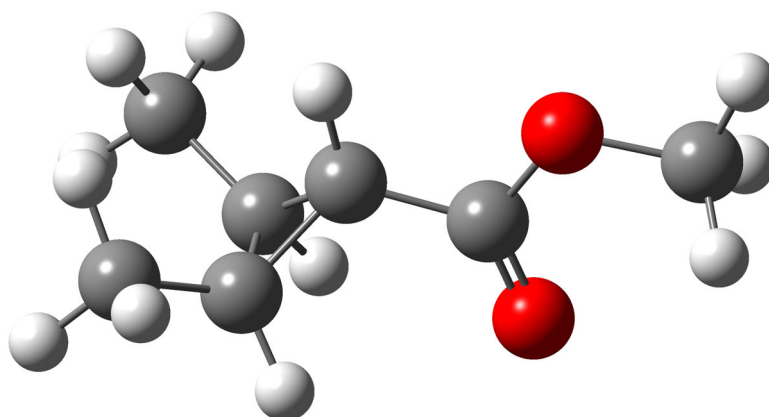
0792497871,-0.103403339,2.297945845\H,0.7936109677,-0.1230894605,3.1113458567\C,-0.958183803,0.83136584,2.2383099647\O,-1.5980493448,1.113870336,1.1966946077\C,0.200682392,-1.0636068431,1.141106348\H,-0.6150560407,-1.7952669432,1.1095851362\C,1.5397799332,-1.8190928985,1.1774057088\H,1.6333673768,-2.5060524344,0.3339707453\H,2.3929834396,-1.1378947131,1.1687806381\H,1.5886480579,-2.4009685012,2.1010889658\H,-0.8169845263,-0.1867793784,-0.6082358334\C,1.0125292558,0.951735667,-0.335491418\H,1.3078976434,0.823183443,-1.3866296137\H,0.5087814888,1.924600939,-0.2844907788\H,1.8949901312,0.9852211872,0.3018621171\O,-1.2911473103,1.4543239164,3.4050473128\H,-1.9768918138,2.0961626161,3.1765177168\\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1044033\RMSD=4.518e-09\RMSF=1.281e-05\Thermal=0.\Dipole=0.7375218,-0.3009354,-0.8535737\PG=C01 [X(C6H10O2)]\

11 (Me/COOH)



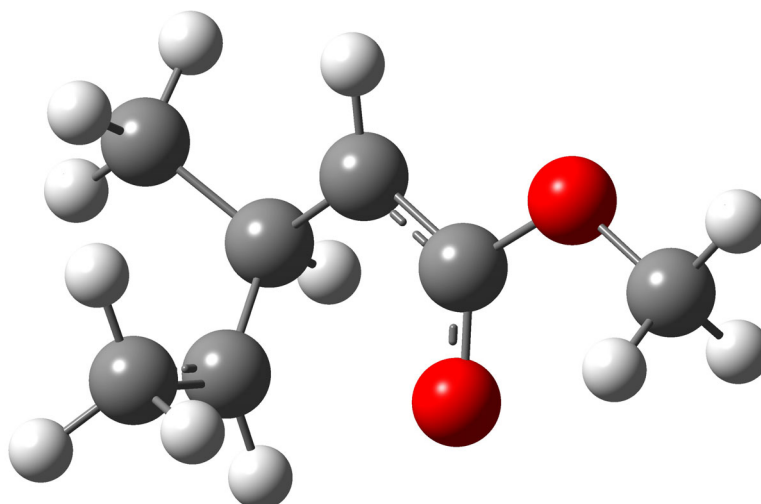
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHEI\29-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Me_COOH_3\0,1\C,-0.0081940448,-0.1577506773,-0.0375008109\C,0.0347271642,-0.1863135623,2.5856938564\C,0.8285904609,-0.0598502727,1.2814228474\H,1.3217472352,0.9239154758,1.2990738159\C,1.8534669435,-1.1476888436,1.0435356835\H,-0.7178315545,0.6025463721,2.682582204\H,0.7095048259,-0.0937887831,3.441357441\C,1.7980579521,-1.4941793218,-0.2481838407\O,0.8450831754,-0.8833895273,-0.9850094217\H,-0.4674637703,-1.1525472399,2.6684525999\H,-0.164313916,0.8268767493,-0.4814491888\C,-1.330895796,-0.9041041952,0.0490059087\H,-2.0451114578,-0.373926889,0.6841492395\H,-1.7642830882,-0.9955469926,-0.9490234436\H,-1.191005326,-1.9101583607,0.4510747224\O,2.52489357,-2.3518608584,-0.9872183714\H,3.2361669136,-2.7039644416,-0.4402373896\H,2.5575178699,-1.5150946351,1.7772187892\\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1672495\RMSD=3.751e-09\RMSF=8.949e-06\Thermal=0.\Dipole=0.1741118,0.0363781,0.7609824\PG=C01 [X(C6H10O2)]\

10 (Me/COOMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\10-Jun-2010\
0\# opt freq rb3lyp/6-311g(d) geom=connectivity\DA_Me_COOR_1\0,1\C,-0.0
108880506,-0.0357030732,-0.0535890324\H,0.0055952726,-0.068688321,1.03
21108172\C,1.3854073452,-0.0670313872,-0.669694707\H,1.5291925848,0.47
12323385,-1.5996158174\C,2.5526749533,-0.0870686003,0.2408248808\C,0.4
762861756,-1.2927383153,-0.7058299062\H,0.7789035385,-2.0639866052,-0.
0031914814\C,-0.0494369907,-1.8150835014,-2.0240178491\H,-0.9654722871
,-2.3957782191,-1.8764519483\H,-0.2776921759,-1.0149260994,-2.73135538
97\H,0.684322708,-2.4716680608,-2.500434328\O,2.5907947715,-0.63252949
61,1.3200903054\C,-1.084070811,0.8545963506,-0.638820839\H,-2.08153507
33,0.4840183625,-0.3822240769\H,-0.9991205162,1.872157077,-0.246605674
\H,-1.0274968154,0.9197653798,-1.7275035299\O,3.599327919,0.5915503645
,-0.2846588821\C,4.7831402571,0.6290769446,0.5273441353\H,5.5085010881
,1.2058176038,-0.0422021155\H,4.5775614761,1.1100577817,1.4845484444\H
,5.1550557785,-0.3796921301,0.7114785306\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-424.5091328\RMSD=6.161e-09\RMSF=2.719e-06\Thermal=0.\Dipol
e=-0.0434989,0.2705235,-0.5535169\PG=C01 [X(C7H12O2)]\
```

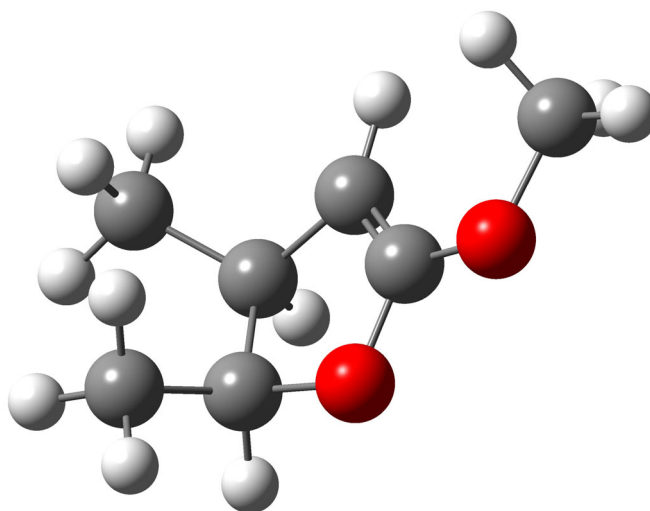
TS₁₀₋₁₁ (Me/COOMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\10-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=ti
ght\DA_Me_COOR_TS\0,1\C,0.0133928711,-0.1698446659,0.0902161964\C,0.
0835489718,-0.3479491831,2.3454073074\H,0.8052938029,-0.3465629947,3.1
```

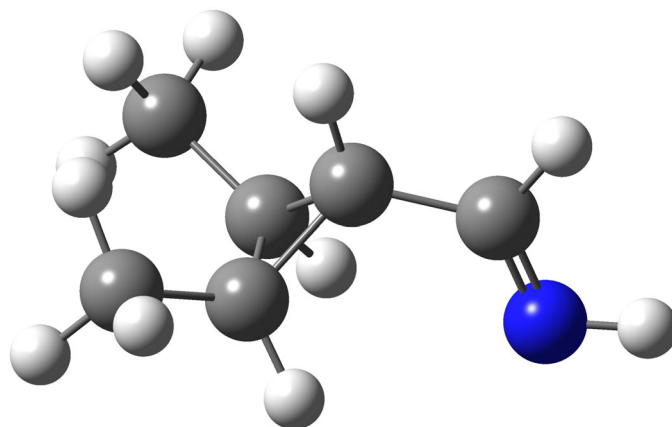
526785783\C,-1.071837056,0.4444791006,2.3723072491\O,-1.7496697745,0.7265870363,1.3556903628\C,0.3037371863,-1.1862223757,1.1122173091\H,-0.4128463167,-2.0118211467,1.0261149068\C,1.7277972155,-1.7654615675,1.0725824638\H,1.8905461566,-2.3634624171,0.1736655875\H,2.4877798097,-0.9825319429,1.112734184\H,1.8687825863,-2.4099852348,1.9438393659\H,-0.846189227,-0.3119025009,-0.5557537021\C,0.8262685359,1.0290405259,-0.2001081522\H,1.1201604003,1.0236593694,-1.2595363713\H,0.2061927914,1.9236398769,-0.0671269241\H,1.7072444438,1.1229807826,0.4334623276\O,-1.4480127393,0.8933650868,3.6012028975\C,-2.5974041462,1.7421408999,3.6324725593\H,-2.6390855067,2.1412850607,4.6448795653\H,-2.5080118473,2.512541322,2.9051598925\H,-3.5069008619,1.1775876227,3.416949565\Version=AM64L-G03RevC.02\State=1-A\HF=-424.4156738\RMSD=5.698e-09\RMSF=6.721e-06\Thermal=0.\Dipole=0.6534641,-0.0851711,-0.6985439\PG=C01 [X(C7H12O2)]\

11 (Me/COOMe)



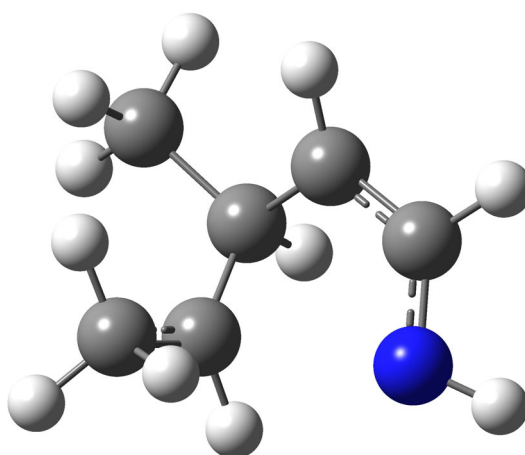
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\10-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Me_COOR_2\0,1\C,-0.0193321768,-0.13254967,-0.0190888088\C,-0.0537632362,-0.1737607133,2.6036380345\C,0.7844029476,-0.1224252709,1.3219632387\H,1.3725438355,0.8070963594,1.3592882554\C,1.7061333047,-1.304358341,1.1100680541\H,-0.7244888707,0.6873075532,2.6866471903\H,0.6030782521,-0.1552727342,3.4778756767\C,1.6520068672,-1.6465585001,-0.1850725338\O,0.7824947033,-0.9359699224,-0.9450293931\H,-0.6544234938,-1.0839479472,2.6647257169\H,-0.0649666495,0.8646042683,-0.4607189447\C,-1.412728535,-0.7422228698,0.0272105275\H,-2.0886984482,-0.1430590022,0.6426301782\H,-1.8236009927,-0.7898664467,-0.9833369033\H,-1.3862640401,-1.7572504856,0.4302908885\O,2.2980014869,-2.5642859789,-0.9117189739\H,2.3472725979,-1.7308473132,1.8659762366\C,3.2719410403,-3.3295484283,-0.2103872847\H,2.8074272626,-3.9043395126,0.5969221053\H,3.7064169042,-4.0072787047,-0.9419682048\H,4.0501821988,-2.6823213414,0.2054651799\Version=AM64L-G03RevC.02\State=1-A\HF=-424.4823552\RMSD=7.160e-09\RMSF=2.577e-05\Thermal=0.\Dipole=0.2056071,-0.0989461,0.6590989\PG=C01 [X(C7H12O2)]\

10 (Me/CHNH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1\TSCHNEI\10-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHNH_1\0,1\C,-0.0275409136,0.0167193371,0.0275958698\H,0.1248023005,0.0421793353,1.103226489\C,1.2938165768,-0.0055132434,-0.7410959587\H,1.2881385864,0.4852472839,-1.7105135805\C,2.5726273052,0.0712687477,-0.0025920109\C,0.4224333835,-1.255788644,-0.6192781231\H,0.8396802475,-1.9798079857,0.0753690168\C,-0.241500113,-1.856384507,-1.8381090272\H,-1.1186707711,-2.4478808301,-1.5560450345\H,-0.5732041973,-1.0979069556,-2.5508401692\H,0.4473843593,-2.5216108019,-2.3672191956\C,-1.1952450152,0.8406902086,-0.4669477392\H,-2.1428889491,0.4486263026,-0.0833954732\H,-1.1083849422,1.8781486598,-0.1305238257\H,-1.2646095877,0.8568726304,-1.55700733\N,2.7235954032,-0.4586982548,1.1447527588\H,3.3774421326,0.6170483811,-0.5161757017\H,3.6679078967,-0.3038178771,1.4969333037\Version=AM64L-G03RevC.02\State=1-A\HF=-290.0331466\RMSE=9.230e-09\RMSE=4.948e-06\Thermal=0.\Dipole=0.1369767,0.3211076,-0.5362373\PG=C01 [X(C6H11N1)]\

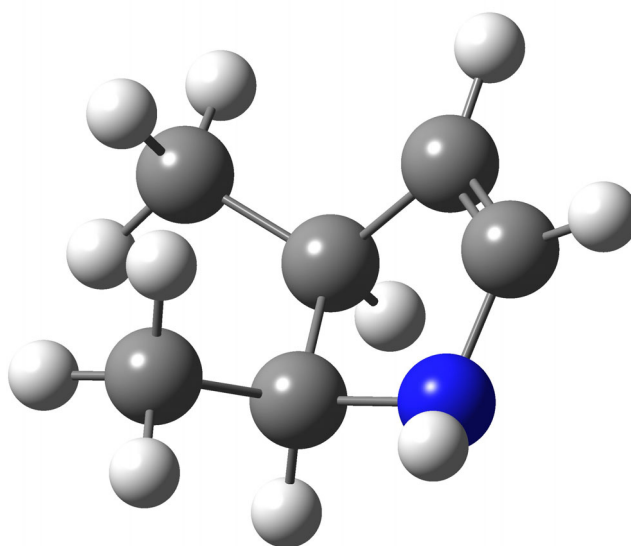
TS₁₀₋₁₁ (Me/CHNH)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H11N1\TSCHNEI\10-Jun-2010\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) geom=connectivity in t=ultrafine scf=tight\DA_Me_CHNH_TS\0,1\C,0.0834943764,-0.1342942412,-0.0444654244\C,0.0601792183,0.0242872473,2.21223725\H,0.8690109432,0.1153229325,2.9336409919\C,-0.9846858944,0.9478597705,2.2015804235\C,0.1921672824,-1.0214221532,1.117592246\H,-0.653520821,-1.7165040795,1.1

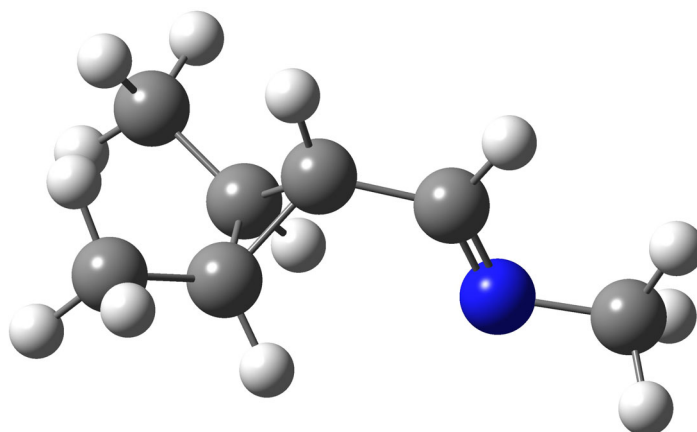
330802306\C,1.4987009776,-1.8132157801,1.2553049273\H,1.5874108341,-2.5698516817,0.4728878111\H,2.3758842338,-1.1640391472,1.2042658767\H,1.5139713001,-2.3165696149,2.2262446766\H,-0.8015364887,-0.2026206731,-0.6635702795\C,1.059863014,0.9061994543,-0.4407271651\H,1.3204647147,0.7962854039,-1.5019875488\H,0.5884666706,1.893000321,-0.3411326353\H,1.9706351106,0.901601824,0.1597201072\N,-1.6027587589,1.3141045553,1.1048977456\H,-2.5178175239,1.7246433942,1.3077705757\H,-1.2747584996,1.3650533009,3.176853123\\Version=AM64L-G03RevC.02\State=1-A\HF=-289.9530898\RMSD=7.022e-09\RMSF=2.342e-06\Thermal=0.\Dipole=0.2842137,-0.2768631,-0.1114607\PG=C01 [X(C6H11N1)]\\

11 (Me/CHNH)



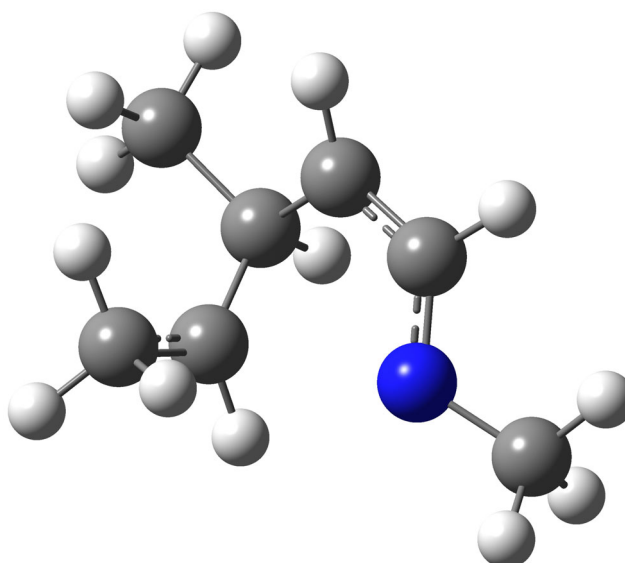
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1\TSCHNEI\10-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHNH_2\0,1\C,-0.0094782532,-0.0718274053,-0.0390012123\C,0.0306320399,-0.1749827474,2.5900609006\C,0.8239674279,-0.0503181931,1.2869654131\H,1.3546606033,0.914076084,1.316503997\C,1.8398782909,-1.1473745828,1.0309159403\H,-0.7067780615,0.626955611,2.6963673423\H,0.7063396422,-0.1074162924,3.4475700211\C,1.8626856519,-1.4185620872,-0.2770556349\H,-0.4934714475,-1.1308962313,2.6622607672\H,-0.2679981743,0.9475205602,-0.3390131836\C,-1.2884706461,-0.9136902172,0.0155990257\H,-2.0137666742,-0.5052282175,0.724032356\H,-1.7717714811,-0.9305540781,-0.9667820948\H,-1.0721414524,-1.9456629665,0.3048473345\H,2.5158846145,-1.5445318453,1.776196867\N,0.9589523818,-0.6377459494,-1.0167651119\H,2.5152308758,-2.1041613293,-0.8052430576\H,0.5275551155,-1.1089507947,-1.8035084984\\Version=AM64L-G03RevC.02\State=1-A\HF=-290.0507705\RMSD=7.038e-09\RMSF=7.994e-06\Thermal=0.\Dipole=-0.3386566,-0.197756,-0.1525251\PG=C01 [X(C6H11N1)]\\

10 (Me/CHNMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1\TSCHNE\10-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHNR_1\0,1\C,-0.0520262648,-0.03599
49941,0.0590285169\H,0.0874204833,-0.077323125,1.1359558057\C,1.273996
6139,0.0453226178,-0.6944927121\H,1.253144703,0.5982911653,-1.62968890
13\C,2.5490601053,0.1339039788,0.0510686821\C,0.4564652779,-1.24452727
83,-0.6667543881\H,0.8954498348,-1.9965609795,-0.0166173705\C,-0.17441
33247,-1.7902206249,-1.9284013083\H,-1.029618435,-2.432766913,-1.69452
65488\H,-0.5306849981,-1.0003873279,-2.5936742425\H,0.5443390186,-2.39
16687901,-2.4930346152\C,-1.2507796555,0.7682636654,-0.3924991448\H,-2
.1840161677,0.3105008343,-0.0483377992\H,-1.2126777501,1.7833539359,0.
0140691726\H,-1.310566515,0.8558425126,-1.4797491143\N,2.7394399772,-0
.4516258981,1.1588754167\H,3.3386044052,0.7469633359,-0.4160350796\C,4
.0256682823,-0.3004592061,1.8077220486\H,3.8836323641,0.1303835133,2.8
037278579\H,4.4796434556,-1.2857569706,1.9521403032\H,4.7317525825,0.3
333099203,1.2481868531\Version=AM64L-G03RevC.02\State=1-A\HF=-329.35
32346\RMSD=7.613e-09\RMSF=1.501e-05\Thermal=0.\Dipole=0.0691773,0.240
4874,-0.3519114\PG=C01 [X(C7H13N1)]\

TS₁₀₋₁₁ (Me/CHNMe)



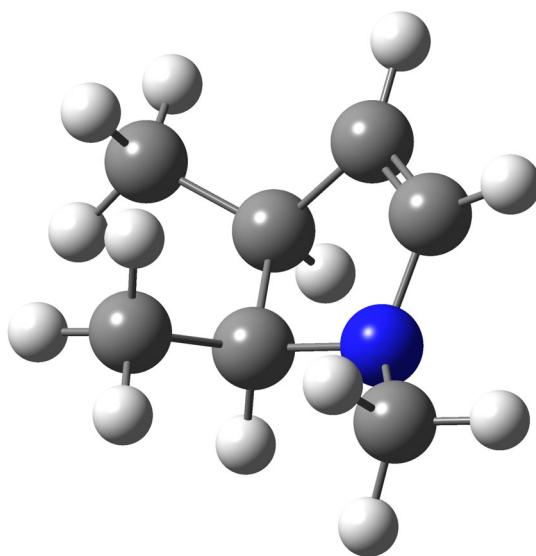
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1\TSCHNE\10-Jun-2010\

```

0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight
\\DA_Me_CHNR_TS\\0,1\\C,0.0083737844,-0.1798327047,0.0046544433\\C,0.1
106464156,0.0492017336,2.2561170874\\H,0.9566304054,0.1846049419,2.926
5171367\\C,-0.9493525792,0.9563987506,2.2784069435\\C,0.2058016721,-1.02
4477534,1.1886330265\\H,-0.6196100202,-1.7388485231,1.273411909\\C,1.535
8475095,-1.7845743253,1.2715014137\\H,1.5953367166,-2.5631413052,0.5080
630437\\H,2.3936385794,-1.1191160317,1.1488738262\\H,1.620059112,-2.2571
068742,2.2544366313\\H,-0.9039673105,-0.2951443741,-0.5665058024\\C,0.93
08933613,0.8761345482,-0.4717232903\\H,1.1346799778,0.7484064059,-1.543
3194388\\H,0.4427169925,1.8545144737,-0.3663373106\\H,1.8739224365,0.908
7110895,0.0760306705\\N,-1.6571546855,1.2713963223,1.2252396192\\H,-1.18
71564734,1.4157835983,3.2506865719\\C,-2.9788021772,1.8343520928,1.4312
559554\\H,-3.1081592404,2.2667752906,2.4357806737\\H,-3.1772935483,2.613
4527656,0.6890358223\\H,-3.7561578162,1.0683307739,1.3088595276\\Version
=AM64L-G03RevC.02\\State=1-A\\HF=-329.271487\\RMSD=8.060e-09\\RMSF=6.
834e-06\\Thermal=0\\Dipole=0.2649897,-0.2702756,-0.2360415\\PG=C01 [X(C7H
13N1)]\\

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11 (Me/CHNMe)



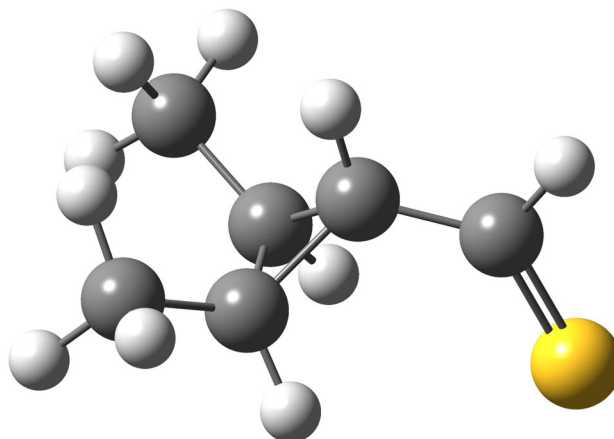
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1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H13N1\\TSCHNEI\\10-Jun-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_Me_CHNR_2\\0,1\\C,-0.0646022641,-0.03854
63352,0.0003823269\\C,0.041205929,-0.2130918181,2.6239533521\\C,0.798956
9799,-0.0431803511,1.3057698376\\H,1.3203645195,0.9265646802,1.34932257
03\\C,1.8240104747,-1.1176217434,0.9912529638\\H,-0.7014921349,0.5773561
302,2.7727704272\\H,0.7393915123,-0.1619321485,3.464490929\\C,1.83735556
63,-1.3153138276,-0.3319586911\\H,-0.4704430674,-1.1764134628,2.6831638
597\\H,-0.3586297821,0.9833954263,-0.2607721351\\C,-1.3275215673,-0.9082
903335,0.0796315878\\H,-2.0071190064,-0.5349145357,0.84898385\\H,-1.8757
400696,-0.8947066897,-0.8656245604\\H,-1.0852314174,-1.9476740141,0.315
8965476\\H,2.5215369829,-1.533379016,1.7054981457\\N,0.9027236212,-0.534
0445631,-1.0147135713\\H,2.5003771243,-1.9548053162,-0.903767015\\C,0.43
83668207,-0.9341124133,-2.327542171\\H,-0.1411387671,-0.1226445153,-2.7
752631871\\H,1.3006680839,-1.1130682319,-2.9743691813\\H,-0.1843394542,-
1.8420777394,-2.3329003233\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-32

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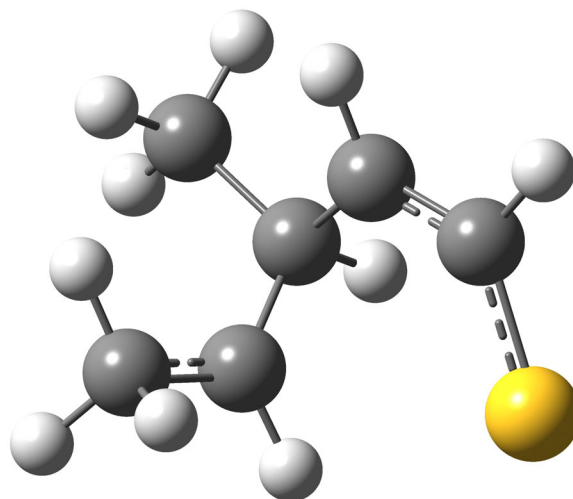
9.3652907\RMSD=3.963e-09\RMSF=1.534e-05\Thermal=0.\Dipole=-0.2396672
,-0.0405273,-0.2708521\PG=C01 [X(C7H13N1)]\

10 (Me/CHS)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10S1\TSCHNEI\07-Sep-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHS_1\0,1\C,-0.027303395,-0.0189541
087,0.005617096\H,-0.0402936662,-0.0204034608,1.0925090893\C,1.4160843
712,-0.0175700912,-0.5463160201\H,1.5445572997,0.4973211883,-1.4941237
669\C,2.5644093927,0.038872736,0.3483399087\C,0.5047930009,-1.26445250
17,-0.5988384695\H,0.8120893646,-2.0156543223,0.1241896508\C,0.0636995
493,-1.8145385461,-1.9355050241\H,-0.8404486879,-2.4210513467,-1.82125
48866\H,-0.1573879991,-1.0304431713,-2.6626194744\H,0.8386220494,-2.45
45977048,-2.3657742127\H,3.4164383715,0.5959417593,-0.0476469216\C,-1.
0771720424,0.8559583001,-0.6394670265\H,-2.0806225141,0.4819262044,-0.
4123461849\H,-1.0131552107,1.880086868,-0.2621409883\H,-0.981576515,0.
8985965961,-1.7263998247\S,2.7063432597,-0.6237889365,1.8406783849\V
ersion=AM64L-G03RevC.02\State=1-A\HF=-632.8843775\RMSD=8.820e-09\R
MSF=4.248e-05\Thermal=0.\Dipole=-0.7708144,0.2347348,-1.1623943\PG=C0
1 [X(C6H10S1)]\

TS₁₀₋₁₁ (Me/CHS)



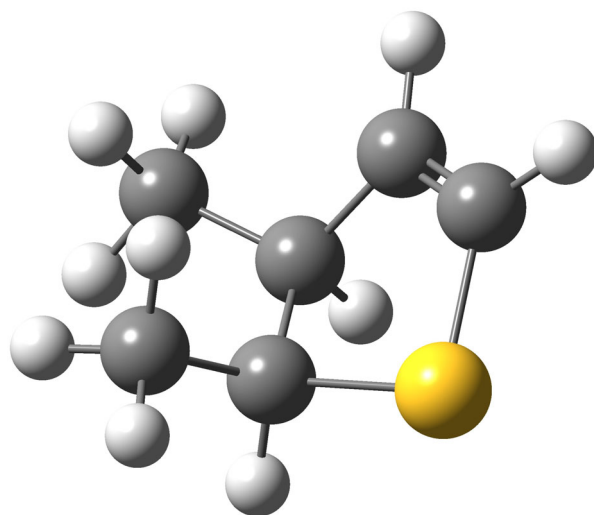
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10S1\TSCHNEI\07-Sep-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_CHS_1\0,1\C,-0.027303395,-0.0189541
087,0.005617096\H,-0.0402936662,-0.0204034608,1.0925090893\C,1.4160843
712,-0.0175700912,-0.5463160201\H,1.5445572997,0.4973211883,-1.4941237
669\C,2.5644093927,0.038872736,0.3483399087\C,0.5047930009,-1.26445250
17,-0.5988384695\H,0.8120893646,-2.0156543223,0.1241896508\C,0.0636995
493,-1.8145385461,-1.9355050241\H,-0.8404486879,-2.4210513467,-1.82125
48866\H,-0.1573879991,-1.0304431713,-2.6626194744\H,0.8386220494,-2.45
45977048,-2.3657742127\H,3.4164383715,0.5959417593,-0.0476469216\C,-1.
0771720424,0.8559583001,-0.6394670265\H,-2.0806225141,0.4819262044,-0.
4123461849\H,-1.0131552107,1.880086868,-0.2621409883\H,-0.981576515,0.
8985965961,-1.7263998247\S,2.7063432597,-0.6237889365,1.8406783849\V
ersion=AM64L-G03RevC.02\State=1-A\HF=-632.8843775\RMSD=8.820e-09\R
MSF=4.248e-05\Thermal=0.\Dipole=-0.7708144,0.2347348,-1.1623943\PG=C0
1 [X(C6H10S1)]\

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0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\\DA_Me_CHS_TS\\0,1\\C,-0.0546673807,0.0769107965,-0.0045743621\\C,0.
0032611264,0.061495085,2.232266375\\H,0.8842282017,0.1358031767,2.86771
80504\\C,-1.1063406701,0.8150715125,2.5132483207\\H,-1.149929646,1.20384
64989,3.5334424774\\C,0.1128979361,-0.9135110097,1.0527688246\\H,-0.7322
780406,-1.6064043542,1.0583042924\\C,1.4370770097,-1.685098192,1.088140
6317\\H,1.5164622875,-2.365650842,0.23788482\\H,2.3030005886,-1.01947283
88,1.0745803567\\H,1.4855611843,-2.2754130583,2.0064660564\\H,-0.9873204
576,0.0864932092,-0.5534110082\\C,0.9255160828,1.1157507762,-0.38862639
97\\H,1.170724366,1.0037851386,-1.4547199748\\H,0.4723829099,2.110407497
5,-0.2956563177\\H,1.845183014,1.0968043245,0.1950520676\\S,-2.413331731
3,1.1981655782,1.5088808503\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-63
2.824572\\RMSD=5.353e-09\\RMSF=1.247e-05\\Thermal=0.\\Dipole=1.8522599,-0.
7003059,-0.7218158\\PG=C01 [X(C6H10S1)]\\

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11 (Me/CHS)

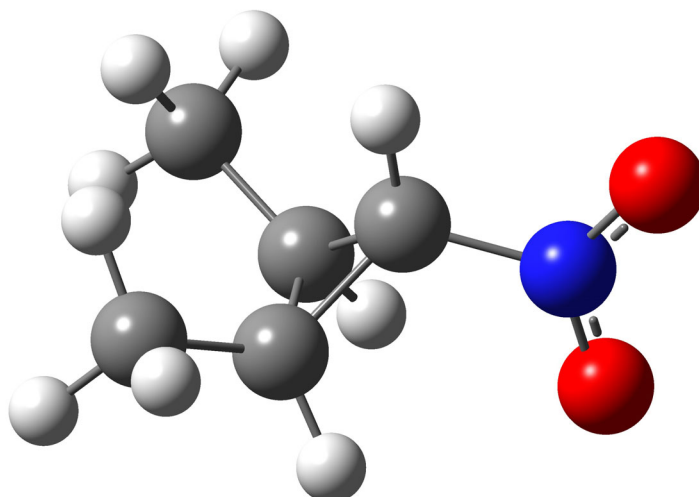


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1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C6H10S1\\TSCHNEI\\07-Sep-2010\\
0\\# opt freq b3lyp/6-311g(d)\\DA_Me_CHS_2\\0,1\\C,-0.023421479,-0.10150259
82,-0.0185709991\\C,0.041933534,-0.1139163922,2.5806328736\\C,0.84094040
16,-0.0823830238,1.2731284675\\H,1.4114523468,0.8598045079,1.2554630617
\\C,1.844902889,-1.2067100551,1.1237515342\\H,2.3545300899,-1.6372300414
,1.9795758095\\H,-0.6712126612,0.7135234324,2.6362651421\\H,0.7171599621
,-0.0190011147,3.435644804\\C,2.106531515,-1.5534426572,-0.1350918274\\H
,-0.5117152161,-1.0479362199,2.7006229292\\H,2.8350999114,-2.2804707855
,-0.4712439573\\H,-0.3204424535,0.9134576912,-0.2887904847\\C,-1.2494663
233,-1.0114885243,0.0281493715\\H,-1.9683757016,-0.665263913,0.77712610
68\\H,-1.7562699962,-1.0209372212,-0.9386904686\\H,-0.9705923998,-2.0396
943351,0.2702870221\\S,1.1466263446,-0.6897738039,-1.3542166152\\Versio
n=AM64L-G03RevC.02\\State=1-A\\HF=-632.9079133\\RMSD=6.656e-09\\RMSF=
2.520e-05\\Thermal=0.\\Dipole=-0.2092174,0.0509724,0.6745895\\PG=C01 [X(C6
H10S1)]\\

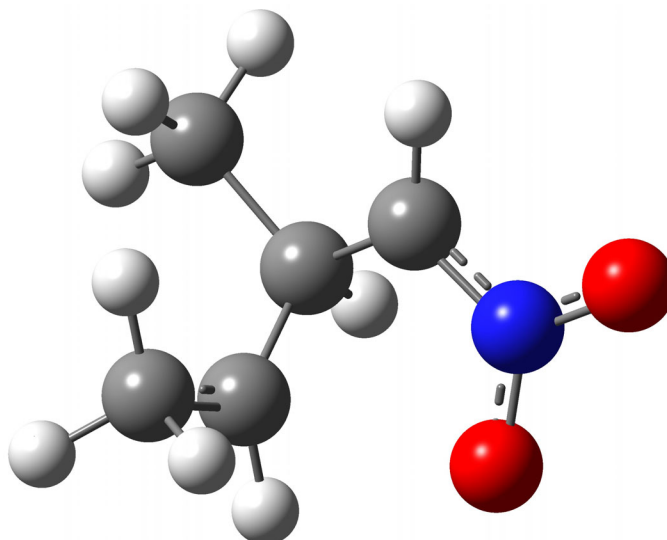
```

10 (Me/NO₂)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\10-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_NO2_1\0,1\C,0.0272292084,0.0143036
915,-0.022533315\H,0.227876872,0.0808654514,1.0422878611\C,1.293842398
8,-0.0110131927,-0.8521895088\H,1.3247035934,0.4617589925,-1.823840090
5\C,0.4929588726,-1.2780306219,-0.6365966644\H,0.9597228968,-1.9493952
097,0.0775072608\C,-0.1824774094,-1.9570403276,-1.8069692083\H,-1.0117
085231,-2.5814152821,-1.4621066788\H,-0.5855871902,-1.2465404203,-2.53
15067807\H,0.521838451,-2.6035976002,-2.3369699879\C,-1.1753386536,0.7
985137355,-0.4978316699\H,-2.0907540005,0.4123272024,-0.0403689937\H,-
1.0838181864,1.8516557258,-0.2194085093\H,-1.3059332045,0.7550988947,-
1.5810320124\N,2.5882010592,0.1295147546,-0.1664771245\O,3.4659557756,
0.731766062,-0.7691400282\O,2.7064094383,-0.3586662933,0.951476403\Ve
rsion=AM64L-G03RevC.02\State=1-AHF=-401.1299588\RMSD=6.902e-09\RMS
F=1.421e-05\Thermal=0\Dipole=-1.5924317,-0.3001487,-0.5759531\PG=C01 [X(
C5H9N1O2)]\
```

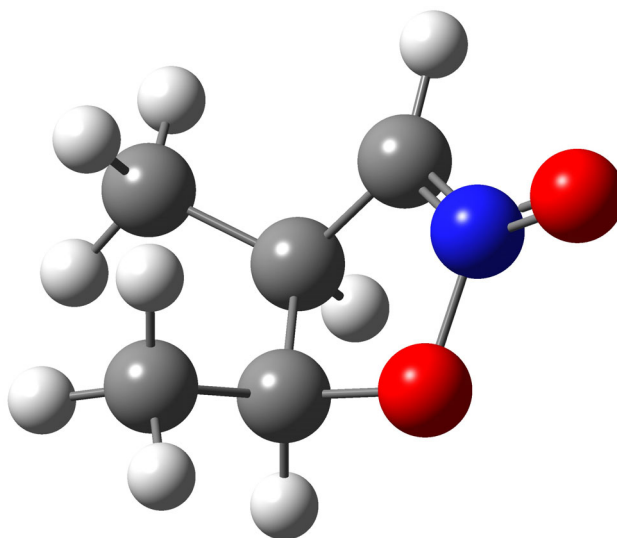
TS₁₀₋₁₁ (Me/NO₂)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\10-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=t
```

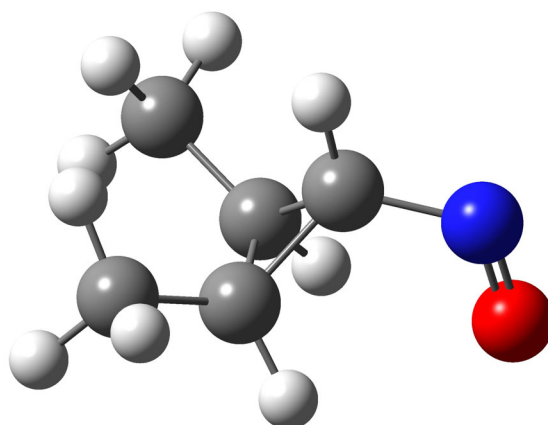
ight\\DA_Me_NO2_TS\\0,1\\C,0.0878071349,-0.0596256701,-0.0091156688\\C,0.1111973861,0.0610368425,2.1922910212\\H,0.8511265807,0.1833129169,2.9695020169\\O,-1.6819916515,1.0060137218,1.1699068442\\C,0.1776916504,-0.9890376067,1.1261229503\\H,-0.6925750101,-1.6523622989,1.1402508047\\C,1.467354253,-1.812230338,1.2395798383\\H,1.5320562842,-2.5469585683,0.4352271783\\H,2.3605882833,-1.1853988446,1.206636015\\H,1.4679962588,-2.3449166332,2.1932620027\\H,-0.7953065294,-0.0909500551,-0.6346870842\\C,1.1213154785,0.9111507638,-0.4241647864\\H,1.3939263717,0.71370697,-1.4710747659\\H,0.7000851837,1.9236006395,-0.4186618365\\H,2.0135047478,0.9043155929,0.2003170298\\O,-1.2006238555,1.5806107251,3.2371273761\\N,-0.9540420286,0.9218415073,2.2179395136\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-401.0443697\\RMSD=9.335e-09\\RMSF=6.678e-06\\Thermal=0.\\Dipole=1.7056474,-1.2734966,-1.4735051\\PG=C01 [X(C5H9N1O2)]\\

11 (Me/NO₂)



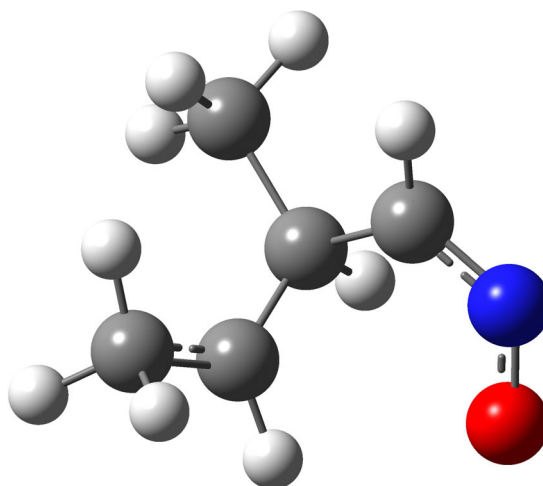
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C5H9N1O2\\TSCHNEI\\10-Jun-2010\\0\\# opt freq rb3lyp/6-311g(d)\\DA_Me_NO2_2\\0,1\\C,-0.0318775016,-0.1180186801,-0.0331051779\\C,0.0422208251,-0.1308238845,2.5884128857\\C,0.8142079153,-0.0443759619,1.2699444344\\H,1.3651318708,0.9082992253,1.2663468972\\C,1.7766226989,-1.161854883,1.0242122925\\H,-0.6721253538,0.6919426444,2.6788426606\\H,0.7286739651,-0.0577460623,3.4358518604\\O,0.8651211183,-0.7007765844,-1.0066868994\\H,-0.504341497,-1.0707337312,2.6843222207\\H,-0.2539627576,0.8842883372,-0.4059038781\\C,-1.3037325617,-0.9530516404,0.0382523424\\H,-2.0454074076,-0.4971135124,0.6993478824\\H,-1.7397096823,-1.0315009518,-0.9592934162\\H,-1.0975673925,-1.964951863,0.395276573\\H,2.4520262905,-1.6484045587,1.7105002596\\O,2.496352116,-2.2887557335,-0.8751084684\\N,1.8286993536,-1.502521642,-0.2336306127\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-401.1297269\\RMSD=6.272e-09\\RMSF=1.160e-04\\Thermal=0.\\Dipole=-0.8378613,0.859894,1.3528465\\PG=C01 [X(C5H9N1O2)]\\

10 (Me/NO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1\TSCHNEI\25-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Me_NO_1\0,1\C,0.0292532671,-0.0178832
213,-0.0214589441\H,0.2539196821,0.0551061484,1.0404497109\C,1.3236005
995,-0.0358516107,-0.8457564452\H,1.3295895175,0.4377711277,-1.8204575
387\C,0.4728838918,-1.2957747803,-0.6390159853\H,0.9575750405,-1.97353
62986,0.0603985101\C,-0.2085904605,-1.9552001473,-1.8151247044\H,-1.05
01212059,-2.5681467583,-1.4775083466\H,-0.5972175382,-1.2320971926,-2.
5349423749\H,0.4858080486,-2.6102280145,-2.3474913749\C,-1.1600269179,
0.7870092725,-0.4904601489\H,-2.0826568317,0.4075714205,-0.0402329618\
H,-1.0566701095,1.8356567158,-0.2001076888\H,-1.2869726574,0.756023046
1,-1.5744098151\N,2.5954023449,0.0857853366,-0.1818448418\O,2.65236160
27,-0.4278849273,0.9180131567\Version=AM64L-G03RevC.02\State=1-A\HF=-
325.8939436\RMSD=9.077e-09\RMSF=4.823e-05\Thermal=0\Dipole=-1.204536
1,-0.1065227,-0.6440368\PG=C01 [X(C5H9N1O1)]\
```

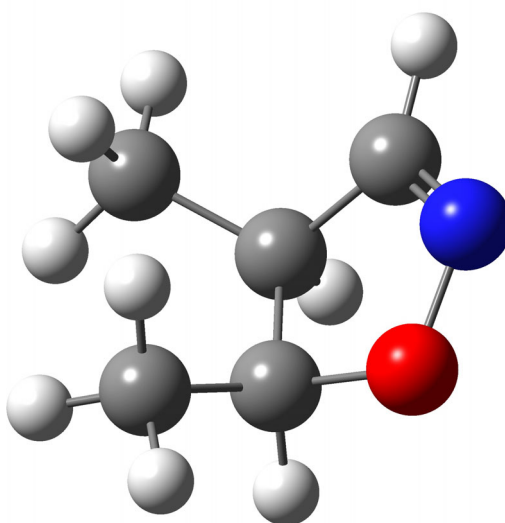
TS₁₀₋₁₁ (Me/NO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O1\TSCHNEI\25-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=t
ight\DA_Me_NO_TS\0,1\C,0.0696770758,0.0399625648,-0.0642523752\C,-0.
0939405913,0.0591201437,2.2177127689\H,0.7334247771,0.105661249,2.914
8450734\O,-2.0177448735,0.9599704897,1.5249768498\C,-0.0126359461,-0.9
434374069,0.97921432\H,-0.9753239559,-1.4604836258,0.955191648\C,1.151
```

0611636,-1.9113617362,1.1953361739\H,1.2287657263,-2.611610273,0.36089
66308\H,2.1098988132,-1.3976230659,1.2934356583\H,0.9885702727,-2.4866
761398,2.1093068776\H,-0.8605134658,0.3421871975,-0.5295751584\C,1.292
7765525,0.7769959104,-0.4716654547\H,1.526486994,0.5483393877,-1.52190
19923\H,1.1295416164,1.8597840227,-0.436926724\H,2.1719535838,0.540136
3269,0.127972265\N,-1.1690646545,0.7386165009,2.4110913233\\Version=AM
64L-G03RevC.02\State=1-A\HF=-325.8459249\RMSD=6.948e-09\RMSF=5.793e
-06\Thermal=0.\Dipole=1.5583199,-0.7342703,-0.8361959\PG=C01 [X(C5H9N1O
1)]\

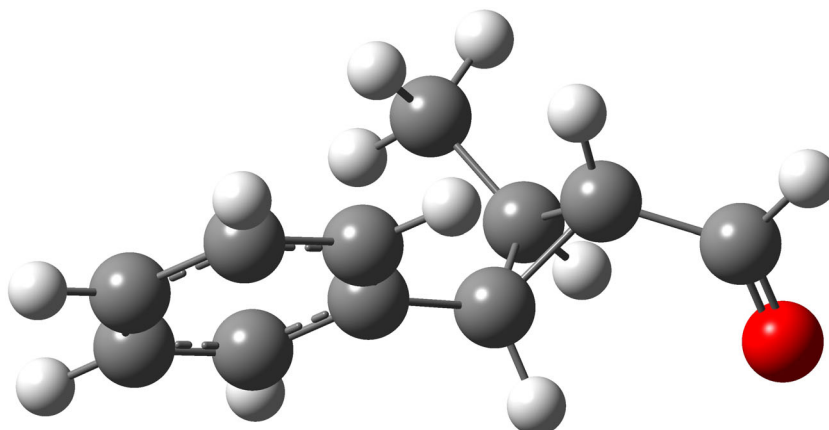
11 (Me/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O1\TSCHNEI\25-Jun-2010\
0\\# opt freq rb3lyp/6-311g(d)\DA_Me_NO_2\\0,1\C,0.0053110708,-0.0231092
809,-0.0069678509\C,-0.0053888965,-0.0516215019,2.6285554213\C,0.79493
26719,0.0148179045,1.3246322895\H,1.4096531536,0.9254253327,1.35105528
48\C,1.7199594738,-1.1531749032,1.0815439823\H,-0.677326627,0.80491991
25,2.7259954284\H,0.6691701883,-0.0328474785,3.4886220198\O,0.84291728
69,-0.8396141089,-0.8891787551\H,-0.6049311108,-0.9611868295,2.6981841
257\H,-0.0392093302,0.9635993352,-0.471735363\C,-1.3818039277,-0.64934
329,0.0388021429\H,-2.0726560233,-0.0560741396,0.6444631789\H,-1.78417
02728,-0.710321512,-0.9740457958\H,-1.3458376624,-1.6630271152,0.44482
7386\H,2.3721818387,-1.6122460007,1.8162486982\N,1.7419496333,-1.58261
49109,-0.1160456722\\Version=AM64L-G03RevC.02\State=1-A\HF=-325.938547
9\RMSD=1.909e-09\RMSF=5.804e-06\Thermal=0.\Dipole=-0.504711,0.7327459,
1.142398\PG=C01 [X(C5H9N1O1)]\

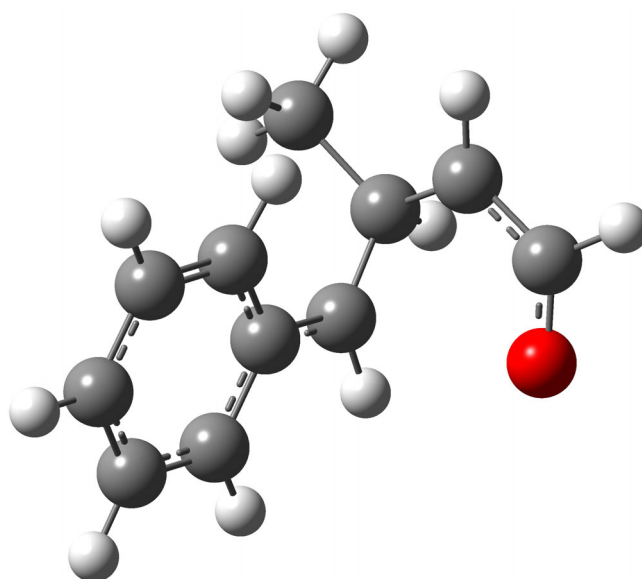
Ph-Donor

10 (Ph/CHO)



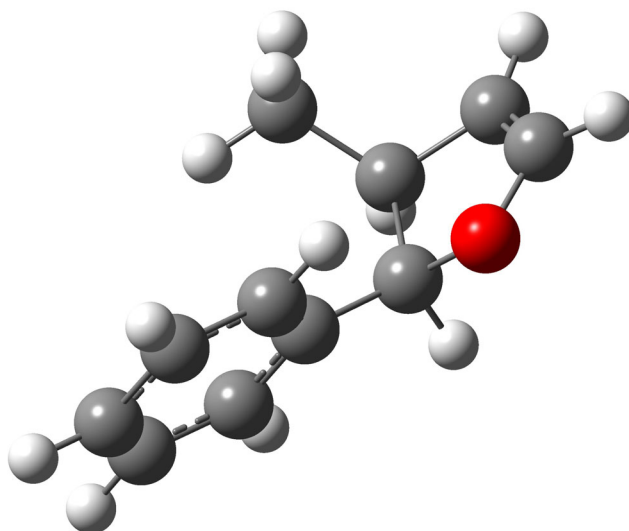
```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12O1\TSCHEI\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHO_1\0,1\C,-0.0087122495,0.038262
6779,-0.1450449459\H,-0.0007473609,0.1470757423,0.9372924694\C,1.40241
82265,-0.0597733622,-0.7234158163\H,1.5629810387,0.3353505509,-1.72136
30006\C,2.5483742969,0.0407980409,0.207730925\C,0.4922064352,-1.289648
7734,-0.6227303158\H,0.7880410433,-1.9679168709,0.1728908154\C,-0.0137
145303,-1.9492964337,-1.8837654478\H,-0.9114715571,-2.5410300637,-1.67
95196543\H,-0.2738717436,-1.2178358104,-2.6514784303\H,0.7401820078,-2
.6239411731,-2.2992737462\O,2.5240653926,-0.3210304058,1.3625905091\H,
3.4767993895,0.4767948878,-0.2206556354\C,-1.0920318303,0.8020456094,-
0.8441721403\C,-2.4183274694,0.3627115561,-0.7387038217\C,-0.834670944
7,1.9704489703,-1.5667420622\C,-3.4549135584,1.067873625,-1.3428983561
\H,-2.6358253386,-0.5400039546,-0.1754955495\C,-1.8706236,2.6783177701
,-2.1746232606\H,0.1843084515,2.335126908,-1.648403412\C,-3.1838174728
,2.2288580379,-2.0657918533\H,-4.4757417565,0.7104648164,-1.2504795587
\H,-1.6496847598,3.584138733,-2.7305369447\H,-3.9909469366,2.778865404
1,-2.5388697326\\Version=AM64L-G03RevC.02\State=1-A\HF=-501.6969046\R
MSD=5.476e-09\RMSF=2.464e-06\Thermal=0.\Dipole=-0.4644433,0.0994241,-1
.031057\PG=C01 [X(C11H12O1)]\
```

TS₁₀₋₁₁ (Ph/CHO)



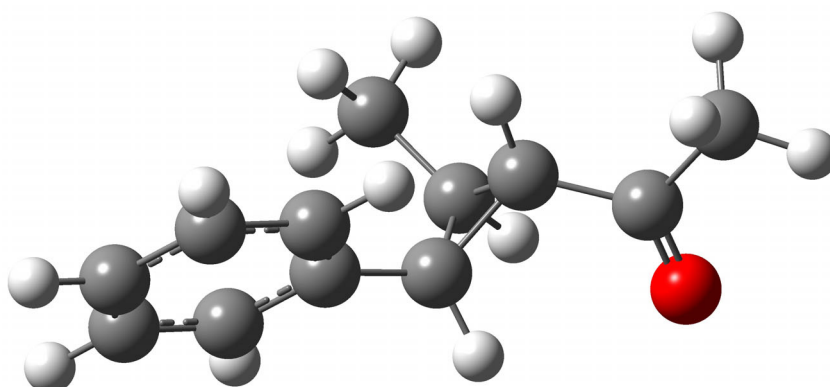
```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C11H12O1\TSCHNE\03-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=t
ight\DA_Ph_CHO_TS\0,1\C,0.3861456389,-0.2854976282,-0.0295550123\C,-
0.1638195103,0.1872015161,2.1581693471\H,0.3547367951,0.4020028661,3.0
879604911\C,-1.2832535784,0.9086043433,1.7434679493\H,-1.8222596864,1.
4649150155,2.5367859311\O,-1.7578011817,0.911477226,0.5890025363\C,0.2
926277592,-0.9622257776,1.2801268804\H,-0.4958191347,-1.7201709991,1.2
099236182\C,1.5633825953,-1.6522789722,1.7990243165\H,1.8482726337,-2.
4833979893,1.1503043601\H,2.4118414899,-0.9702635946,1.865065682\H,1.3
702842992,-2.0509569332,2.7983316165\H,-0.3460392401,-0.5710184691,-0.
7753809809\C,1.3540831231,0.6662279296,-0.4915448933\C,1.4098017428,0.
8950479495,-1.8865039496\C,2.2995690235,1.337304977,0.3212912138\C,2.3
945618036,1.6968755098,-2.44753888\H,0.6725549992,0.4205945475,-2.5259
938337\C,3.2823014318,2.1305804924,-0.2432378589\H,2.2158650776,1.2689
932459,1.3982325425\C,3.3404810008,2.3114505936,-1.6301167839\H,2.4181
432521,1.8515190994,-3.5211127022\H,3.9957987948,2.6384899923,0.397388
2185\H,4.1028374532,2.9506777751,-2.0630227545\\Version=AM64L-G03RevC.
02\State=1-A\HF=-501.6256589\RMSD=6.539e-09\RMSF=1.234e-05\Thermal=0.\
Dipole=1.5337628,-0.2650237,-0.2530244\PG=C01 [X(C11H12O1)]\
```

11 (Ph/CHO)



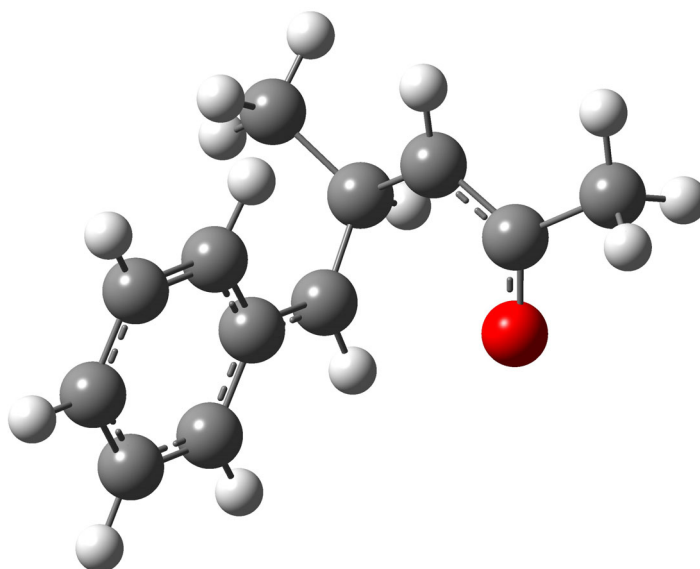
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12O1\TSCHNE\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHO_2\0,1\C,-0.0768070122,-0.36312
46663,0.0642598045\C,0.2040731572,-0.4147670178,2.6835836508\C,0.74578
67882,0.0663941544,1.329742404\H,0.8044324047,1.1597381792,1.347331869
9\C,2.0813039772,-0.5678036639,0.9907963245\H,3.0002910336,-0.40773195
02,1.5372746849\H,-0.7656903287,0.033770246,2.9133435775\H,0.898889291
6,-0.141693017,3.4831259619\C,1.8994957747,-1.4512517471,0.0134175892\
O,0.6285719054,-1.5069194674,-0.4914646755\H,0.0863979874,-1.500763163
,2.702071559\H,2.5903298629,-2.1480808009,-0.4425291277\H,0.0197984867
,0.4363947596,-0.680775815\C,-1.5366385489,-0.6823495218,0.2630079803\
C,-2.4582661483,0.3655335333,0.3613060127\C,-1.9960389013,-1.996469287
5,0.3710728502\C,-3.8085494203,0.1075283179,0.5800286578\H,-2.11788157
86,1.3930029273,0.26096785\C,-3.3489673493,-2.2558177301,0.583217072\H
, -1.2907785348,-2.8124675228,0.2704840351\C,-4.2586533161,-1.206989633
6,0.6927254803\H,-4.5105218348,0.932244127,0.6535838216\H,-3.692529077
8,-3.2827820868,0.6596187337\H,-5.3118695599,-1.4111643786,0.857001954
4\\Version=AM64L-G03RevC.02\State=1-A\HF=-501.6986303\RMSE=2.865e-09
\RMSF=9.641e-06\Thermal=0.\Dipole=0.0527916,0.2805319,0.3012827\PG=C01
[X(C11H12O1)]\

10 (Ph/COMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H14O1\TSCHNEI\03-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COR_1\0,1\C,0.0085540996,0.0001487826,-0.0119799647\H,0.0123457872,-0.0098875692,1.0756501791\C,1.4186206364,-0.0038143935,-0.592927531\H,1.5588762695,0.4967595913,-1.5457072788\C,2.5692203325,0.027740956,0.3569987277\C,0.5456621958,-1.2586979494,-0.6261454803\H,0.8545633652,-2.0082398826,0.0970286625\C,0.054222415,-1.7968692415,-1.9494757821\H,-0.830580362,-2.4258582741,-1.8107395473\H,-0.2208240639,-0.9971231022,-2.6404778176\H,0.8230877227,-2.4089914905,-2.4299349497\O,2.5000529237,-0.4820023911,1.4578206655\C,-1.0981892677,0.8011449473,-0.6275199528\C,-2.4118381519,0.3172531044,-0.5661757501\C,-0.8772491507,2.0448926746,-1.225972063\C,-3.4702664777,1.0519761693,-1.0922109566\H,-2.6019846597,-0.6444664241,-0.0988750075\C,-1.9348851644,2.7831306719,-1.7554384767\H,0.1308882426,2.444531462,-1.2713676228\C,-3.2347977204,2.2887630494,-1.6913677367\H,-4.4804898656,0.6586643253,-1.0354671139\H,-1.7415352715,3.7476432688,-2.2146189268\H,-4.0589963232,2.8624370765,-2.1029979089\C,3.8287723652,0.7215125705,-0.1241326038\H,3.6224190222,1.77298648,-0.350838167\H,4.6025996646,0.6609621683,0.6400030625\H,4.1907081085,0.2629176902,-1.050270293\Version=AM64L-G03RevC.02\State=1-AHF=-541.0304064\RMSD=9.469e-09\RMSF=4.697e-06\Thermal=0.\Dipole=-0.1744309,0.3018335,-1.022319\PG=C01 [X(C12H14O1)]\

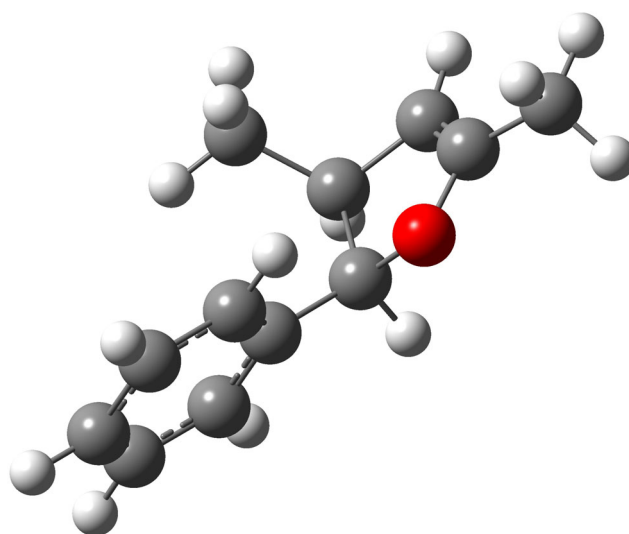
TS₁₀₋₁₁ (Ph/COME)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C12H14O1\TSCHNEI\03-Jun-2010\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_Ph_COR_TS\0,1\C,0.0106997068,-0.0118690997,0.0126434784\C,0.0397380077,-0.0049153565,2.3108031527\H,0.7927432251,0.0047576901,3.0925846391\C,-1.1203858944,0.7832824357,2.3608150136\O,-1.8473748084,0.9861843106,1.3601846663\C,0.1959463465,-0.9498353326,1.1394399359\H,-0.6316559927,-1.6681196254,1.1153913209\C,1.5096923836,-1.7447101452,1.1716683358\H,1.5773234842,-2.4227054574,0.3180220207\H,2.3885734214,-1.098865896,1.1589947057\H,1.5424246165,-2.3434953163,2.0857307475\H,-0.8917161781,-0.129933894,-0.5746789648\C,0.8948106685,1.0093651297,-0.4700368229\C,0.6324791769,1.5221563499,-1.7621466367\C,2.0432101463,1.4

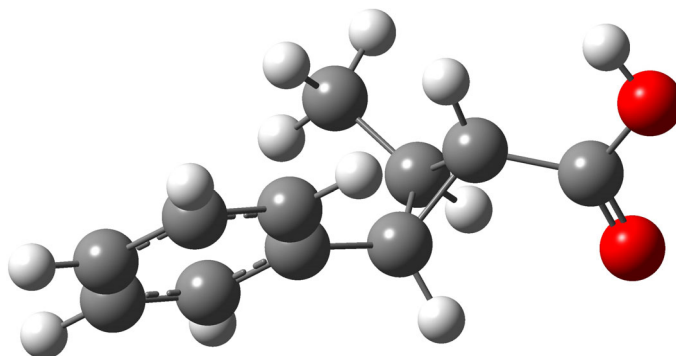
900356401,0.204731815\C,1.5021339304,2.4141074882,-2.3752979976\H,-0.2
615966937,1.1969333866,-2.284126696\C,2.910035636,2.3735656674,-0.4132
619465\H,2.2116414113,1.2013176768,1.2341692927\C,2.6493600453,2.83739
41202,-1.7080623633\H,1.2799157597,2.7876155275,-3.3694058684\H,3.7836
111375,2.7311140876,0.1220814866\H,3.3239561618,3.5456711726,-2.177654
2364\C,-1.5669800102,1.3489033713,3.7038778413\H,-1.7690006489,2.41781
98891,3.5979210598\H,-2.5061845764,0.8713591332,3.9970000541\H,-0.8356
438256,1.1980918031,4.4998025572\\Version=AM64L-G03RevC.02\State=1-A\
HF=-540.9552139\RMSD=8.218e-09\RMSF=3.906e-06\Thermal=0.\Dipole=1.28
24492,-0.1435253,-0.530685\PG=C01 [X(C12H14O1)]\\

11 (Ph/COMe)



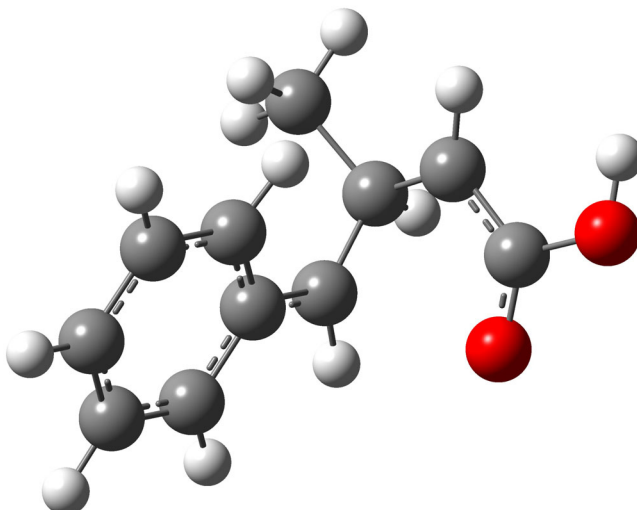
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H14O1\TSCHNEI\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COR_2\0,1\C,-0.0087010859,-0.01049
25719,0.0036220379\C,0.0077375247,-0.013445428,2.6362492129\C,0.820487
5399,-0.0003035753,1.3330132849\H,1.4609322874,0.8884206252,1.33326534
86\C,1.6130226851,-1.2754727206,1.138614663\H,2.4371224087,-1.58913141
66,1.7649546707\H,-0.5729351225,0.904165505,2.7615195517\H,0.679584045
6,-0.1060695157,3.494546256\C,1.0487782141,-2.0106491549,0.1791255976\
O,-0.0205046606,-1.3937776755,-0.4331402517\H,-0.6853115738,-0.8577955
068,2.6649701856\H,0.5695804422,0.5389449493,-0.7500879057\C,-1.408483
9848,0.5472639091,0.0533004466\C,-1.5937187519,1.9333559787,0.01269082
16\C,-2.5289865105,-0.2793454033,0.1564431317\C,-2.8700170249,2.483605
879,0.0893728776\H,-0.7320383389,2.5887111292,-0.0858907155\C,-3.80790
79202,0.2703417727,0.226949456\H,-2.3924561647,-1.3538898131,0.1626222
157\C,-3.9833166341,1.6516501961,0.1977657955\H,-2.9962837997,3.561242
8801,0.0555003462\H,-4.6702716586,-0.3849934927,0.3007188907\H,-4.9800
807822,2.0778310233,0.2510501559\C,1.3542576806,-3.3750203025,-0.32992
25395\H,2.196647641,-3.8116986607,0.20761867\H,0.4869800926,-4.0324029
853,-0.2125271229\H,1.5932816374,-3.3468594254,-1.3973638973\\Version=A
M64L-G03RevC.02\State=1-A\HF=-541.0308663\RMSD=2.807e-09\RMSF=1.01
8e-05\Thermal=0.\Dipole=0.221772,0.0691717,0.2064795\PG=C01 [X(C12H14O
1)]\\

10 (Ph/COOH)



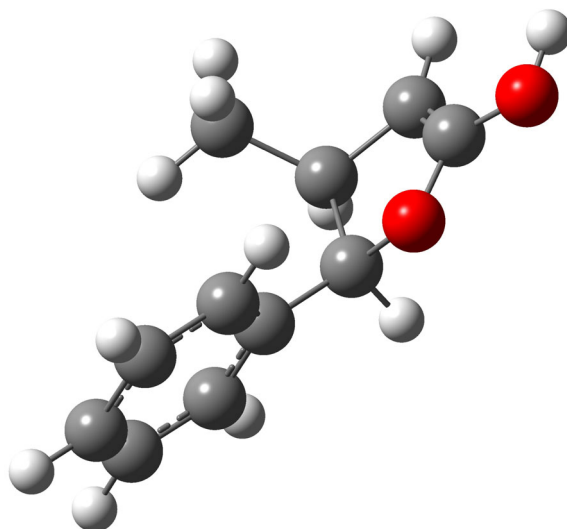
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12O2\TSCHNEI\03-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COOH_1\0,1\C,-0.081628251,-0.0914835216,0.091227002\C,0.1588944702,0.0779118187,2.7213483656\C,0.7531248452,0.0350205526,1.3328260224\H,0.3461130504,0.4053463888,-0.7761287341\H,1.6628377372,0.612492492,1.1991351209\C,0.7580481284,-1.2763434236,0.5522344606\H,0.216781971,-2.0962486819,1.0170924718\O,2.6421192046,-0.8014609178,-0.8271149688\H,-0.1106728782,1.1016129243,2.9978661688\H,0.8770017491,-0.2860355759,3.4618023737\O,2.3206959132,-2.9284709622,-0.2723944574\C,1.9757850609,-1.6112404234,-0.2411381369\H,-0.7459267781,-0.5284429304,2.8002722205\H,1.7028867671,-3.4558691688,0.2488234124\C,-1.5793477029,-0.1408608511,0.109552784\C,-2.3052529164,1.0110330165,0.4385156375\C,-2.2862994324,-1.293192079,-0.2461448936\C,-3.6970216341,1.0080445828,0.4184728299\H,-1.7712622762,1.916922434,0.7092245142\C,-3.6800577136,-1.3000642668,-0.2663044675\H,-1.7414817296,-2.1908839586,-0.521830339\C,-4.3899361104,-0.1495900437,0.0673342946\H,-4.2417705278,1.9104606756,0.6775859387\H,-4.2103969693,-2.2043653786,-0.5478580551\H,-5.4750330681,-0.1532568647,0.0518688616\\Version=AM64L-G03RevC.02\State=1-A\HF=-576.9610027\RMSD=2.955e-09\RMSF=4.304e-06\Thermal=0.\Dipole=-1.3899037,-0.3595208,1.0674674\PG=C01 [X(C11H12O2)]\

TS₁₀₋₁₁ (Ph/COOH)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C11H12O2\TSCHNEI\17-Aug-2010\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_Ph_COOH_TS\0,1\C,0.0082684104,0.0040901951,-0.0116159857\C,0.0061593875,-0.0013656415,2.5416845542\C,0.8171232309,-0.0043526124,1.2346337403\H,1.4329308207,0.9048672393,1.2304329701\C,1.6625494307,-1.2303116073,1.0581876035\H,1.7817880271,-1.944191273,1.8676252681\O,2.0029002554,-0.7037100725,-1.200221036\H,-0.5803008033,0.9145572837,2.6398519478\H,0.6962373017,-0.0553595353,3.3879430238\O,3.3618651027,-2.2287109569,-0.3021933712\C,2.3060867427,-1.3574999824,-0.1927544382\H,-0.6759668868,-0.8505719077,2.6042023387\H,0.1539933261,0.8428207651,-0.6835566661\C,-1.0400876991,-0.8862197258,-0.406427184\C,-1.9073852087,-0.436410368,-1.4305881282\C,-1.3277010841,-2.133989864,0.199157923\C,-3.0405101748,-1.156428549,-1.7819947606\H,-1.6843464583,0.4978462937,-1.9354326796\C,-2.4644659981,-2.8417134546,-0.1475723403\H,-0.6165091826,-2.5529089007,0.8994123851\C,-3.3291189381,-2.3570610759,-1.1361279368\H,-3.6929274766,-0.7883706525,-2.566690343\H,-2.6684930503,-3.7962002393,0.3264031574\H,-4.2045706256,-2.9315911538,-1.4203662666\H,3.5982757593,-2.5567128499,0.5733476864\Version=AM64L-G03RevC.02\State=1-A\HF=-576.877802\RMSD=9.241e-09\RMSF=2.151e-06\Thermal=0.\Dipole=-1.5749306,-0.0916342,1.1431929\PG=C01 [X(C11H12O2)]\

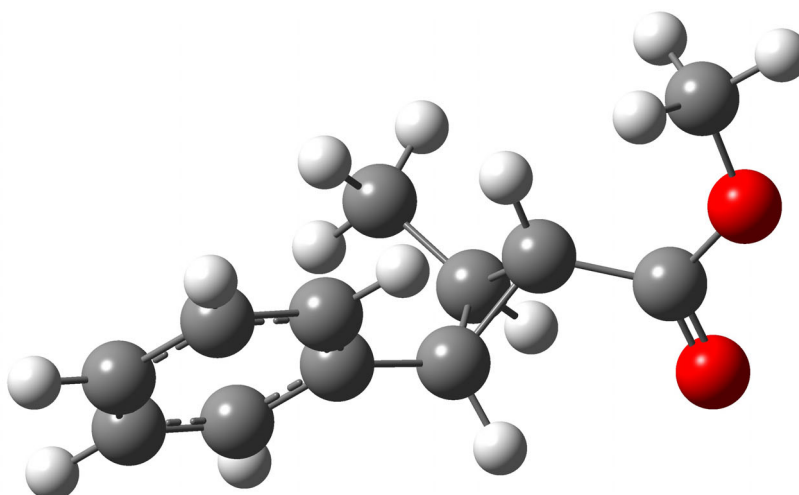
11 (Ph/COOH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12O2\TSCHNEI\29-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COOH_3\0,1\C,0.0618978641,-0.6429152679,-0.0650738745\C,0.3553665612,-0.9233123117,2.5343094917\C,0.7149057049,-0.1335036809,1.2677303887\H,-0.0709068481,0.2253255678,-0.721153016\H,0.4123890934,0.9095396539,1.4130503122\C,2.1758115144,-0.2595312232,0.8888307679\O,1.0767599392,-1.4677341291,-0.7032502608\H,-0.704853486,-0.8312603204,2.7851704026\H,0.9352727174,-0.5482341577,3.3826574301\O,3.3012817793,-1.5881699885,-0.8446607046\C,2.25826709,-1.0673190126,-0.1754180556\H,0.5848604669,-1.9856589601,2.419987715\C,-1.2388207371,-1.3954438813,0.0390231432\C,-2.4278324582,-0.6777026821,0.2063802078\C,-1.2924119422,-2.7897772532,-0.0084403217\C,-3.6449368543,-1.3396220405,0.3396763601\H,-2.4029381561,0.4088251547,0.226993679\C,-2.5119153222,-3.4527696947,0.1182559843\H,-0.3779785739,-3.3492314929,-0

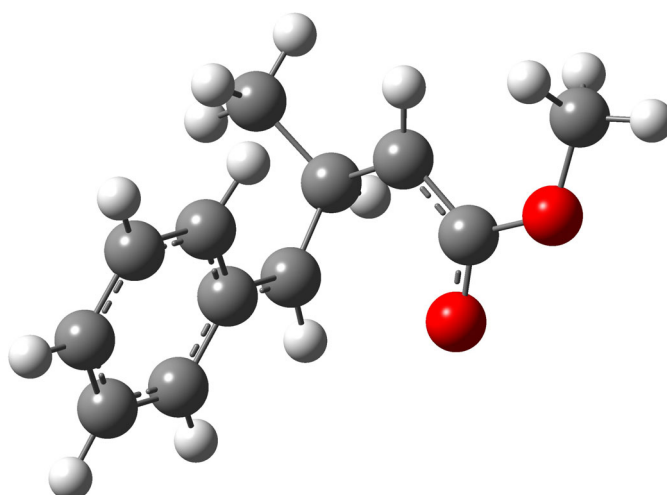
.1637296567\C,-3.6902612231,-2.7322697878,0.2966530561\H,-4.5588962829
 ,-0.7681947505,0.4677864022\H,-2.5398246728,-4.5369807096,0.072689851\
 H,-4.6389157567,-3.2505529736,0.393368051\H,4.1146623233,-1.3441635311
 ,-0.3883369884\H,3.006037993,0.123122728,1.466332303\\Version=AM64L-G0
 3RevC.02\State=1-A\HF=-576.94137\RMSD=3.488e-09\RMSF=1.948e-05\Ther
 mal=0.\Dipole=0.2631666,0.4102351,0.612284\PG=C01 [X(C11H12O2)]\\

10 (Ph/COOMe)



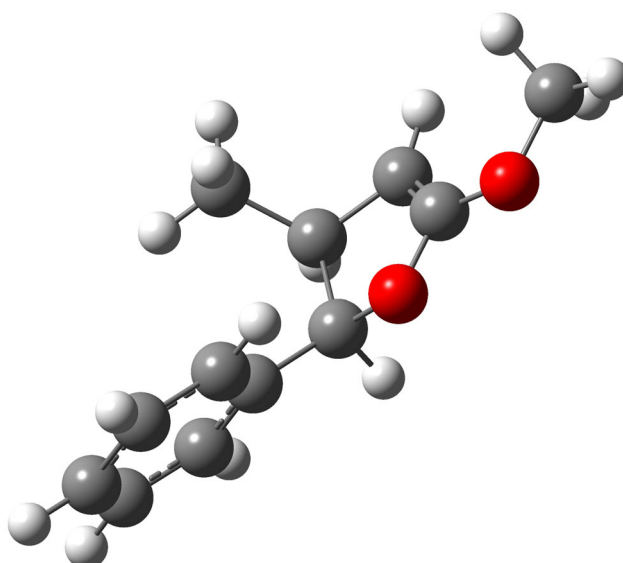
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H14O2\TSCHNEI\04-Jun-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COOR_1\0,1\C,-0.141758977,-0.06436
 72888,0.0942235011\C,0.0871993152,0.0620389879,2.7266292559\C,0.688999
 9067,0.0266774071,1.3412804156\H,0.300252547,0.4392127691,-0.761474484
 \H,1.6102232621,0.5880489579,1.2197167062\C,0.669977988,-1.2754281604,
 0.539988785\H,0.1098051228,-2.0826838253,0.9920757308\O,2.5356606773,-
 0.7643693602,-0.8291634275\H,-0.1584756683,1.0877593619,3.0179677975\H
 ,0.7905366907,-0.330785974,3.4667708801\O,2.3008339058,-2.8976517493,-
 0.3287658929\C,1.889277718,-1.6026284024,-0.2537842301\H,-0.8332024772
 ,-0.5223624246,2.7901584951\C,-1.6402013075,-0.0761166814,0.109456664\
 C,-2.3337119139,1.1069914991,0.3965285416\C,-2.3809571339,-1.21952323
 67,-0.2036776368\C,-3.724887854,1.1432715465,0.3772178645\H,-1.7736361
 555,2.0065642832,0.6339060885\C,-3.7745772454,-1.1874756175,-0.2224426
 372\H,-1.8633342886,-2.1421456918,-0.4470448945\C,-4.4512795022,-0.0063
 035877,0.0695543008\H,-4.2431919644,2.0698621115,0.6033343054\H,-4.330
 7402788,-2.086292755,-0.4699740733\H,-5.5361245608,0.0200473235,0.0556
 240693\C,1.6123711537,-3.9547392651,0.3413125443\H,1.5937204869,-3.804
 9984576,1.423774832\H,0.5934479337,-4.0778947663,-0.0352592934\H,2.181
 8696303,-4.8548364603,0.1181398475\\Version=AM64L-G03RevC.02\State=1-
 A\HF=-616.2700659\RMSD=4.160e-09\RMSF=6.033e-06\Thermal=0.\Dipole=-1.
 2078147,-0.6584805,1.0280707\PG=C01 [X(C12H14O2)]\\

TS₁₀₋₁₁ (Ph/COOMe)



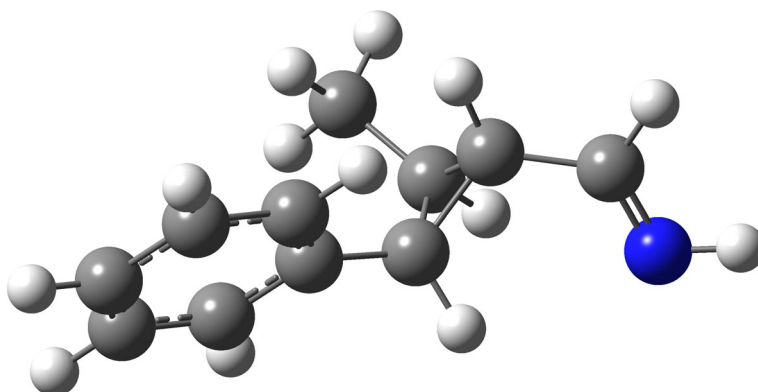
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C12H14O2\TSCHNEI\05-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=t
ight\DA_Ph_COOR_TS\0,1\C,0.0169846395,-0.3025720694,-0.1382242078\C,
-0.0330508704,0.3674275094,2.3299881616\C,0.7956376484,0.0224284576,1.
0826696118\H,1.4189938811,0.8949436609,0.849024458\C,1.6383787884,-1.2
108223533,1.2446540301\H,1.7047049141,-1.697197318,2.2093624275\O,2.06
05637859,-1.2385280573,-1.0574124628\H,-0.6183748599,1.276405493,2.175
1323684\H,0.6445218728,0.5383374196,3.1708446043\O,3.3869073075,-2.50
31553936,0.1815236999\C,2.3305089656,-1.6379161112,0.0876613407\H,-0.7
195607134,-0.4347238949,2.6049176011\H,0.194464925,0.3167914039,-1.009
9997741\C,-1.0310475189,-1.2634558959,-0.3086912509\C,-1.8505115571,-1.
1154990666,-1.4528368527\C,-1.3635707722,-2.2887851838,0.6101547566\C,
-2.9808609163,-1.9001554274,-1.6359652403\H,-1.5919812883,-0.362542865
7,-2.1901336623\C,-2.4966938652,-3.0606370745,0.4279403387\H,-0.689722
7403,-2.4981118454,1.4308412833\C,-3.3142728039,-2.869521626,-0.692498
1489\H,-3.5956566064,-1.7641238738,-2.5193883191\H,-2.7351258936,-3.84
17375999,1.1423852213\H,-4.1876323099,-3.4961846084,-0.8402384315\C,3.
8822457787,-2.8789017285,1.4605002556\H,3.1568883079,-3.4882845494,2.0
102513914\H,4.7727349605,-3.4771997732,1.2715890118\H,4.149288745,-2.0
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73302,1.0555514\PG=C01 [X(C12H14O2)]\
```

11 (Ph/COOMe)



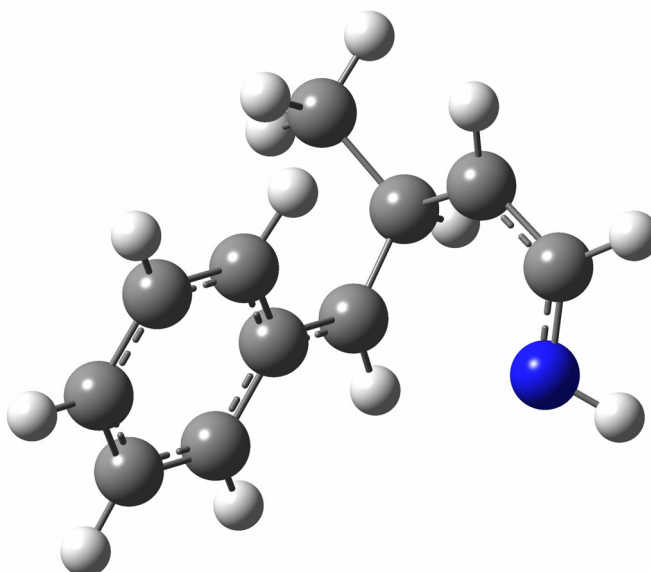
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H14O2\TSCHNEI\04-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_COOR_2\0,1\C,0.0263472368,-0.8721164307,-0.0659269641\C,0.2457417098,-1.0647244582,2.5473386989\C,0.7155593251,-0.3829347535,1.2542756914\H,0.0114787577,-0.0261282022,-0.7637538202\H,0.5405243514,0.6946476567,1.3481300128\C,2.1572768136,-0.7011418332,0.9154641164\O,0.9399238596,-1.8446940139,-0.6411584117\H,-0.7975136164,-0.8310674164,2.7765819242\H,0.8583533091,-0.7273054154,3.3884948968\O,3.1297711532,-2.2346688024,-0.7393451537\C,2.160478772,-1.5630163771,-0.111626055\H,0.3429558697,-2.1512469593,2.4816758476\C,-1.3600129392,-1.4518026721,0.0446989552\C,-2.4515054004,-0.5853582678,0.1668669603\C,-1.5880248459,-2.8292172107,0.0455029367\C,-3.7436815658,-1.0842545886,0.3033511232\H,-2.2902450933,0.4895186453,0.1493405087\C,-2.8826532014,-3.3292578935,0.1754627787\H,-0.7491151499,-3.5038497708,-0.0743903398\C,-3.963199935,-2.4609618477,0.3087590828\H,-4.5800450844,-0.3985404865,0.3961488173\H,-3.0460666828,-4.4024277112,0.1680202015\H,-4.9705895112,-2.8524607321,0.4081918653\C,4.4417649969,-2.0548961531,-0.2151145923\H,5.0972757395,-2.6682346566,-0.8292261549\H,4.7459670467,-1.005833379,-0.2816880429\H,4.4929309181,-2.3834708999,0.8273676861\H,3.0109917618,-0.3879608754,1.4965181505\\Version=AM64L-G03RevC.02\State=1-A\HF=-616.2565116\RMSD=4.305e-09\RMSF=1.310e-05\Thermal=0.\Dipole=0.4311971,0.3401473,0.4849297\PG=C01 [X(C12H14O2)]\\

10 (Ph/CHNH)



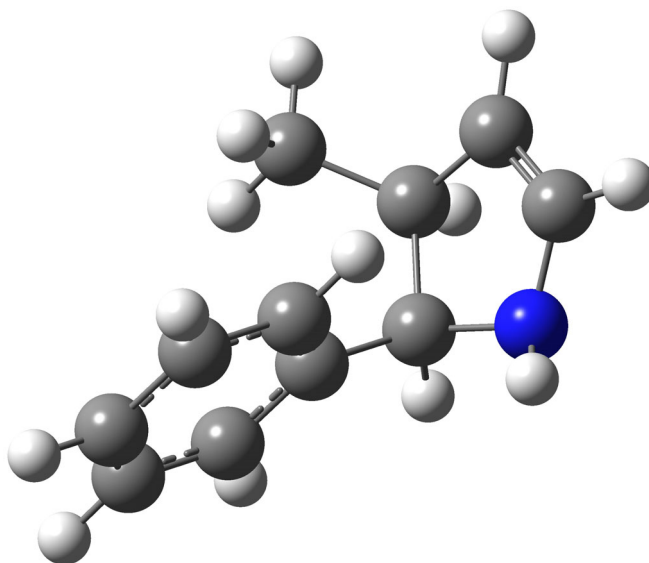
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H13N1\TSCHNEI\08-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHNH_1\0,1\C,-0.0616874353,-0.0457397854,0.1392267385\C,0.1313953728,0.0458822874,2.7743400979\C,0.7555254524,0.0415944842,1.3986587324\H,0.3786666246,0.4807357785,-0.7044595532\H,1.6673876194,0.6234489663,1.2965881663\C,0.77564238,-1.2422953036,0.570147092\H,0.2400022128,-2.0814486185,1.0028022149\H,-0.158558102,1.0589880201,3.0709283938\H,0.8356010933,-0.328892615,3.5232017531\C,1.9908839031,-1.5961707255,-0.1987590682\H,-0.7670507243,-0.5736336395,2.816579441\N,2.6725332537,-0.7207102241,-0.8207436355\H,2.2605152044,-2.6619203601,-0.1841571053\C,-1.5595968626,-0.0812952926,0.1439073304\C,-2.2759148691,1.0920003577,0.4165191545\C,-2.279653533,-1.2412724019,-0.1568923535\C,-3.6674044773,1.1033234328,0.3944573061\H,-1.7318914554,2.0032767511,0.647086844\C,-3.6737874535,-1.2343753543,-0.1786764411\H,-1.7440106178,-2.157432385,-0.3845608944\C,-4.3726453305,-0.0624737064,0.0981329658\H,-4.202856758,2.0228368096,0.610024196\H,-4.2130621031,-2.1463096092,-0.4159216874\H,-5.4578668667,-0.0557885742,0.0821962449\H,3.4766349292,-1.1434381325,-1.2837990575\\Version=AM64L-G03Rev C.02\State=1-A\HF=-481.8081379\RMSD=7.387e-09\RMSF=2.482e-06\Thermal=0.\Dipole=-0.0566076,-0.5687905,0.2656384\PG=C01 [X(C11H13N1)]\\

TS₁₀₋₁₁ (Ph/CHNH)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C11H13N1\TSCHNEI\09-Jun-2010\0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\DA_Ph_CHNH_TS\0,1\C,0.0902668187,-0.4358194562,-0.1779615103\C,-0.0635164341,0.1459077066,2.3129509504\C,0.807798134,-0.0855003663,1.0699790759\H,1.3703588411,0.8362361503,0.8791831406\C,1.7701297467,-1.2382785148,1.2251994475\H,1.7827498465,-1.8014585057,2.1547447614\H,-0.7108144771,1.0155276515,2.180151055\H,0.5813328372,0.3279647675,3.1777312505\C,2.5969572435,-1.5986094611,0.1585472866\H,-0.6977457856,-0.7133260573,2.537306592\N,2.3109218588,-1.3436747743,-1.0925193574\H,3.5397615815,-2.0971626855,0.4287183629\H,3.1468542573,-1.3706056833,-1.6811578489\H,0.2528993166,0.2092304937,-1.0322193893\C,-0.8601275805,-1.4865483412,-0.4008436654\C,-1.667646312,-1.3940864729,-1.5592384977\C,-1.1032703979,-2.5724345801,0.4740520118\C,-2.7009835358,-2.2898342021,-1.795486376\H,-1.4789641024,-0.5923982488,-2.2663012943\C,-2.142111428,-3.4577049337,0.2398450614\H,-0.4363753375,-2.7382124159,1.3108880574\C,-2.9516692439,-3.3217656447,-0.8924184995\H,-3.3073350218,-2.1893233605,-2.6899798727\H,-2.3084380508,-4.2818014577,0.9264308108\H,-3.74965858,-4.0324056177,-1.0809715347\Version=AM64L-G03RevC.02\State=1-A\HF=-481.7331926\RMSD=8.042e-09\RMSF=1.611e-05\Thermal=0.\Dipole=-0.3456577,0.0279869,0.1943973\PG=C01 [X(C11H13N1)]\

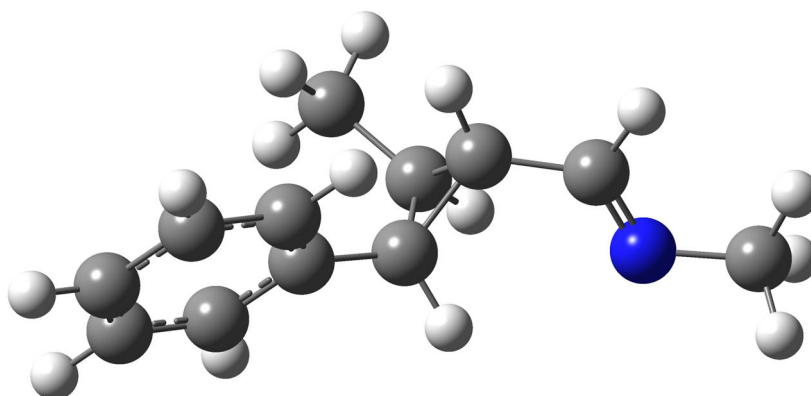
11 (Ph/CHNH)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H13N1\TSCHNEI\09-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHNH_2\0,1\C,-0.0436733183,0.0106941818,0.0784131133\C,0.1500917369,-0.0281591998,2.7144843554\C,0.8743087689,-0.0140506159,1.3662345489\H,1.4858794594,0.8997436598,1.3312047863\C,1.7718967455,-1.2047972619,1.0932396005\H,2.4786027277,-1.6095000605,1.8051999271\H,-0.5059740449,0.8393259115,2.8309658588\H,0.8794150458,0.000519437,3.5295144042\C,1.6509193705,-1.5662855396,-0.1865373282\H,-0.4584078412,-0.9257413396,2.8404347453\H,-0.1341093908,1.0409113879,-0.2745277762\N,0.748125999,-0.7682567308,-0.9060635935\H,0.1943751117,-1.2468972236,-1.605656676\H,2.1958203455,-2.3396580282,-0.7157443159\C,-1.4517704011,-0.5333970166,0.2684798872\C,-2.5302344741,0.3515375021,0.3604633936\C,-1.7122342635,-1.907214195,0.3561345879\C,-3.83

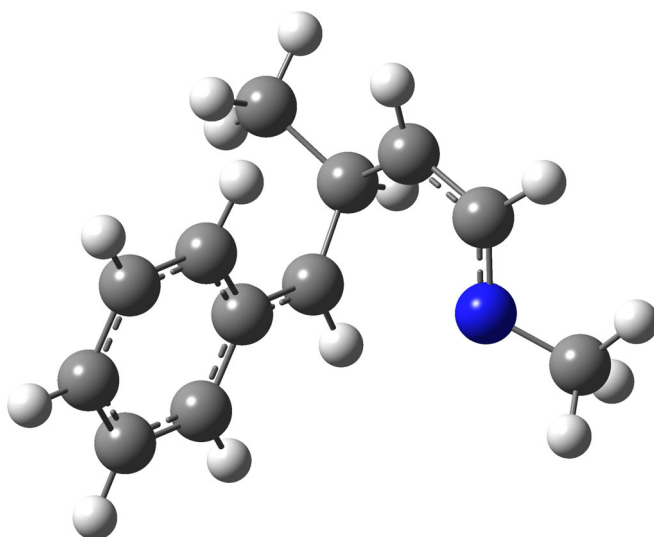
12702862,-0.1136485176,0.5430032066\H,-2.3496928755,1.4202539367,0.2814846424\C,-3.0106195467,-2.3761127379,0.5385674371\H,-0.8909792058,-2.6135459852,0.2965850992\C,-4.0757077878,-1.4812338632,0.6332704021\H,-4.6533180329,0.5925563829,0.6067314781\H,-3.1917772331,-3.4443274963,0.6083468306\H,-5.0875467646,-1.8484836176,0.7721100442\\Version=AM64L-G03RevC.02\State=1-A\HF=-481.8239756\RMSD=5.440e-09\RMSF=8.195e-06\Thermal=0.\Dipole=-0.3211203,-0.1819204,-0.072048\PG=C01 [X(C11H13N1)]\\

10 (Ph/CHNMe)



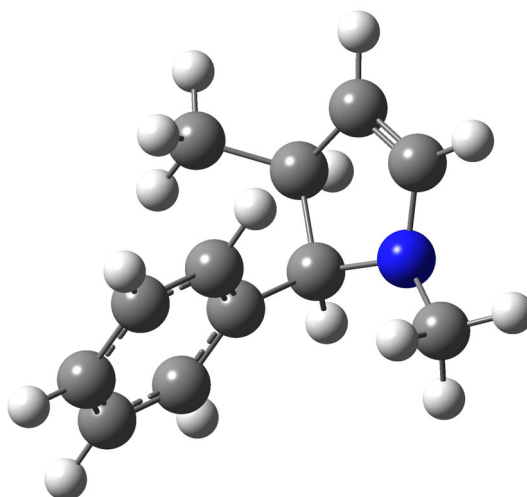
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H15N1\TSCHNEI\09-Jun-2010\0\# opt freq rb3lyp/6-311g(d) geom=connectivity\\DA_Ph_CHNH_1\\0,1\C,-0.0151699728,-0.0122544911,0.2945279062\C,-0.0338101462,0.0988908578,2.9367493402\C,0.6990010298,0.1035335599,1.6155971122\H,0.4738193388,0.5263746817,-0.5138051412\H,1.5971646368,0.7140320782,1.5825559137\C,0.8202141388,-1.17976223,0.7982988791\H,0.2761235992,-2.0320766652,1.193122982\H,-0.3790052963,1.1042728217,3.1985883133\H,0.6190815196,-0.2472976726,3.7436839882\C,2.0996936178,-1.5135056901,0.1291860416\H,-0.9129603647,-0.5488587649,2.9138041659\N,2.8200491287,-0.64168234,-0.4410825721\H,2.3991755762,-2.574557902,0.1626286666\C,-1.5076249089,-0.0819973187,0.1840620019\C,-2.2619698055,1.088820517,0.3415702567\C,-2.1843714407,-1.2690894039,-0.111282612\C,-3.6475861924,1.0718846389,0.2142446134\H,-1.7521297981,2.0215557639,0.564807563\C,-3.5729971033,-1.2907880467,-0.2372902663\H,-1.6195348653,-2.1848286488,-0.254192451\C,-4.3097784315,-0.1210068853,-0.073749914\H,-4.2121866776,1.9904768732,0.3413053132\H,-4.0778068552,-2.2238681367,-0.4681373291\H,-5.3906084517,-0.1367078538,-0.1715462667\C,4.0614752057,-1.0632843773,-1.0570279639\H,4.0491203956,-0.7981186366,-2.1185767633\H,4.8957137905,-0.5177993321,-0.6052481219\H,4.2565820242,-2.1433302649,-0.9657984505\\Version=AM64L-G03RevC.02\State=1-A\HF=-521.1283204\RMSD=4.654e-09\RMSF=3.727e-06\Thermal=0.\Dipole=0.0018341,-0.3776436,0.1872387\PG=C01 [X(C12H15N1)]\\

TS₁₀₋₁₁ (Ph/CHNMe)



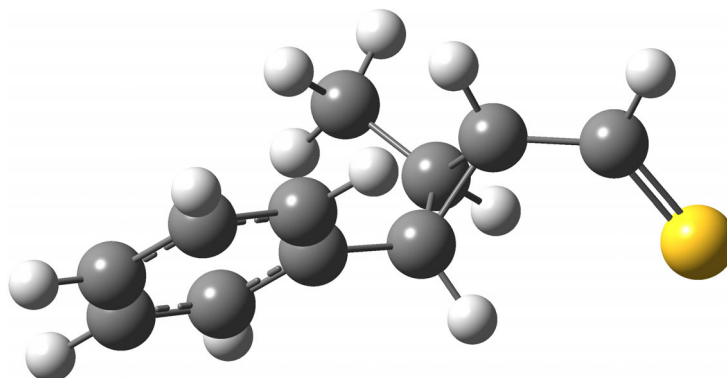
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C12H15N1\TSCHNE\09-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_Ph_CHNR_TS\0,1\C,0.0872888417,-0.4250480276,-0.163296977\C,-0
.031704481,0.0985902813,2.3402073489\C,0.8274494863,-0.1234027826,1.08
64907684\H,1.4045472174,0.7930297975,0.9132544375\C,1.7692271564,-1.29
29679005,1.2122412808\H,1.7837186891,-1.8707330542,2.13295597\H,-0.662
6103157,0.9832899712,2.2303962422\H,0.6213319647,0.2487899739,3.205102
7947\C,2.5775895824,-1.6664234714,0.1349621026\H,-0.6812828909,-0.7532
415849,2.5489636108\N,2.316451291,-1.3803088422,-1.1103205616\H,3.5024
639262,-2.2108639606,0.3843421157\H,0.2454867856,0.2457816689,-0.99909
43412\C,-0.8773447181,-1.4556751518,-0.4054412021\C,-1.7059444921,-1.3
157107681,-1.5453229938\C,-1.1169475551,-2.5695941702,0.4355970036\C,-
2.7530834852,-2.191695119,-1.7923083617\H,-1.5235504167,-0.4907122883,
-2.2269569447\C,-2.1707272626,-3.4343155364,0.1912974319\H,-0.43543439
24,-2.7719954605,1.2524068265\C,-2.9994983724,-3.2514506566,-0.9201927
263\H,-3.3749451811,-2.0536944186,-2.6710847354\H,-2.3335057827,-4.279
7229692,0.8524150743\H,-3.8086627195,-3.9467061718,-1.1180897282\C,3.4
026294476,-1.4056053637,-2.0672084976\H,4.2928527751,-1.9397193284,-1.
6991046915\H,3.0730292434,-1.8750694026,-2.9995620809\H,3.7208762306,
-0.3850787449,-2.3194206589\Version=AM64L-G03RevC.02\State=1-A\HF=-5
21.0522944\RMSE=8.721e-09\RMSE=7.156e-06\Thermal=0.\Dipole=-0.372115
7,0.0722595,0.1076418\PG=C01 [X(C12H15N1)]\
```

11 (Ph/CHNMe)



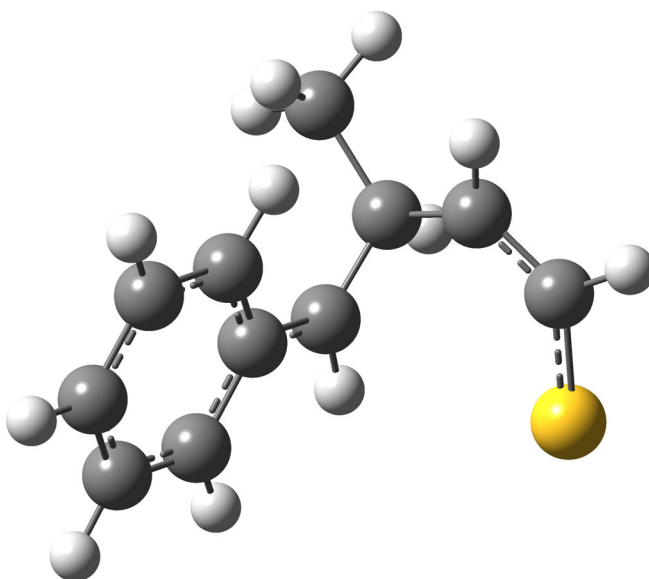
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C12H15N1\TSCHNEI\09-Jun-2010\0\# opt freq rb3lyp/6-311g(d) geom=connectivity\DA_Ph_CHNH_2\0,1\C,-0.0054641752,0.057120253,0.1105049856\C,0.1646872782,-0.0769516176,2.741968288\C,0.8982265262,-0.0314127036,1.4003067055\H,1.527064459,0.8725330309,1.4019064866\C,1.7843247603,-1.2235662233,1.0853401785\H,2.4736223586,-1.6768589678,1.7842244437\H,-0.4806328719,0.7956571888,2.8807108514\H,0.8902341085,-0.0814226361,3.5609278477\C,1.7006988868,-1.4867115558,-0.2239789557\H,-0.4553396682,-0.969719036,2.8405507947\H,-0.11244911,1.1040107232,-0.189853598\N,0.8172119408,-0.6475288686,-0.9006676894\H,2.2602845177,-2.2197948267,-0.7940129886\C,-1.4108896581,-0.5157774472,0.261989322\C,-2.5119415073,0.3444533581,0.2474994322\C,-1.6455398011,-1.8890291607,0.4173746756\C,-3.8109273965,-0.1411748529,0.3941467645\H,-2.3522839992,1.4117781515,0.1179819795\C,-2.9406983462,-2.3786889097,0.5598309013\H,-0.8062889716,-2.5752608866,0.4351527472\C,-4.0293461559,-1.5064845936,0.550538555\H,-4.6500357615,0.5476001589,0.3801106546\H,-3.1018780353,-3.4456411341,0.6800814281\H,-5.0385234186,-1.8903714207,0.6614558743\C,0.2665586001,-0.9931536094,-2.1945943239\H,1.0690208245,-1.362523427,-2.8374748327\H,-0.5276938792,-1.7523066459,-2.158892801\H,-0.1476354038,-0.0986918411,-2.6672211747\Version=AM64L-G03RevC.02\State=1-A\HF=-521.1382091\RMSD=5.935e-09\RMSF=3.720e-06\Thermal=0.\Dipole=-0.1975911,-0.0388635,-0.2756493\PG=C01 [X(C12H15N1)]\

10 (Ph/CHS)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12S1\TSCHNEI\07-Sep-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHS_1\0,1\C,-0.0008817319,0.0044666322,-0.1063222351\H,0.082136464,0.0765977736,0.9765860559\C,1.3802562766,-0.050679229,-0.7789461278\H,1.4320993578,0.3770981433,-1.7752001425\C,2.6080853215,0.0485978827,0.0038680974\C,0.4680059433,-1.2930183033,-0.6666625078\H,0.8284278847,-1.9997163009,0.0760546056\C,-0.0902852918,-1.9051998035,-1.9291857037\H,-0.951768342,-2.541135306,-1.7023654271\H,-0.4234321326,-1.1471527123,-2.6406629638\H,0.6602292566,-2.529734017,-2.4214129517\H,3.4458816568,0.5040823303,-0.5287220435\C,-1.1101049697,0.8130262195,-0.707781144\C,-2.4188843019,0.3145997513,-0.6939251346\C,-0.887510253,2.0880611995,-1.2368607085\C,-3.4745213983,1.0686596647,-1.1991961392\H,-2.6090812013,-0.6705516595,-0.2790972372\C,-1.9421549654,2.8443736193,-1.7444202348\H,0.1191788484,2.4938851652,-1.2460360773\C,-3.2389075036,2.3364976413,-1.7282016709\H,-4.4822415477,0.6656604165,-1.1805523512\H,-1.7496246256,3.8325470864,-2.1502219887\H,-4.0608463182,2.9244224467,-2.1237977326\S,2.8526702003,-0.4444166472,1.5462301146\Version=AM64L-G03RevC.02\State=1-A\HF=-824.6585907\RMSD=7.080e-09\RMSF=1.567e-05\Thermal=0.\Dipole=-0.8113708,0.1127302,-1.1113805\PG=C01 [X(C11H12S1)]\

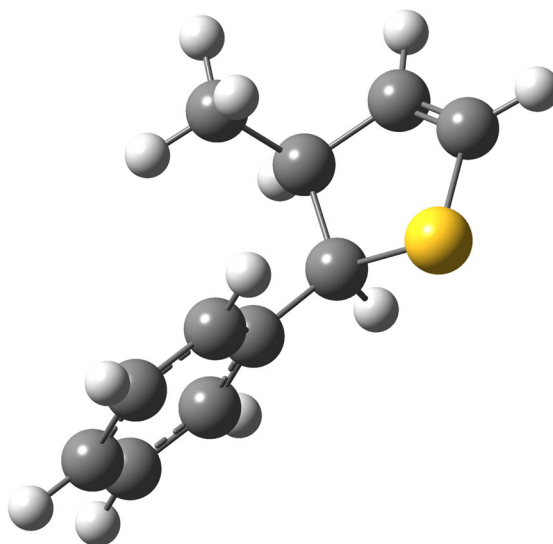
TS₁₀₋₁₁ (Ph/CHS)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C11H12S1\TSCHNEI\07-Sep-2010\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_Ph_CHS_TS\0,1\C,0.020179947,0.0129155209,-0.0252202092\C,-0.0222667166,0.0759801704,2.2830360738\H,0.819935288,0.2492147486,2.9514063038\C,-1.2146330599,0.7071357592,2.5236257959\H,-1.3116151237,1.1407371945,3.5217921346\C,0.2052739023,-0.8911331039,1.1292246718\H,-0.6158365959,-1.6137405317,1.1141726143\C,1.5271574146,-1.663458945,1.2330626965\H,1.6471201176,-2.3420452634,0.3855859953\H,2.401183966,-1.0120921739,1.2641316282\H,1.5212088877,-2.2608303433,2.1484193265\H,-0.8992819023,-0.1197026521,-0.5822437094\C,0.8523486088,1.0664944079,-0.5121142013\C,0.4719317759,1.6711616721,-1.7359044425\C,2.0491797067,1.5193639188,0.0994258261\C,1.2656210983,2.6338330169,-2.3422883728\H,-0.4580674737,1.3651456602,-2.2033139523\C,2.8357830013,2.4788358133,-0.509

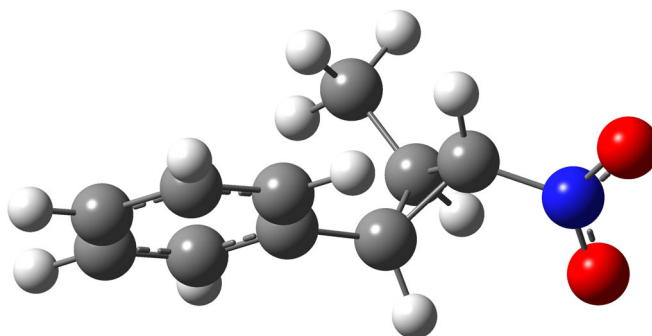
8006396\H,2.3336596875,1.1399394571,1.0717777007\C,2.4535732779,3.0374
434295,-1.7359266786\H,0.9540971593,3.078039485,-3.2815332241\H,3.7467
829435,2.8138632544,-0.0251886834\H,3.0721821097,3.7974440813,-2.20142
47208\S,-2.5691221264,0.8586538294,1.5158214256\\Version=AM64L-G03Rev
C.02\State=1-A\HF=-824.6072151\RMSD=7.347e-09\RMSF=3.719e-06\Thermal=
0.\Dipole=2.2612554,-0.0476507,-1.0095379\PG=C01 [X(C11H12S1)]\\

11 (Ph/CHS)



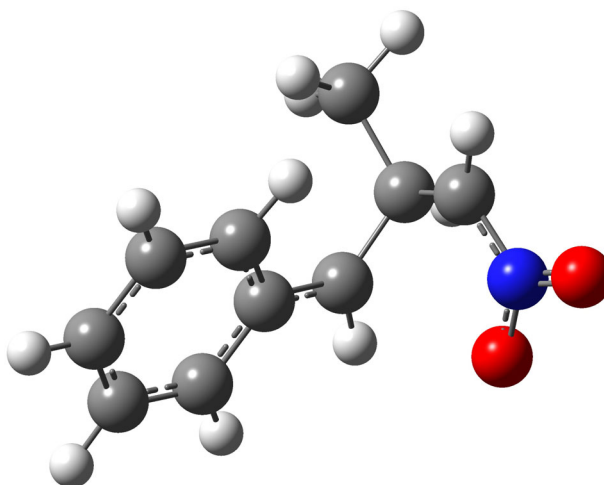
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C11H12S1\TSCHNEI\08-Sep-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Ph_CHS_2\0,1\C,0.0073113485,0.0477297
311,-0.0235516585\C,0.1364296153,0.1264531173,2.5930602189\C,0.8883062
801,-0.0454970958,1.2635526795\H,1.6412819289,0.7485119767,1.193792702
\C,1.5347994088,-1.4131848482,1.1942154489\H,2.4086398411,-1.657609103
5,1.7895351116\H,-0.32052932,1.1153292282,2.6722394135\H,0.8291881218,
0.0077019057,3.4308324754\C,0.8818626174,-2.3129276422,0.4596036603\H,
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0.3497864517\H,0.6848784492,0.2856929742,-0.847232687\C,-1.1074784751,
1.0674455933,-0.013120688\C,-0.8483507064,2.348239922,-0.5161235202\C,
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,1.7963516618,0.5380236555\H,-2.6059353714,-0.1855932726,0.8893559492\
C,-3.081454575,3.0698317227,0.0439185395\H,-1.59910148,4.3283928952,-0
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.840469244,0.0633584666\S,-0.5494774565,-1.6978883817,-0.3896479211\\V
ersion=AM64L-G03RevC.02\State=1-A\HF=-824.6804733\RMSD=7.569e-09\R
MSF=3.151e-05\Thermal=0.\Dipole=0.3270922,0.4534038,0.3606217\PG=C01
[X(C11H12S1)]\\

10 (Ph/NO₂)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C10H11N1O2\TSCHNEI\07-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_NO2_1\0,1\C,-0.0768730758,-0.0793004493,0.0994993874\C,0.1702773034,0.1120087415,2.7399799795\C,0.7607427123,0.0496684415,1.3503230389\H,0.371382716,0.4006565941,-0.7665915805\H,1.6792011527,0.6086176024,1.202121547\C,0.7302865518,-1.2580916975,0.5926548883\H,0.2437981349,-2.1216251661,1.0223637992\H,-0.0827378072,1.1423445616,3.0054699407\H,0.8848876785,-0.2572996688,3.4802895922\O,2.5806020324,-0.7850805171,-0.7207310915\H,-0.743099695,-0.479846593,2.8244597137\N,1.9197869198,-1.6614731524,-0.1767294714\O,2.1655622379,-2.8588913642,-0.2164471242\C,-1.5750222829,-0.1215890532,0.1043685189\C,-2.2970841847,1.0336787152,0.4274868843\C,-2.2798112874,-1.2741164006,-0.2547171483\C,-3.6887133851,1.0346016879,0.3960011749\H,-1.7624623109,1.9381468854,0.7016380829\C,-3.6731949275,-1.2755448325,-0.2852430888\H,-1.7357516992,-2.1747916577,-0.5215122248\C,-4.3814822161,-0.1217851378,0.040890331\H,-4.2329360488,1.9387678683,0.6495711938\H,-4.2041337423,-2.1789916596,-0.5675499483\H,-5.4663675224,-0.1222873543,0.0173743193\\Version=AM64L-G03RevC.02\State=1-A\HF=-592.9043997\RM SD=3.204e-09\RMSF=5.784e-06\Thermal=0.\Dipole=-1.37106,0.7011466,0.8277061\PG=C01 [X(C10H11N1O2)]\\

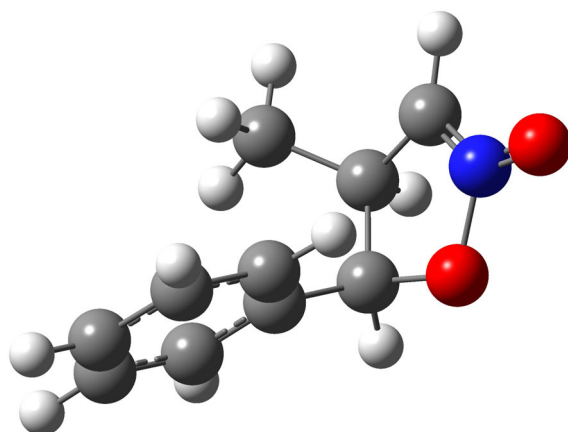
TS₁₀₋₁₁ (Ph/NO₂)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C10H11N1O2\TSCHNEI\09-Jun-2010\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf =tight\DA_Ph_NO2_TS\0,1\C,0.1459478751,-0.3914682077,-0.0925950613\C

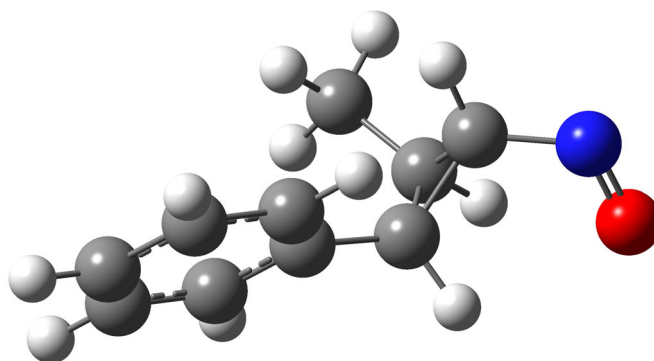
, -0.0771043734, 0.5805329995, 2.2744605478\C, 0.8271916234, 0.0322347051, 1.1610080913\H, 1.5532402951, 0.8087812682, 0.8926400047\C, 1.5237054114, -1.2264559922, 1.5411713728\H, 1.4624645357, -1.7081119275, 2.5057955453\H, -0.5652893636, 1.5034509272, 1.9557082319\H, 0.5317682106, 0.8031972204, 3.154068632\O, 2.3535995871, -1.3638502819, -0.5695044087\H, -0.853224113, -0.1275639336, 2.5674145545\N, 2.3666338855, -1.8016388778, 0.6256335192\O, 3.1427617806, -2.7042780802, 0.985681777\H, 0.4760346359, 0.0877210473, -1.0064963821\C, -0.9425496594, -1.2994712226, -0.2662606123\C, -1.5989672306, -1.2682928477, -1.5215906829\C, -1.4660745608, -2.1613494321, 0.7309588537\C, -2.7550417297, -2.0013352753, -1.7466970088\H, -1.1925191144, -0.6456720399, -2.3116786277\C, -2.6214415347, -2.8841423394, 0.5018116291\H, -0.9250704827, -2.2919110094, 1.659069317\C, -3.2750979673, -2.8055497534, -0.7345510867\H, -3.2439014282, -1.9566667747, -2.7138290686\H, -3.0065146198, -3.5406945256, 1.2746585797\H, -4.1691218496, -3.3937771807, -0.9123859523\\Version=AM64L-G03RevC.02\State=1-A\HF=-592.8264114\RMSD=5.830e-09\RMSF=3.051e-05\Thermal=0.\Dipole=-2.8670338, 0.9307477, 0.1547098\PG=C01[X(C10H11N1O2)]\

11 (Ph/NO₂)



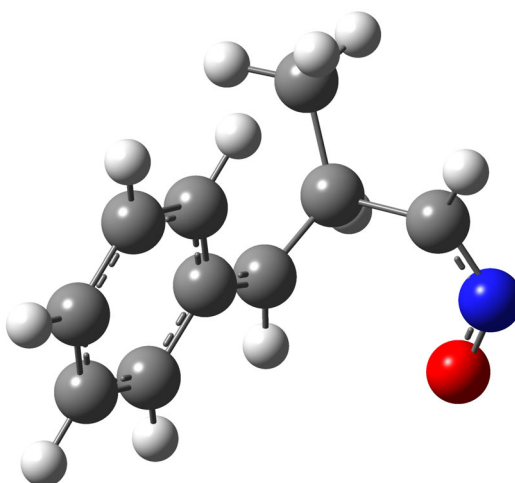
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C10H11N1O2\TSCHEI\07-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_NO2_2\0,1\C, -0.0301961102, -0.111953371, 0.0246323017\C, 0.0738499043, 0.1501778775, 2.6507150674\C, 0.831850011, 0.065351411, 1.324396022\H, 1.4213754891, 0.9868613867, 1.2110214532\C, 1.7403885737, -1.1141239224, 1.2090303231\H, 2.3892630447, -1.5478952365, 1.9539228529\H, -0.5950193413, 1.0136785792, 2.6698992791\H, 0.7798853934, 0.2650081741, 3.4775319871\O, 0.7986317155, -0.898694048, -0.8493203248\H, -0.5240927711, -0.7437959039, 2.833381875\N, 1.7379797171, -1.6368092659, 0.0175472786\O, 2.327104855, -2.55736972, -0.5144710705\H, -0.152603844, 0.8543681208, -0.4691638021\C, -1.3894610597, -0.7585147329, 0.2108389362\C, -2.5003842969, 0.0401983049, 0.4971708737\C, -1.5615728167, -2.1399832572, 0.0926573495\C, -3.7564706312, -0.5296133356, 0.688514337\H, -2.3866563124, 1.1192605616, 0.5613548529\C, -2.8179565293, -2.7108552907, 0.2838912253\H, -0.7194702698, -2.7654471894, -0.1798449745\C, -3.9171102971, -1.9098968466, 0.5868426514\H, -4.6101780344, 0.1045146724, 0.9054730493\H, -2.9388850433, -3.7848920012, 0.1856818031\H, -4.8955711754, -2.3569864224, 0.7297752228\\Version=AM64L-G03RevC.02\State=1-A\HF=-592.9022269\RMSD=9.920e-09\RMSF=1.550e-05\Thermal=0.\Dipole=-0.7457576, 0.9947838, 1.2520692\PG=C01[X(C10H11N1O2)]\

10 (Ph/NO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C10H11N1O1\TSCHNEI\25-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Ph_NO_1\0,1\C,0.074969298,0.0774650
167,-0.0785835525\H,0.3529188858,0.2550545002,0.9598025728\C,1.3251298
502,-0.1072182092,-0.9396360918\H,1.3171680421,0.2354331284,-1.9668744
122\C,0.4259960972,-1.2900681546,-0.561339697\H,0.8984949628,-1.914970
2754,0.1931972731\C,-0.3330232821,-2.0202548842,-1.642991507\H,-1.1619
741995,-2.5925601541,-1.2153516247\H,-0.7559273482,-1.336888212,-2.381
8913364\H,0.3204789431,-2.7243598525,-2.1647132011\N,2.6318195185,0.01
32278733,-0.3401709148\O,2.6945197038,-0.3293644096,0.8231292505\C,-1.
0945618224,0.8676446808,-0.5786161029\C,-2.3968011533,0.4056682864,-0.
3522958507\C,-0.9233427569,2.0980182358,-1.221014102\C,-3.4985332428,1
.152159376,-0.7619200473\H,-2.5458153815,-0.5427243785,0.1545690462\C,
-2.024289613,2.8457274449,-1.6332756141\H,0.0798481467,2.4744854505,-1
.3948398779\C,-3.3152673335,2.3743779354,-1.4059404761\H,-4.5010001306
,0.7787613206,-0.578135262\H,-1.872320028,3.7985496502,-2.1303227326\H
,-4.1732657086,2.9560283653,-1.7271821682\Version=AM64L-G03RevC.02\S
tate=1-A\HF=-517.6682013\RMSD=9.247e-09\RMSF=4.228e-06\Thermal=0.\Di
pole=-1.2221997,-0.1031709,-0.613451\PG=C01 [X(C10H11N1O1)]\
```

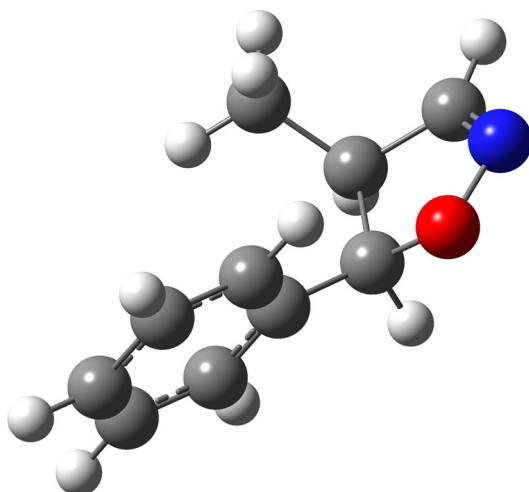
TS₁₀₋₁₁ (Ph/NO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C10H11N1O1\TSCHNEI\26-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf
=tight\DA_Ph_NO_TS\0,1\C,0.1130311517,0.3660909022,0.2436771914\C,0.
1658918485,-0.4024943189,2.4806536387\H,1.0648169457,-0.6774937376,3.0
```

182278235\O,-1.7024559309,0.8479158114,2.4777584522\C,-0.0364201797,-0.8781796366,0.9794331918\H,-1.0908586391,-1.1679112924,0.9351481912\C,0.8542232646,-2.0928889358,0.6946100354\H,0.9079711484,-2.3016690017,-0.3759336718\H,1.8730229882,-1.9775839552,1.067154706\H,0.4320234562,-2.9686884767,1.1918044242\H,-0.8163431486,0.9107649947,0.1166764525\N,-0.7576093572,0.2745361706,3.0506125429\C,1.2759909102,1.0582262168,-0.2182581907\C,2.6112889633,0.5964305279,-0.0995604531\C,1.0744616189,2.2984625476,-0.8775695815\C,3.6665603169,1.3273700605,-0.6199216809\H,2.8205660364,-0.3329541862,0.4106220321\C,2.1339541125,3.0226946739,-1.3989200959\H,0.0631531142,2.6813527133,-0.9692287839\C,3.4378021967,2.5406673323,-1.2745693174\H,4.6798422763,0.9535897824,-0.5144303459\H,1.9480143321,3.9675690439,-1.8986788568\H,4.2703327804,3.1066737408,-1.6788408728\\Version=AM64L-G03RevC.02\State=1-A\HF=-517.6295211\RMSD=8.617e-09\RMSF=7.846e-06\Thermal=0.\Dipole=1.5646648,-0.3085892,-1.3452308\PG=C01 [X(C10H11N1O1)]\\

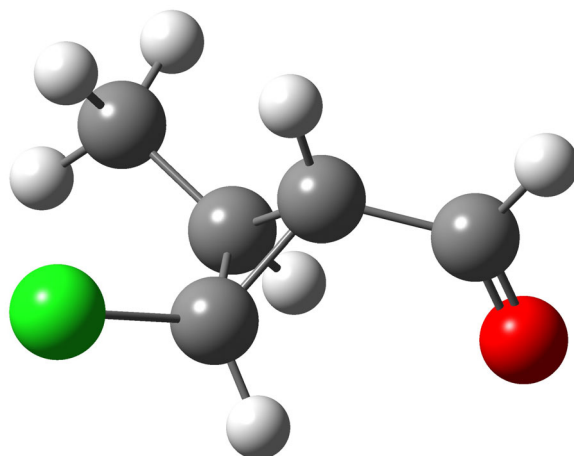
11 (Ph/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C10H11N1O1\TSCHNEI\25-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Ph_NO_2\0,1\C,0.0337442675,-0.326439634,-0.015857583\C,0.0741401461,-0.526875761,2.6127038871\C,0.6719699269,0.0918503153,1.3401055884\H,0.657376376,1.1813373281,1.434848207\C,2.0684180438,-0.4186843941,1.0814164018\H,-0.9508594817,-0.1849661496,2.7700497149\H,0.6635553332,-0.2391866021,3.4876916535\O,0.9350008556,-1.3416958586,-0.5372097392\H,0.0597225056,-1.6172848494,2.5598903153\H,0.0975425238,0.5267619487,-0.7028526473\H,2.9386134155,-0.2320666148,1.7010761217\N,2.1788144826,-1.2169514213,0.0957430118\C,-1.3822745006,-0.8446957809,0.0108960348\C,-2.4457441519,0.0634246425,-0.0095230604\C,-1.6610593397,-2.2120589636,0.0726127495\C,-3.7629901544,-0.3834101225,0.0509268219\H,-2.2434690667,1.1291482015,-0.0797290772\C,-2.9796647304,-2.6595606165,0.1251268553\H,-0.8412774318,-2.9200723132,0.0571305053\C,-4.0337112939,-1.7489088905,0.119553269\H,-4.5774770014,0.3338644212,0.0340455819\H,-3.1827457788,-3.7250865178,0.1655307014\H,-5.0597917097,-2.1002338244,0.1589474604\\Version=AM64L-G03RevC.02\State=1-A\HF=-517.7124417\RMSD=6.173e-09\RMSF=7.550e-06\Thermal=0.\Dipole=-0.6402831,0.8159817,0.912012\PG=C01 [X(C10H11N1O1)]\\

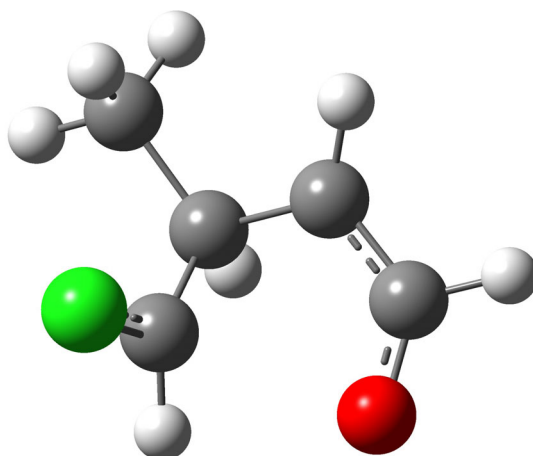
Cl-Donor

10 (Cl/CHO)



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1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H7Cl1O1\TSCHNEI\19-Jan-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_CHO_1\0,1\C,0.0079424292,-0.00963
16104,-0.0015822667\H,0.0047090382,0.0314891503,1.0795697324\C,1.36940
27631,0.0138625715,-0.6739714844\H,1.4361866578,0.5463559054,-1.616544
6181\C,2.5621363146,0.0541126513,0.2064580288\C,0.4865694224,-1.246951
4344,-0.6635361683\H,0.8310606077,-1.9955695443,0.0458946082\C,-0.0908
018007,-1.7873470343,-1.9490254757\H,-0.9765446245,-2.3948859976,-1.74
2905403\H,-0.3888551628,-0.9914515732,-2.633137077\H,0.639019237,-2.42
02856071,-2.4599973951\O,2.6131934143,-0.4732744274,1.2939824738\H,3.4
371806314,0.6080770548,-0.1926205428\Cl,-1.3162236589,0.9667181955,-0.
6834701576\Version=AM64L-G03RevC.02\State=1-A\HF=-730.219626\RMSD
=6.458e-09\RMSF=9.999e-06\Thermal=0.\Dipole=0.1586402,-0.2340661,-0.826
3184\PG=C01 [X(C5H7Cl1O1)]\
```

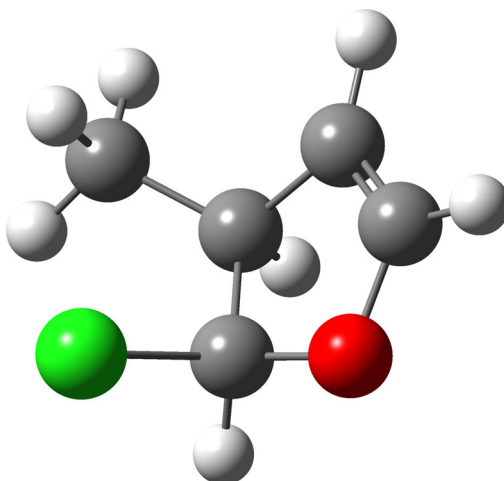
TS₁₀₋₁₁ (Cl/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H7Cl1O1\TSCHNEI\19-Jan-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_Cl_CHO_TS\0,1\C,-0.0012578226,0.006750425,0.0186788509\C,0.0
706636664,0.0340708995,2.2812451435\H,0.8668712541,0.0626750609,3.0178
248006\C,-1.007240063,0.9113193012,2.2963352982\H,-1.2924350034,1.3190
```

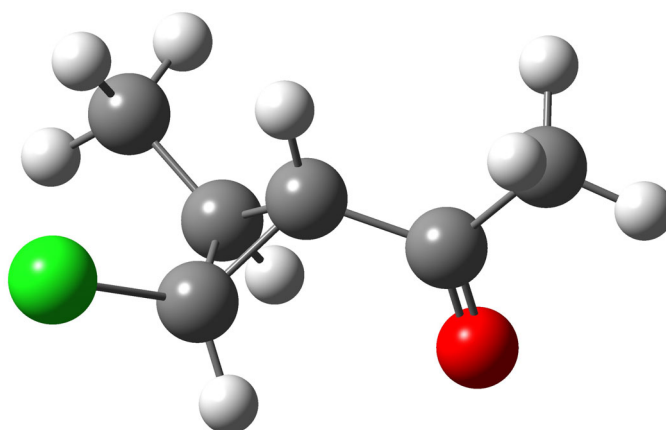
810089,3.2847305193\O,-1.7086497419,1.21027683,1.3058361193\C,0.174678
 7165,-0.9435334267,1.1090793197\H,-0.6743995427,-1.6353597567,1.092515
 7527\C,1.49108182,-1.7283329306,1.1412575807\H,1.5677286831,-2.4035883
 89,0.2871216252\H,2.3551347631,-1.0618553508,1.1349565385\H,1.52698182
 11,-2.3214721371,2.0574879029\H,-0.903028859,0.0811528934,-0.56634118\
 Cl,1.2148004035,1.0873906459,-0.5171158597\\Version=AM64L-G03RevC.02\
 State=1-A\HF=-730.1378046\RMSD=2.501e-09\RMSF=1.659e-05\Thermal=0.\D
 ipole=0.7897731,-0.9297064,-0.0770208\PG=C01 [X(C5H7Cl1O1)]\\

11 (Cl/CHO)



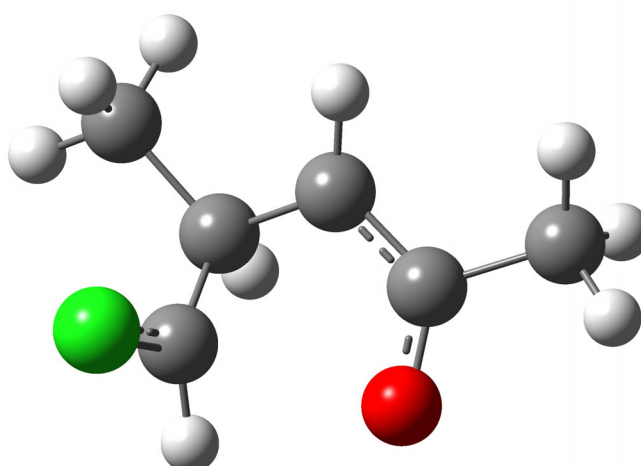
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H7Cl1O1\TSCHNEI\19-Jan-2010\
 0\# opt freq rb3lyp/6-311g(d)\DA_Cl_CHO_2\0,1\C,0.0556101354,0.046763
 4134,-0.0544547384\C,0.0005922831,-0.0791015759,2.5756101906\C,0.82087
 4906,-0.0111039292,1.2888831268\H,1.4240500361,0.909962618,1.319779712
 3\C,1.7464304431,-1.1800874523,1.0176693122\H,2.3513887574,-1.68094104
 42,1.7590596841\H,-0.6973945208,0.7582543774,2.6488007858\H,0.66810170
 61,-0.0327344686,3.4401166341\C,1.7146331588,-1.440633922,-0.282249322
 1\O,0.8509239751,-0.6237271168,-0.994483567\H,-0.5734233021,-1.0035965
 602,2.6352511809\H,2.244170227,-2.1595042513,-0.8897174278\H,-0.173497
 4431,1.039905985,-0.4250925051\Cl,-1.6073475506,-0.7865330196,0.016109
 4265\\Version=AM64L-G03RevC.02\State=1-A\HF=-730.2272613\RMSD=8.632
 e-09\RMSF=6.744e-06\Thermal=0.\Dipole=0.9298026,0.3259794,0.6021047\PG
 =C01 [X(C5H7Cl1O1)]\\

10 (Cl/COMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H9Cl1O1\TSCHNEI\03-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_CI_COR_1\0,1\C,0.010589343,-0.001087
7959,0.0052673575\H,0.0182410694,-0.0089444638,1.086894058\C,1.3604473
852,-0.000814833,-0.682631325\H,1.4248121535,0.5666121704,-1.604817510
1\C,2.5731001912,-0.0395367018,0.1915697909\C,0.437456894,-1.227082891
7,-0.7155482839\H,0.7585767709,-2.0164634185,-0.0402309786\C,-0.176103
4433,-1.6927498025,-2.0138867909\H,-1.0791576787,-2.2790960133,-1.8216
806558\H,-0.4560231313,-0.8588980145,-2.6594255248\H,0.5246664309,-2.3
273830715,-2.5625593631\O,2.5644634331,-0.6391021656,1.2476716126\Cl,-
1.2877033861,1.0506706314,-0.6179381428\C,3.7949355146,0.7012930709,-0
.3082420509\H,4.0990908444,0.3219014623,-1.2893474847\H,3.5683459733,1
.7650046837,-0.4364765908\H,4.6155072082,0.5865530108,0.3985405788\\Ve
rsion=AM64L-G03RevC.02\State=1-AHF=-769.5538779\RMSD=5.931e-09\RMS
F=4.674e-06\Thermal=0.\Dipole=0.4406343,-0.0677178,-0.8675829\PG=C01 [X
(C6H9Cl1O1)]\

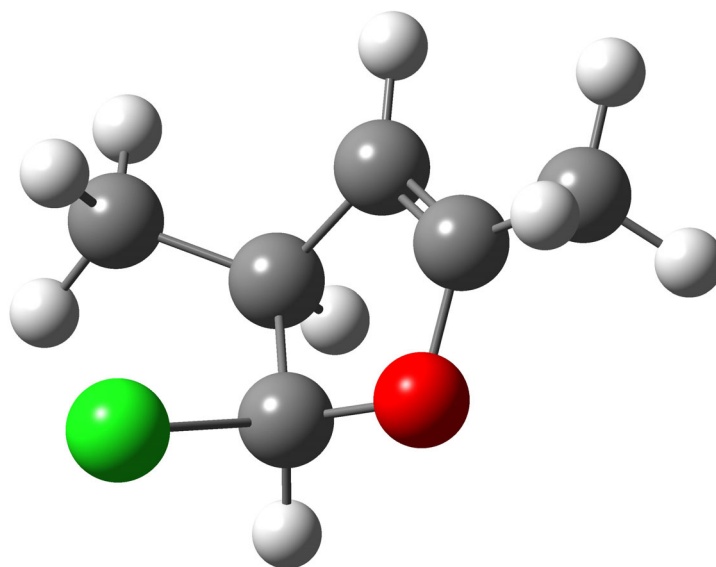
TS₁₀₋₁₁ (Cl/COMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H9Cl1O1\TSCHNEI\03-Jun-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_CI_COR_TS\0,1\C,-0.0260728049,-0.0165758521,0.0044960105\C,
0.0359006005,0.0152070222,2.2586749969\H,0.8365471184,0.035970804,2.98
98324626\C,-1.0529808552,0.8943888288,2.2817093969\O,-1.7239590661,1.1

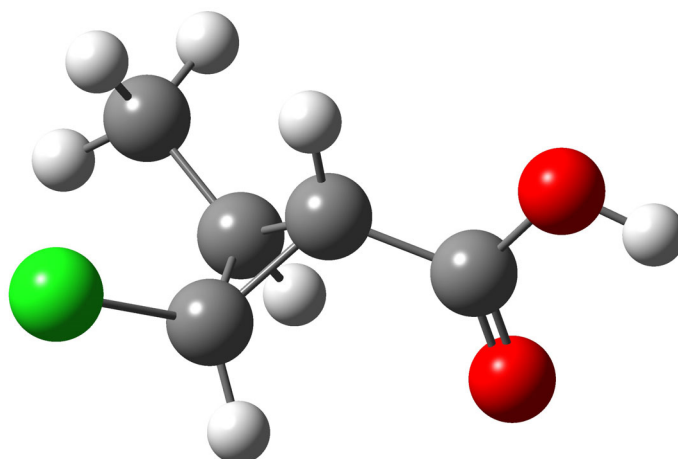
611000983,1.2551165435\C,0.1301995363,-0.9684734228,1.0982634638\H,-0.7276555729,-1.6500450782,1.0746535787\C,1.4349300463,-1.771649056,1.1354193265\H,1.5066234688,-2.448551468,0.2820042977\H,2.308062264,-1.1169641814,1.1326381796\H,1.4591347259,-2.3645888539,2.0523786523\H,-0.9136696083,0.0584188657,-0.6012105127\Cl,1.2086322633,1.0510648785,-0.5213133097\C,-1.4975060241,1.4714883106,3.6205805662\H,-2.1574256757,0.7662217854,4.1348728551\H,-0.645092597,1.6641466544,4.2770114019\H,-2.0466355645,2.3984708707,3.4574050186\\Version=AM64L-G03RevC.02\State=1-A\HF=-769.4670894\RMSD=3.115e-09\RMSF=1.792e-04\Thermal=0.\Dipole=0.6366659,-0.8374921,0.1056958\PG=C01 [X(C6H9Cl1O1)]\\

11 (Cl/COMe)



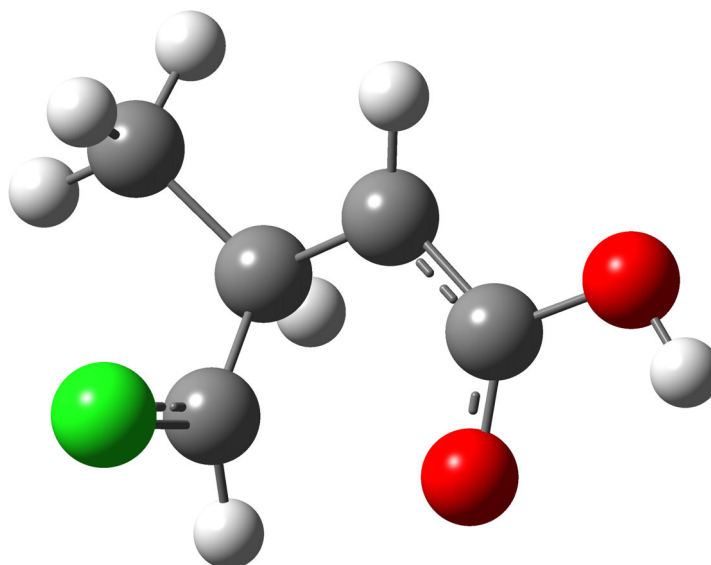
1\1\GINC-WERZ01\FOpt\RB3LYP/6-311G(d)\C6H9Cl1O1\TSCHNEI\03-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Cl_COR_2\0,1\C,-0.0124159987,-0.0236563846,0.0017247502\C,0.015429372,0.0100493121,2.6337164047\C,0.7939171487,0.0015999694,1.3194716648\H,1.3899039711,0.9274927438,1.2756540105\C,1.7116323188,-1.1781630807,1.0864011546\H,2.3362011877,-1.633370648,1.8414561842\H,-0.6844267136,0.8480245694,2.6784821021\H,0.7101847456,0.1116804771,3.471732432\C,1.6556397003,-1.5261927697,-0.1960323755\O,0.7591684898,-0.7360375269,-0.9200367318\H,-0.5509529322,-0.9112877694,2.7688093518\H,-0.269670526,0.943704458,-0.4162853626\Cl,-1.6666498538,-0.8706218608,0.1740042737\C,2.3570178659,-2.5564546997,-1.0016076896\H,2.9113819256,-2.0926298231,-1.8233377307\H,3.0572345467,-3.1194684216,-0.3837833933\H,1.6392615755,-3.2517372048,-1.4466749599\\Version=AM64L-G03RevC.02\State=1-A\HF=-769.560452\RMSD=6.091e-09\RMSF=7.899e-06\Thermal=0.\Dipole=1.0540914,0.2243193,0.3979113\PG=C01 [X(C6H9Cl1O1)]\\

10 (Cl/COOH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H7Cl1O2\TSCHNEI\22-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_COOH_1\0,1\C,0.0315071735,-0.0021
790651,0.0037124139\H,0.0242727246,0.0335735371,1.0844092749\C,1.38375
11628,0.0025819316,-0.6753115942\H,1.4618881359,0.534844444,-1.6147956
034\C,2.578036522,0.0335340958,0.2015711443\C,0.4985675026,-1.24817640
69,-0.6618370454\H,0.8257405281,-2.0038809438,0.0473934142\C,-0.085781
6934,-1.7800771167,-1.9483244099\H,-0.9720520126,-2.3868530224,-1.7429
008261\H,-0.3839088306,-0.9790595316,-2.6262495646\H,0.6410713798,-2.4
108847672,-2.4662535119\O,2.6533211903,-0.4780820421,1.2936288427\Cl,-
1.283222051,0.9897911064,-0.6753721431\O,3.6035101465,0.7084710598,-0.
3644048007\H,4.3410711984,0.6837281863,0.2647465848\\Version=AM64L-G
03RevC.02\State=1-A\HF=-805.4937189\RMSD=4.506e-09\RMSF=7.599e-06\T
hermal=0.\Dipole=0.4742045,-0.3301487,-0.3995154\PG=C01 [X(C5H7Cl1O2)]\
```

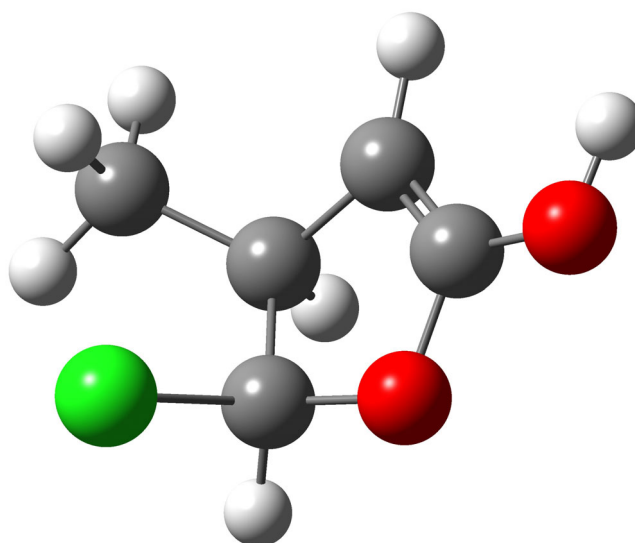
TS₁₀₋₁₁ (Cl/COOH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H7Cl1O2\TSCHNEI\22-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_Cl_COOH_TS\0,1\C,-0.0592977276,0.0168705699,0.0953590053\C,0
.0525866899,-0.1067466843,2.3741423909\H,0.8036029137,-0.1291313533,3.
```

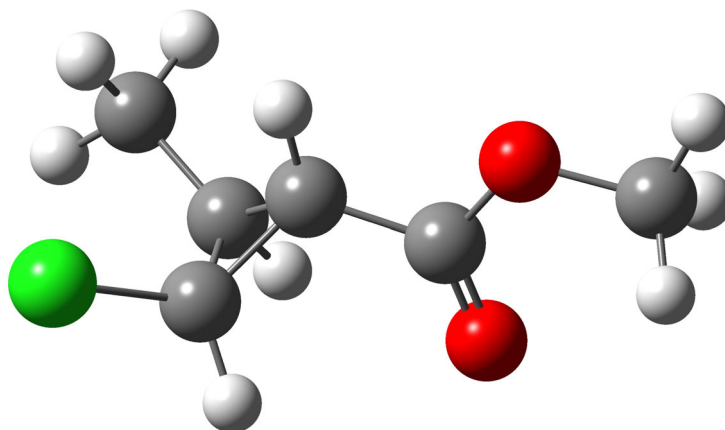
1525450289\C,-1.0231562644,0.7880102072,2.3881256003\O,-1.6968778476,1.0940028325,1.3751908071\C,0.1749020963,-0.977146509,1.1505049701\H,-0.6327190294,-1.7174565272,1.0805984737\C,1.5275008363,-1.7021715507,1.0867555737\H,1.6077022975,-2.3172285548,0.1887266185\H,2.3587747566,-0.9955232095,1.1037648107\H,1.6160188758,-2.3508731984,1.9609079221\H,-0.9282892337,0.0123324561,-0.5443828972\Cl,1.0625656981,1.2238463261,-0.3542740271\O,-1.3607017762,1.323856532,3.5918449553\H,-2.0746491584,1.9519424519,3.4171200859\\Version=AM64L-G03RevC.02\State=1-A\HF=-805.3957581\RMSD=6.555e-09\RMSF=1.625e-06\Thermal=0.\Dipole=0.4121438,-0.5585313,-0.5351001\PG=C01 [X(C5H7Cl1O2)]\\

11 (Cl/COOH)



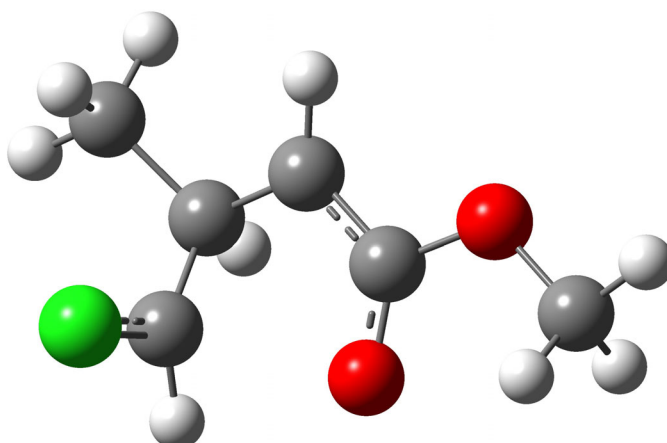
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H7Cl1O2\TSCHNEI\29-Jul-2010\0\\# opt freq rb3lyp/6-311g(d)\\DA_Cl_COOH_3\\0,1\C,0.0747839861,0.0111332668,-0.0497737796\C,-0.0108354772,-0.0945304596,2.5738776341\C,0.8293394406,0.0007975637,1.3022438119\H,1.3759127589,0.9573208906,1.3337169235\C,1.8016588546,-1.1325969258,1.0534148241\H,-0.7460206916,0.7123056976,2.6295565856\H,0.6392130023,-0.0118262092,3.4490297919\C,1.8017266833,-1.3793953496,-0.2579920993\O,0.925813253,-0.6098901113,-0.9811321896\H,-0.5424264893,-1.0443093058,2.6314842862\H,-0.1999702109,0.9892142926,-0.4291819746\Cl,-1.5277651942,-0.9165001181,-0.0069929323\O,2.4856210464,-2.2112166127,-1.0525739732\H,2.409219565,-1.6134851817,1.8055562796\H,3.1413889804,-2.682635274,-0.5258717557\\Version=AM64L-G03RevC.02\State=1-A\HF=-805.4688089\RMSD=7.482e-09\RMSF=1.500e-05\Thermal=0.\Dipole=1.150751,0.1777571,0.9270224\PG=C01 [X(C5H7Cl1O2)]\\

10 (Cl/COOMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H9Cl1O2\TSCHNEI\22-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_CI_COOR_1\0,1\C,0.0539511895,-0.0199
898419,0.0139592168\H,0.0422554211,-0.0097662308,1.0951426601\C,1.4068
519829,-0.0650818396,-0.6595513938\H,1.5137291863,0.4835578778,-1.5868
303654\C,2.6012686375,-0.1073062682,0.2224351203\C,0.4642860579,-1.271
8784908,-0.6791566788\H,0.7497009288,-2.0589695097,0.0139275947\C,-0.1
419222142,-1.7444446517,-1.9788419318\H,-1.0673571826,-2.2962486396,-1
.7915530115\H,-0.3811188611,-0.9143830618,-2.645093826\H,0.5477620031,
-2.4117965155,-2.5019976731\O,2.6406764188,-0.6481837647,1.3032142789\
Cl,-1.2128539803,1.0469634152,-0.6458123593\O,3.6463698638,0.534303191
8,-0.3356695706\C,4.8551709441,0.550666078,0.4439525489\H,5.5788063813
,1.0972699433,-0.1558008909\H,4.6876984623,1.0535355776,1.3969169356\H
,5.2015848433,-0.4657813838,0.6334968728\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-844.8067844\RMSD=6.868e-09\RMSF=3.156e-06\Thermal=0.\Dipole
=0.703086,-0.2541169,-0.4171592\PG=C01 [X(C6H9Cl1O2)]\
```

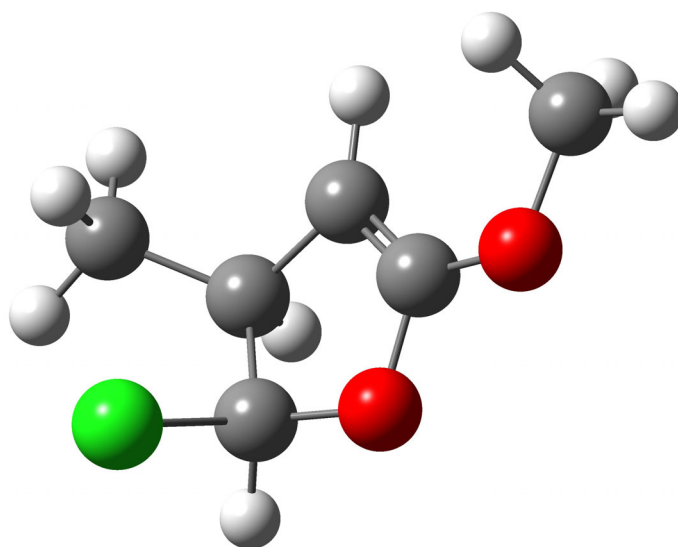
TS₁₀₋₁₁ (Cl/COOMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H9Cl1O2\TSCHNEI\22-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_CI_COOR_TS\0,1\C,-0.1257452579,-0.0290451682,0.1478876918\C,
0.0457882719,-0.3149064893,2.4096367983\H,0.8045148994,-0.302262974,3.
```

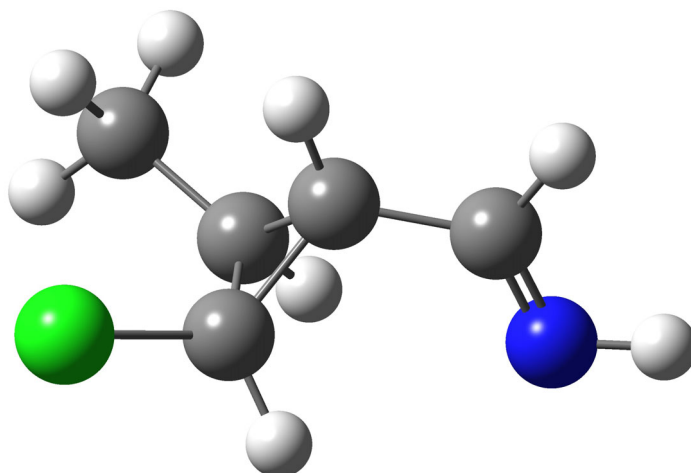
1809080867\C,-1.141875015,0.426017226,2.503744734\O,-1.8583679627,0.7176522832,1.5165673409\C,0.2573481308,-1.0616304893,1.1197883487\H,-0.4472960342,-1.8949448825,0.9970406133\C,1.6913218511,-1.5951607361,0.9844243825\H,1.8324734614,-2.1225010967,0.0393167074\H,2.4231587749,-0.7882901816,1.0486765762\H,1.8826891153,-2.2924235032,1.8030893495\H,-0.9934349381,-0.1025786204,-0.4893623164\Cl,0.8181345161,1.3511590069,-0.2101576341\O,-1.5069676852,0.7954283257,3.7571318614\C,-2.6933926889,1.5894681946,3.8577474755\H,-2.7128905684,1.9560247952,4.8827172413\H,-2.6667501448,2.4206658762,3.1512656094\H,-3.5822832519,0.9874158693,3.6597163701\\Version=AM64L-G03RevC.02\State=1-A\HF=-844.7073834\RMSD=6.233e-09\RMSF=7.989e-06\Thermal=0.\Dipole=0.3495559,-0.4106165,-0.3751483\PG=C01 [X(C6H9Cl1O2)]\\

11 (Cl/COOMe)



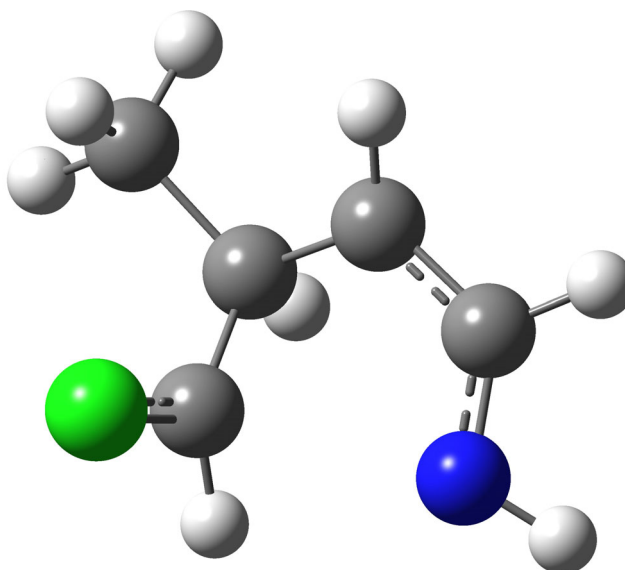
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H9Cl1O2\TSCHNEI\22-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Cl_COOR_2\0,1\C,0.0948177194,0.043551079,-0.0350774839\C,-0.1111088136,-0.087316168,2.5809047811\C,0.7862472742,-0.0044574558,1.3480188884\H,1.3594033493,0.9346908298,1.4148209221\C,1.7367458236,-1.1624712022,1.1318804321\H,2.2933313426,-1.6621266017,1.90837447\H,-0.8262415517,0.7386768599,2.6121714704\H,0.50174818,-0.0300056391,3.4845105175\C,1.7875609833,-1.4004656073,-0.1826082619\O,0.9663332281,-0.5887134283,-0.9340947524\H,-0.6701921615,-1.022649088,2.6060743424\H,-0.1390779317,1.0330527937,-0.412459316\Cl,-1.5380527209,-0.8394560798,-0.0728096451\O,2.4702084636,-2.2390179436,-0.9554735442\C,3.3873171733,-3.0925980844,-0.2732441399\H,3.8607613474,-3.6980891646,-1.0421447549\H,4.1420489113,-2.504141874,0.2568016923\H,2.8592445472,-3.7372956729,0.4351944094\\Version=AM64L-G03RevC.02\State=1-A\HF=-844.784642\RMSD=3.200e-09\RMSF=7.910e-06\Thermal=0.\Dipole=1.2069664,-0.0011339,0.8631317\PG=C01 [X(C6H9Cl1O2)]\\

10 (Cl/CHNH)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H8Cl1N1\TSCHNEI\22-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_CHNH_1\0,1\C,-0.0545254543,0.0690
185286,-0.0747116685\H,-0.0846024682,0.1918030501,0.9996182823\C,1.317
288337,0.0624605755,-0.7149695618\H,1.3820290324,0.5176593493,-1.69740
04722\C,2.5041076408,0.2189465999,0.1588508088\C,0.4639871326,-1.20935
32371,-0.6304808537\H,0.8024693651,-1.8938193738,0.1435423101\C,-0.080
27363,-1.8575240525,-1.8805663526\H,-0.962144472,-2.4614966632,-1.6479
472639\H,-0.3748193427,-1.1215018156,-2.6305362057\H,0.6688078146,-2.5
164510964,-2.3276549989\H,3.3416786086,0.778652561,-0.2787251495\Cl,-1
.3914611724,0.9576610555,-0.857955714\N,2.5284629222,-0.2681413168,1.3
329961708\H,3.4132268354,-0.0672087075,1.798100214\\Version=AM64L-G03
RevC.02\State=1-A\HF=-710.332468\RMSE=9.003e-09\RMSE=4.176e-06\Therm
al=0.\Dipole=0.9437386,-0.1685235,-0.297587\PG=C01 [X(C5H8Cl1N1)]\
```

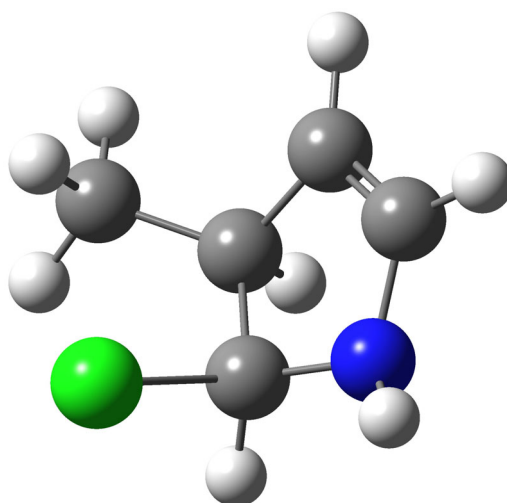
TS₁₀₋₁₁ (Cl/CHNH)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H8Cl1N1\TSCHNEI\22-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_Cl_CHNH_TS\0,1\C,-0.0082784123,-0.0177387207,-0.008875929\C,
0.0467862046,0.0252794343,2.2779384193\H,0.8819406958,0.1164182967,2.9
```

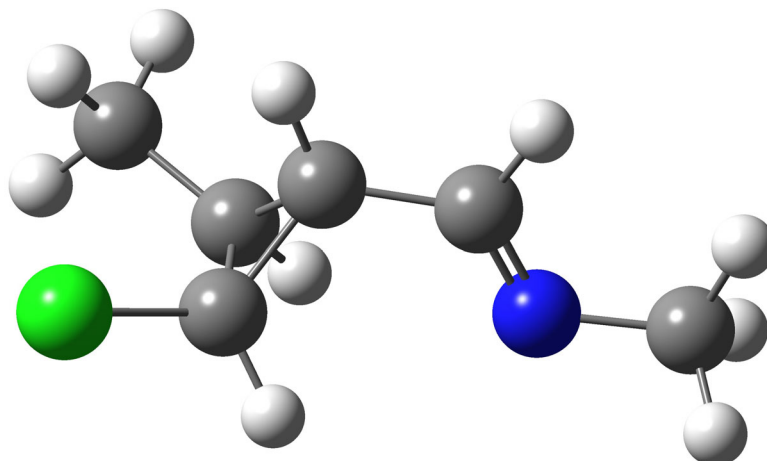
669905029\C,-1.0355470846,0.9010991127,2.3381287108\H,-1.33235026,1.2405958631,3.3404700848\C,0.1711566364,-0.9405601828,1.1106453431\H,-0.6751182901,-1.6368867889,1.0953647051\C,1.485556292,-1.726988195,1.1481862261\H,1.554856338,-2.4207219429,0.3081572254\H,2.3495428693,-1.0603866156,1.1159506047\H,1.5330968382,-2.2989898351,2.0784250737\H,-0.8840929553,0.0052162732,-0.6334938424\Cl,1.1743685047,1.1334450587,-0.4964411175\N,-1.6897653187,1.2999790297,1.2770732278\H,-2.6274650055,1.6388406724,1.5079132637\\Version=AM64L-G03RevC.02\State=1-A\HF=-710.2470563\RMSD=3.918e-09\RMSF=1.895e-05\Thermal=0.\Dipole=-0.1146055,-0.6133145,0.2507154\PG=C01 [X(C5H8Cl1N1)]\\

11 (Cl/CHNH)



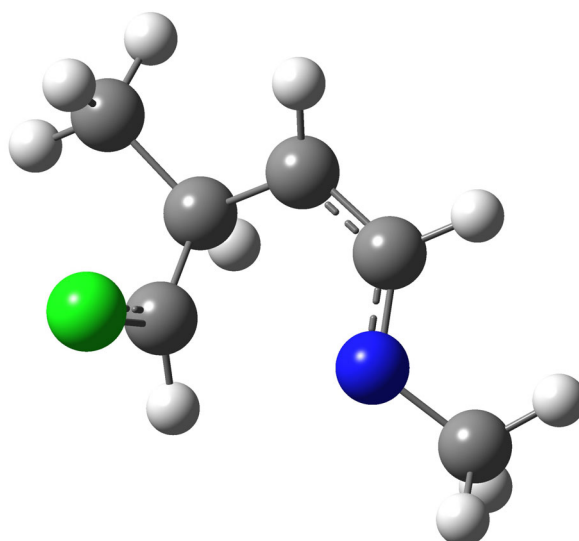
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H8Cl1N1\TSCHNEI\22-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Cl_CHNH_2\0,1\C,0.1170467844,0.1043699867,-0.0588141716\C,-0.012880534,-0.0872260755,2.5590610939\C,0.8440272831,-0.0172919931,1.2982166218\H,1.4556520169,0.899518428,1.3541205963\C,1.7780623689,-1.1817882692,1.0349480468\H,2.3477453852,-1.69774809,1.7938472789\H,-0.6892178009,0.7683590868,2.6301375988\H,0.6300988765,-0.077557961,3.4433388166\C,1.8420540279,-1.3820451485,-0.2823055303\H,-0.6148722579,-0.9952655619,2.581705436\H,2.442553919,-2.086060776,-0.8421522718\H,-0.2309361345,1.0959838718,-0.3261807876\Cl,-1.5492152403,-0.8763929997,-0.0684482334\N,1.0259671222,-0.4650989525,-0.980581115\H,0.6777119254,-0.7122660876,-1.8953872134\\Version=AM64L-G03RevC.02\State=1-A\HF=-710.3614571\RMSD=4.525e-09\RMSF=5.146e-05\Thermal=0.\Dipole=0.9512747,0.2767279,-0.1407795\PG=C01 [X(C5H8Cl1N1)]\\

10 (Cl/CHNMe)



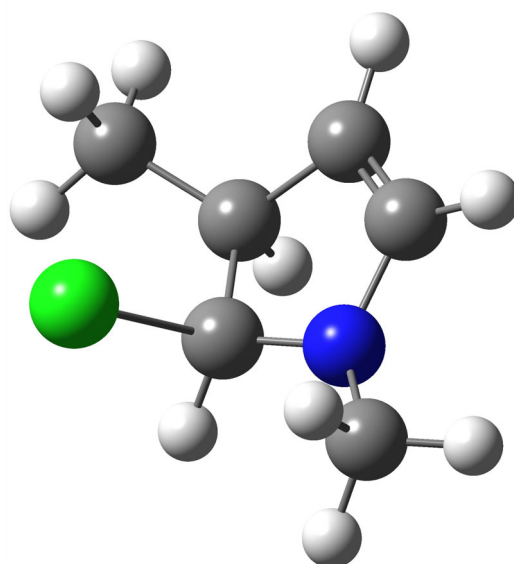
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10Cl1N1\TSCHNEI\22-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_Cl_CHNR_1\0,1\C,-0.3456589843,0.051792736,-0.259461927\H,-0.5378330676,0.2454480124,0.7871894801\C,1.0882320598,0.1864855792,-0.7207363441\H,1.2239972869,0.5720080066,-1.7255246606\C,2.1247245099,0.5754030521,0.2657521046\C,0.4026303668,-1.1812407673,-0.6296047062\H,0.715300802,-1.75557591,0.2390996584\C,0.1172516047,-1.9885317061,-1.873051759\H,-0.7039138485,-2.6896791012,-1.6975407675\H,-0.1649301214,-1.3570379128,-2.7171075314\H,0.9971910603,-2.568925321,-2.1633084547\H,2.943672552,1.2071690366,-0.1141235762\Cl,-1.6698264448,0.6866313689,-1.2782986093\N,2.0723412769,0.2044404334,1.47545995\C,3.1231693464,0.6290820786,2.3782955321\H,2.6828562827,1.1906482993,3.2075060158\H,3.604362264,-0.2518500264,2.8134074802\H,3.8929985006,1.2524624707,1.8985888436\\Version=AM64L-G03RevC.02\State=1-A\HF=-749.652827\RMSD=3.639e-09\RMSF=1.025e-05\Thermal=0.\Dipole=0.9378308,-0.1540453,0.0307957\PG=C01 [X(C6H10Cl1N1)]\\

TS₁₀₋₁₁ (Cl/CHNMe)



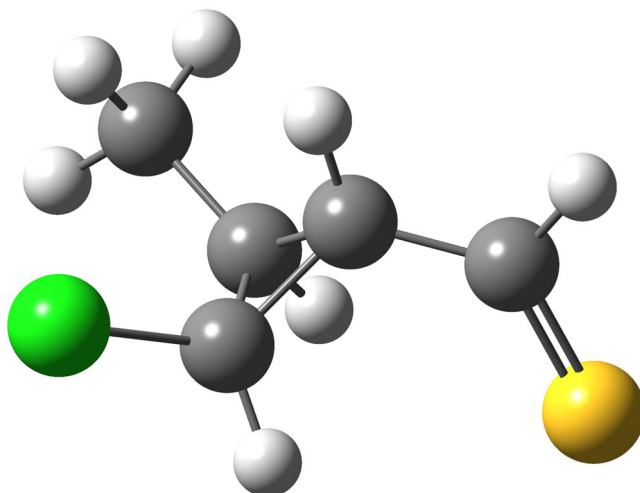
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10Cl1N1\TSCHNEI\22-Jun-2010\0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra fine\DA_CI_CHNR_TS\0,1\C,-0.0995432114,-0.1074914073,-0.0015118862\C,0.0964580044,0.090739482,2.2714313803\H,0.97097194,0.241621702,2.8989355489\C,-0.9863257894,0.9674867881,2.3431648749\H,-1.214779252,1.3898243503,3.3332790821\C,0.1661428005,-0.9474568394,1.1671899988\H,-0.6658907555,-1.6562741251,1.2504331448\C,1.4931350588,-1.713759015,1.1724206701\H,1.5200710298,-2.4627277526,0.3786727291\H,2.3418871299,-1.0401570767,1.0386411208\H,1.6102909217,-2.2197368516,2.1343538548\H,-1.0103887644,-0.1437353459,-0.5734812659\Cl,1.0236865699,1.0346364272,-0.6328667809\N,-1.730531006,1.2855385511,1.3194072469\C,-3.0677306916,1.7946986829,1.557547214\H,-3.2103490969,2.1602038689,2.5857459184\H,-3.2883198589,2.6092318017,0.8615343561\H,-3.8183755538,1.0119385005,1.3869608193\Version=AM64L-G03RevC.02\State=1-A\HF=-749.5659556\RMSD=5.936e-09\RMSF=6.003e-06\Thermal=0.\Dipole=-0.1577828,-0.5552457,0.1933054\PG=C01 [X(C6H10Cl1N1)]\

11 (Cl/CHNMe)



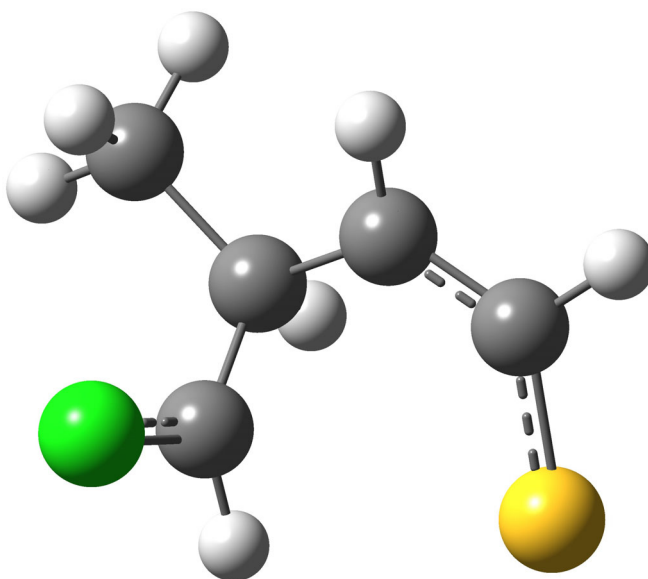
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10Cl1N1\TSCHNEI\22-Jun-2010\0\# opt freq rb3lyp/6-311g(d)\DA_CI_CHNR_2\0,1\C,0.2021162275,0.205202632,-0.0482807552\C,-0.0676475429,-0.1792121125,2.5403640299\C,0.8489775035,-0.0043161332,1.3325950322\H,1.4408365324,0.9144294081,1.4891559989\C,1.8214633548,-1.1288862631,1.0384585044\H,2.3627070711,-1.6891737227,1.786515042\H,-0.7673799184,0.6548636537,2.6333630143\H,0.5320264022,-0.2162245814,3.4541477851\C,1.9504267529,-1.2334550776,-0.2855568547\H,-0.6476985911,-1.0982928457,2.4697606409\H,2.5897945969,-1.8851243551,-0.8657900091\H,-0.1687885092,1.197998305,-0.2780349298\Cl,-1.5107705907,-0.8011267271,-0.180011696\N,1.1339345713,-0.2999292906,-0.9575696572\C,0.8659217612,-0.3714924845,-2.3814682003\H,1.7998001881,-0.5498097972,-2.9168568371\H,0.1500810067,-1.1643953732,-2.6233924792\H,0.454415425,0.5797555132,-2.7228507597\Version=AM64L-G03RevC.02\State=1-A\HF=-749.679512\RMSD=7.582e-09\RMSF=1.896e-05\Thermal=0.\Dipole=1.2554823,0.4429514,-0.2348023\PG=C01 [X(C6H10Cl1N1)]\

10 (Cl/CHS)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H7Cl1S1\TSCHNEI\07-Sep-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_CI_CHS_1\0,1\C,-0.0254353945,-0.0105
703185,0.0026281859\H,-0.0426324629,-0.008533979,1.084885989\C,1.35805
64279,-0.0193880546,-0.6437054976\H,1.4324675549,0.539037669,-1.570876
5438\C,2.559686976,-0.0316206742,0.1903160261\C,0.4028400902,-1.236620
561,-0.7006436864\H,0.7024495195,-2.0308762541,-0.0205893032\C,-0.1614
55008,-1.6902822655,-2.0241349072\H,-1.0794400533,-2.2638199454,-1.866
2971771\H,-0.4054785247,-0.8518249043,-2.677938684\H,0.5519787268,-2.3
340814293,-2.5440910949\H,3.4096646253,0.5068009962,-0.2330655347\Cl,-
1.2767848005,1.0663505495,-0.6622431362\S,2.7409627583,-0.7531057748,1
.6466471206\Version=AM64L-G03RevC.02\State=1-A\HF=-1053.1812604\RMS
D=7.226e-09\RMSF=5.480e-05\Thermal=0.\Dipole=-0.0677453,-0.2571388,-0.89
58251\PG=C01 [X(C5H7Cl1S1)]\

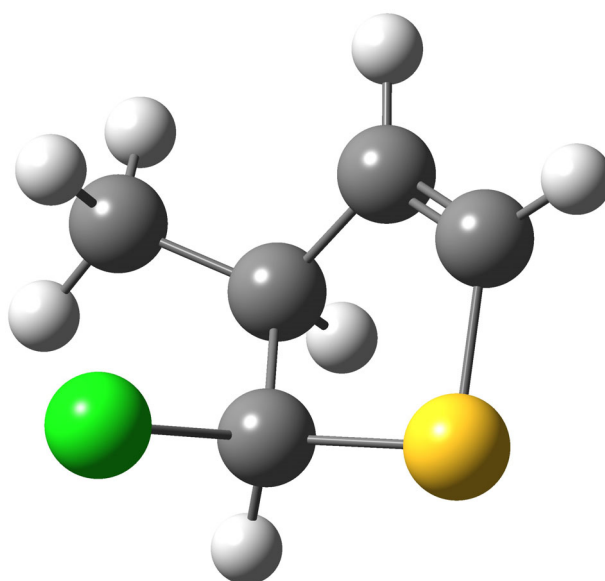
TS₁₀₋₁₁ (Cl/CHS)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H7Cl1S1\TSCHNEI\07-Sep-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=

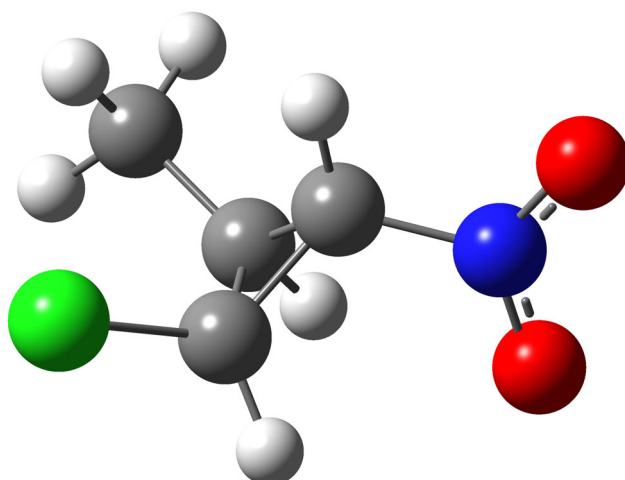
tight\\DA_CI_CHS_TS\\0,1\\C,0.0187591557,0.0631686467,-0.0220006292\\C,-
 0.0010166776,0.0702030884,2.2521502787\\H,0.8645758927,0.1484189286,2.9
 063047202\\C,-1.1220718813,0.8185256316,2.4869270808\\H,-1.2126316259,1.
 2050854099,3.5048201078\\C,0.1318458384,-0.8960007896,1.0682165734\\H,-0
 .7464629945,-1.5477326882,1.0267439405\\C,1.4198942342,-1.7211779429,1.
 1408174494\\H,1.5050451353,-2.3909073076,0.2829553898\\H,2.3059499791,-1
 .0842496303,1.1691268828\\H,1.4067088619,-2.3238239411,2.0516009338\\H,-
 0.8683683793,0.180804214,-0.6221852063\\Cl,1.2709888989,1.1357533845,-0
 .4733718816\\S,-2.3970120862,1.1803836203,1.4376502396\\Version=AM64L-G
 03RevC.02\\State=1-A\\HF=-1053.1177613\\RMSD=3.888e-09\\RMSF=5.748e-05\\T
 hermal=0.\\Dipole=1.4181945,-0.9987226,-0.2772497\\PG=C01 [X(C5H7Cl1S1)]\\

11 (Cl/CHS)



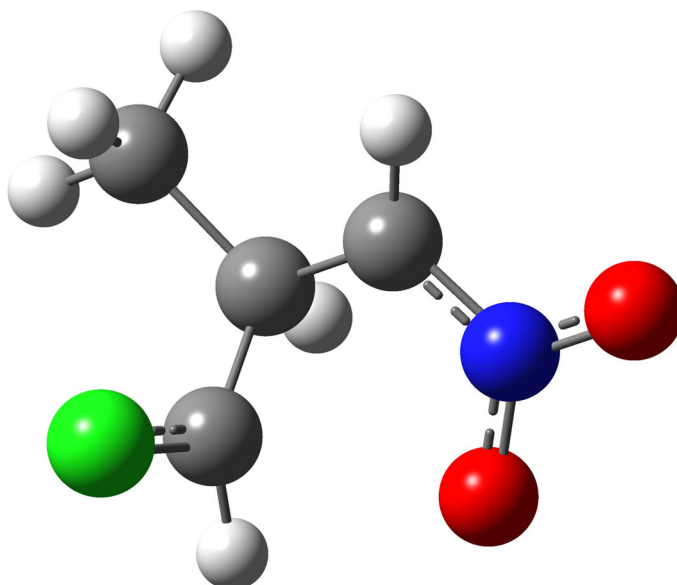
1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C5H7Cl1S1\\TSCHNEI\\07-Sep-2010\\
 0\\# opt freq rb3lyp/6-311g(d)\\DA_CI_CHS_2\\0,1\\C,0.0050860574,0.001647
 672,-0.0358574665\\C,0.0002979574,-0.0759987475,2.571128334\\C,0.8147624
 355,-0.0801104115,1.2764975187\\H,1.4294574031,0.8357018755,1.263399841
 3\\C,1.7632289405,-1.2456192385,1.1105577493\\H,2.2293432609,-1.72802900
 24,1.962184636\\H,-0.6835096764,0.7750530476,2.61012759\\H,0.6743087686,
 -0.0012074306,3.4286901772\\C,2.0154235137,-1.5763146575,-0.1529218671\\
 H,-0.5885454906,-0.987252029,2.6784825591\\H,2.6956681145,-2.337791323,
 -0.5107963228\\H,-0.3101388622,1.0122769855,-0.2761287353\\Cl,-1.5698955
 839,-0.9608780909,0.0300910352\\S,1.1053621277,-0.6277135894,-1.3516946
 108\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-1053.2075774\\RMSD=4.578
 e-09\\RMSF=7.273e-06\\Thermal=0.\\Dipole=0.7537441,0.3508289,0.6622922\\PG
 =C01 [X(C5H7Cl1S1)]\\

10 (Cl/NO₂)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C4H6Cl1N1O2\TSCHNEI\22-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_NO2_1\0,1\C,0.0305971805,-0.036
7833364,-0.001239998\H,0.1872523092,-0.0104380802,1.0681072484\C,1.262
6541037,-0.0159976552,-0.8637409742\H,1.2679494994,0.537824131,-1.7912
637716\C,0.4280248043,-1.278540851,-0.7345845232\H,0.868549274,-2.0190
629168,-0.0731798158\C,-0.3091464546,-1.8236291663,-1.9346502665\H,-1.
1471751345,-2.4462247564,-1.6110745098\H,-0.711298844,-1.0304938085,-2
.5663662324\H,0.3559442423,-2.4411351283,-2.5426599702\O,2.6768705622,
-0.5095589961,0.8991096049\Cl,-1.3693172084,0.9421141537,-0.4859692529
\N,2.5712591081,0.0471591476,-0.1874091198\O,3.459247945,0.6510128607,
-0.767389201\Version=AM64L-G03RevC.02\State=1-A\HF=-821.4243371\RMSD=
8.018e-09\RMSF=1.306e-05\Thermal=0.\Dipole=-0.8927938,-0.7000179,-0.55
29991\PG=C01 [X(C4H6Cl1N1O2)]\
```

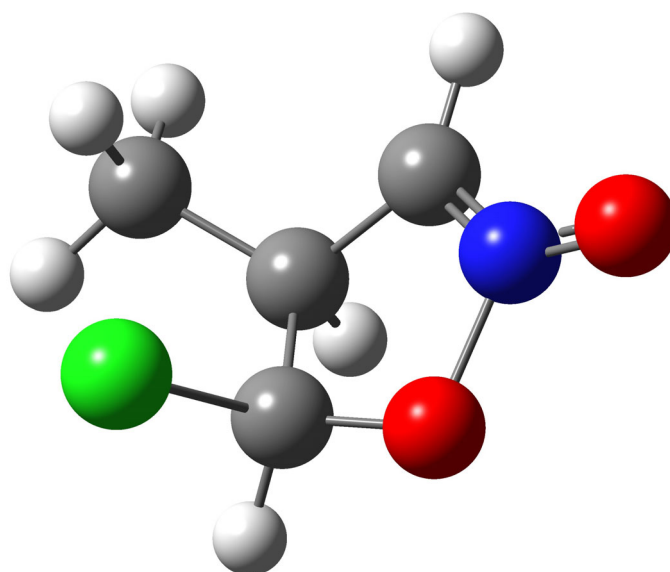
TS₁₀₋₁₁ (Cl/NO₂)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C4H6Cl1N1O2\TSCHNEI\22-Jun-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
fine\DA_Cl_NO2_TS\0,1\C,0.0082775241,0.0511491028,0.0387189343\C,0
.0907655818,0.0357577287,2.2708472258\H,0.8583196008,0.1580473093,3.01
```

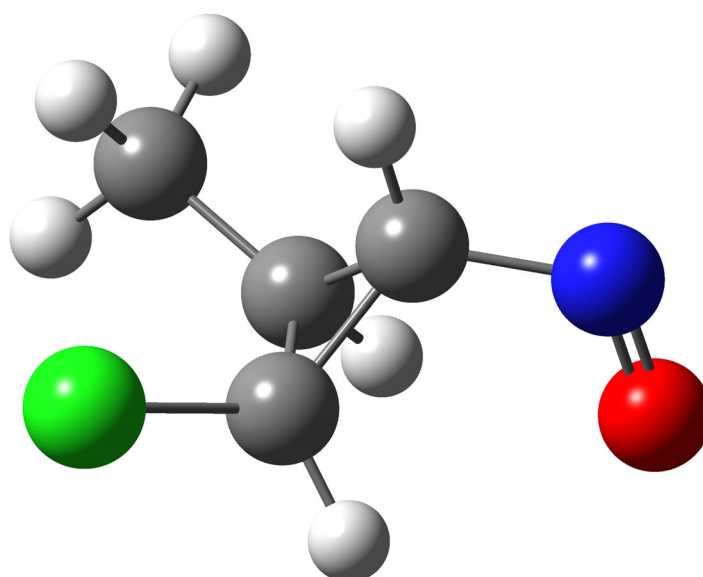
98331861\O,-1.7505841562,0.9629134276,1.3202710016\C,0.165368575,-0.92
50602636,1.1254289545\H,-0.7007568319,-1.595708158,1.0970791171\C,1.46
65922893,-1.7344440038,1.1383946144\H,1.5226447417,-2.3952313886,0.272
024542\H,2.3446784398,-1.0867750806,1.1386707935\H,1.4938067264,-2.345
1350968,2.0430265194\H,-0.8608718753,0.1048815043,-0.5962427816\Cl,1.2
285257723,1.1412759705,-0.4430092363\N,-0.9918517381,0.86903483,2.3478
799331\O,-1.2369043026,1.4826518381,3.3940021053\\Version=AM64L-G03R
evC.02\State=1-A\HF=-821.3347236\RMSD=5.307e-09\RMSF=4.852e-06\Therm
al=0.\Dipole=1.4085837,-1.4468305,-1.2244177\PG=C01 [X(C4H6Cl1N1O2)]\\

11 (Cl/NO₂)



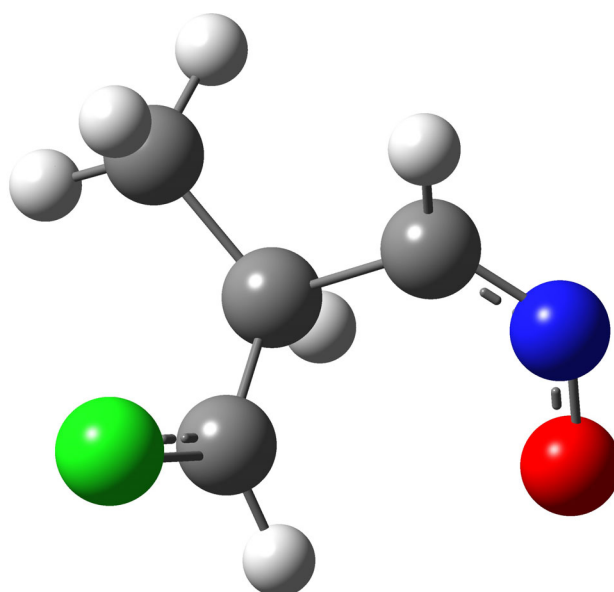
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C4H6Cl1N1O2\TSCHNEI\22-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_NO2_2\0,1\C,0.0091021564,0.0131
589113,-0.051732774\C,-0.0035990579,-0.0677892437,2.5805727488\C,0.792
6523367,-0.033839532,1.2781202643\H,1.4164248802,0.8740796404,1.280551
785\C,1.6705234077,-1.2161539289,1.0204418106\H,2.2557445111,-1.791364
0483,1.7208612131\H,-0.6796466151,0.7876832003,2.6416365712\H,0.676290
7098,-0.0152328964,3.4345586062\O,0.8299079771,-0.5439740448,-1.004088
7342\H,-0.5978986785,-0.9767961296,2.6657201387\H,-0.2806891906,1.0105
246441,-0.3719340487\Cl,-1.6003710101,-0.9174165659,0.0405478484\O,2.3
218645647,-2.32737017,-0.9198022137\N,1.7355472876,-1.5288767449,-0.23
80220919\\Version=AM64L-G03RevC.02\State=1-A\HF=-821.4315874\RMSD=
4.067e-09\RMSF=5.776e-05\Thermal=0.\Dipole=0.3584007,1.0430045,1.51169
89\PG=C01 [X(C4H6Cl1N1O2)]\\

10 (Cl/NO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C4H6Cl1N1O1\TSCHNEI\25-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_Cl_NO_1\0,1\C,0.0642950119,-0.0544
508131,-0.0295984405\H,0.2417474396,0.0538533407,1.0334931216\C,1.3154
212579,-0.034638777,-0.8898384879\H,1.2782118219,0.4552067316,-1.85426
29969\C,0.4864739095,-1.3135887007,-0.6831514772\H,0.9758340597,-1.994
5747364,0.0111533723\C,-0.2367377361,-1.9512317889,-1.8429213806\H,-1.
0555380872,-2.5778822379,-1.4782986808\H,-0.6648210637,-1.209573737,-2
.518641442\H,0.4435060151,-2.5850850118,-2.4161970939\N,2.6054088324,0
.0990174567,-0.2459538906\O,2.6732737571,-0.4034726576,0.8555801505\Cl
, -1.3674386367,0.8519987146,-0.556856855\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-746.1895241\RMSD=9.681e-09\RMSF=4.120e-05\Thermal=0.\Dipole
=-0.4857971,-0.5951986,-0.5496557\PG=C01 [X(C4H6Cl1N1O1)]\

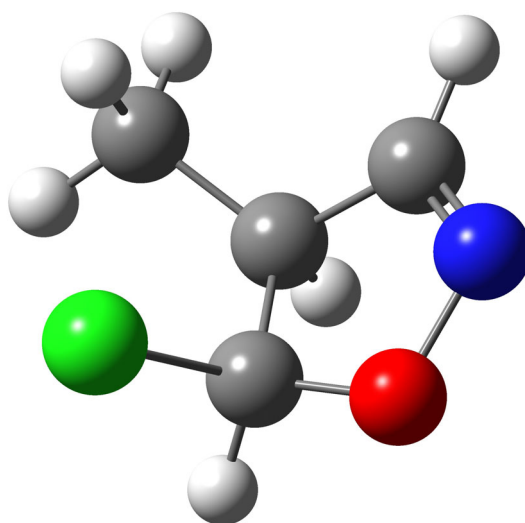
TS₁₀₋₁₁ (Cl/NO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C4H6Cl1N1O1\TSCHNEI\28-Jun-2010\
0\# opt=(calcf,ts,noigentest) freq rb3lyp/6-311g(d) int=ultrafine

scf=tight\\DA_CI_NO_TS\\0,1\\C,0.136028818,-0.0394040666,-0.1446451827\\C,-0.027793558,0.0964444067,2.1894413124\\H,0.8330298644,0.2020603006,2.836088773\\O,-2.0070177633,0.9336561618,1.53193181\\C,0.029704197,-0.9419297523,0.9558586746\\H,-0.9690748196,-1.390207571,0.9415535862\\C,1.1397090073,-1.960024279,1.2013021986\\H,1.1907569758,-2.6760359239,0.378694024\\H,2.1169159591,-1.4824815387,1.2930472447\\H,0.9407886781,-2.5075480667,2.1241455946\\H,-0.7318521736,0.4126895533,-0.6017712211\\N,-1.1014316771,0.7609170771,2.3615915134\\Cl,1.6323920629,0.6178906549,-0.6814310223\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-746.1434148\\RMSD=3.105e-09\\RMSF=2.354e-05\\Thermal=0.\\Dipole=1.0415073,-0.9610615,-0.2969806\\PG=C01 [X(C4H6Cl1N1O1)]\\

11 (Cl/NO)



1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C4H6Cl1N1O1\\TSCHNEI\\25-Jun-2010\\0\\# opt freq rb3lyp/6-311g(d)\\DA_CI_NO_2\\0,1\\C,0.0191183823,0.0110106765,-0.0544715311\\C,-0.0100615749,-0.0857328149,2.5874929347\\C,0.7759586598,-0.0199414839,1.2803760809\\H,1.4059082874,0.8827092469,1.2935239558\\C,1.6856618284,-1.1828169239,0.9760569127\\H,-0.7005933004,0.7557711666,2.6700445952\\H,0.6756391907,-0.0385183373,3.4371054031\\O,0.8545170796,-0.6381609596,-0.9648961271\\H,-0.5903328268,-1.0046931934,2.6626049559\\H,-0.2235853276,0.9948933105,-0.4417220779\\H,2.3024164415,-1.7180955899,1.688610767\\N,1.7380219914,-1.5086044893,-0.2506128215\\Cl,-1.6204561509,-0.8603040523,0.0289943034\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-746.2405469\\RMSD=9.817e-09\\RMSF=1.306e-05\\Thermal=0.\\Dipole=0.4986868,0.9104032,1.3979645\\PG=C01 [X(C4H6Cl1N1O1)]\\

Solvent Calculations

PhMe (Toluene)

10 (MeO/CHO)

```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\
0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA_O_
CHO_1_PhMe_PCM\0,1\C,-0.0058857825,-0.0107590726,0.0008812829\O,-0
.0009860411,-0.0108378585,1.3841269731\C,1.3077747636,0.0057689372,1.9
418022365\H,0.5630673537,-0.8136419833,-0.4703587124\C,0.0792304639,1.
3546052263,-0.7357390099\H,0.1011052057,2.2291411696,-0.0922124014\C,0
.8700118316,1.4140441721,-1.9707621587\H,1.8473723982,0.9170783341,1.6
580989873\H,1.1887910769,-0.0239130848,3.0242140992\H,1.8871319153,-0.
8667420963,1.6165990506\C,-1.2001370516,0.502057077,-0.6958774866\H,-1
.4046511214,0.0150756416,-1.6465439998\C,-2.4077295234,1.0054423991,0.
0593359383\H,-3.0965054715,0.181630272,0.268817498\H,-2.12678999,1.449
9909207,1.0148413148\H,-2.9485125544,1.7539281114,-0.5259274967\O,0.90
35771702,0.5315430856,-2.8080644152\H,1.4781278873,2.3335743634,-2.108
7064048\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1493685\RMSD=2.4
30e-09\RMSF=6.204e-05\Thermal=0.\Dipole=0.0946042,0.5105645,1.0337339\
PG=C01 [X(C6H10O2)]\
```

TS₁₀₋₁₁ (MeO/CHO)

```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent
=toluene) scf=tight int=ultrafine\DA_O_CHO_TS_PhMe_PCM\0,1\C,0.00047
72242,0.0135202741,-0.0033299099\C,-0.0331184483,-0.0118151902,2.29746
41933\H,0.7364767327,-0.0118947268,3.0637173155\C,-1.1081218355,0.8504
227924,2.3275198096\H,-1.309011213,1.3261032988,3.3104180485\O,-1.8899
937391,1.1190188065,1.368180741\C,0.1661602697,-0.9451119497,1.0886257
499\H,-0.6449518364,-1.680239022,1.0217833689\C,1.5275187341,-1.646998
2773,1.1351306593\H,1.6709462839,-2.3025581808,0.2729700112\H,2.345111
7163,-0.9246094747,1.1615054654\H,1.5835781395,-2.2555349738,2.0399190
284\O,0.9845564924,0.7599991557,-0.3896099388\C,0.6971899872,1.8842309
75,-1.2551570184\H,1.6101198474,2.0775903345,-1.8119339465\H,-0.124857
7306,1.6413520926,-1.9297511823\H,0.4380909486,2.736733884,-0.62819653
71\H,-0.9583077913,0.1548807461,-0.4903709809\Version=AM64L-G03RevC.0
2\State=1-A\HF=-385.0915592\RMSD=7.952e-09\RMSF=1.235e-06\Thermal=0.\
Dipole=1.4982563,-0.1887411,-1.7792282\PG=C01 [X(C6H10O2)]\
```

11 (MeO/CHO)

```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\
0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA
_O_CHO_2_DMSO_PCM\0,1\C,-0.0001726693,0.0047115382,0.0030554029\O,0.0
007315154,0.0190882754,1.3942238918\C,1.2996058562,-0.0038080857,1.973
9969904\C,-2.4797054904,-0.6299465748,0.4532211858\C,-1.4523605114,-0.
0782728857,-0.5390268658\H,-1.4408478245,-0.7322529529,-1.4225917319\C
,-1.6821411692,1.3531384437,-0.9796005602\H,-2.6333269886,1.7597414317
,-1.2965508625\H,-2.2330681537,-1.6501830618,0.7581000338\H,-3.4703966
```

641,-0.6499826424,-0.0096501723\H,1.1595515561,-0.059142039,3.05290274
67\H,1.8638406924,-0.8833585345,1.6371132051\C,-0.5254097722,2.0045130
293,-0.9392133824\O,0.5445403566,1.2516304803,-0.5122690913\H,1.861710
5516,0.8997800664,1.7237960647\H,-2.5307332248,-0.0138975031,1.3510623
467\H,-0.2791288043,3.0272994736,-1.1968524973\H,0.662667761,-0.784617
6362,-0.3704615175\\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1599879
\RMSD=4.280e-09\RMSF=4.955e-06\Thermal=0.\Dipole=0.0543273,-0.2515462,
-0.0799113\PG=C01 [X(C6H10O2)]\

10 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\
0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA_O_
COOR_1_PhMe_PCM\0,1\C,0.0135423634,0.0124346908,0.0036795248\O,0.0
198762069,0.0173981917,1.3980134953\C,1.3380684912,-0.0135688142,1.936
0740968\C,-0.0958251932,-2.6137923048,-0.0564846804\C,-0.0846767605,-1
.272877412,-0.7525228677\H,0.5577530408,0.8338292069,-0.4622262856\H,0
.3678034267,-1.2498167763,-1.7401768068\C,-1.313312363,-0.357069778,-0
.6308580253\H,-2.0617554324,-0.6855241271,0.0775301887\O,-0.9458096059
,0.7813097857,-2.6753873009\H,0.9179682899,-3.0186821543,0.0171045492\
H,-0.7007252298,-3.3387499812,-0.6081918439\H,1.2345285338,0.009916174
9,3.0204889796\H,1.8718328529,-0.9239527341,1.6411521812\O,-3.04132816
48,0.7068116662,-2.0073858535\C,-1.7303781439,0.4083526658,-1.83334938
57\C,-4.0400397889,0.3401392045,-1.0454336481\H,-4.1306318459,-0.74494
16217,-0.9576465309\H,-3.8351797129,0.7816215868,-0.0679295348\H,-4.97
2051759,0.7457103589,-1.4333895134\H,1.9173246814,0.8592585724,1.61066
43565\H,-0.4970957069,-2.5355126518,0.9556749198\\Version=AM64L-G03Re
vC.02\State=1-A\HF=-499.7224328\RMSD=6.185e-09\RMSF=1.101e-04\Thermal
=0.\Dipole=-0.1985891,-0.8791425,1.4341238\PG=C01 [X(C7H12O3)]\

TS₁₀₋₁₁ (MeO/COOMe)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent
=toluene) scf=tight int=ultrafine\DA_O_COOR_TS_PhMe_PCM\0,1\C,-0.008
1632066,-0.0093624344,-0.011639159\C,-0.0332373646,-0.0386422474,2.512
5887538\C,0.7936228712,-0.0152664188,1.2215725949\H,1.4337041506,0.875
8194155,1.2024920727\C,1.5966621345,-1.2983301235,1.0389095748\H,1.525
7006378,-2.0425212582,1.820767176\O,2.0072483866,-0.8408616694,-1.2325
003994\H,-0.6072945577,0.8820853149,2.6406964157\H,0.6435884011,-0.140
5707031,3.3634197064\O,3.098887349,-2.5603220874,-0.3587990586\C,2.199
9945949,-1.5264888933,-0.1989537854\C,3.5098361406,-3.309604286,0.7776
272762\H,3.892040812,-2.6578779468,1.5687297232\H,2.6897455317,-3.9163
070653,1.1775863176\H,4.3031228127,-3.9726804901,0.4326501696\H,-0.723
626837,-0.8839625384,2.5250076141\O,-1.0651999877,-0.7404439363,-0.123
9341634\C,-1.6478813732,-0.9220783362,-1.4378891641\H,-2.7107342517,-1
.0824958073,-1.2780182895\H,-1.4745051562,-0.0384818322,-2.0532077939\
H,-1.1862761431,-1.7989212233,-1.8898640532\H,0.2650375619,0.602077165
6,-0.865410104\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.6573015\RM
SD=3.086e-09\RMSF=8.236e-07\Thermal=0.\Dipole=-2.3099133,0.5328581,0.58
12677\PG=C01 [X(C7H12O3)]\

11 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA_O_C OOR_2_PhMe_PCM\0,1\C,0.0006361215,0.0034390394,0.0039679622\O,0.007113047,0.0182895892,1.3924689179\C,1.2992391254,-0.0059512381,1.9751923071\C,-2.475021395,-0.6352320231,0.4380630896\C,-1.4508363989,-0.0597297187,-0.5433173987\H,0.6583640571,-0.7884477506,-0.3721715862\H,-1.4379073195,-0.7020134451,-1.4363523853\C,-1.6765279422,1.3828374903,-0.9431094655\H,-2.6281547666,1.8001774638,-1.2357169204\O,0.5612547901,1.2447852209,-0.5111074297\H,-2.2303693011,-1.6643322165,0.7152410509\H,-3.4667936006,-0.6417209219,-0.0231780025\H,1.1560227313,-0.0657031967,3.0533689024\H,1.8644694601,-0.8836635058,1.6357805002\O,-0.1117368098,3.2626058,-1.1815049066\C,-0.4974765651,2.0135524336,-0.9021085004\C,-1.1434758774,4.136009831,-1.6400093619\H,-1.5933758038,3.7529843407,-2.560671073\H,-1.9174971307,4.2536484151,-0.8760205824\H,-0.6640573856,5.0932719238,-1.8317309642\H,1.860277237,0.899448455,1.7298912702\H,-2.5233361973,-0.0414255233,1.3509909674\Version=AM64L-G03RevC.02\State=1-A\HF=-499.7183313\RMSD=3.081e-09\RMSF=3.474e-05\Thermal=0.\Dipole=-0.323938,0.0251678,-0.2111102\PG=C01 [X(C7H12O3)]\

10 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\28-Jan-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA_N_CHO_1_PhMe_PCM\0,1\C,-0.0077279738,-0.0025166989,0.0029424056\H,0.0129298949,0.0118378173,1.0989976166\C,1.3893881442,-0.0166273249,-0.6279149848\H,1.4887689454,0.5077212996,-1.5733186012\C,2.5638943478,0.0008120626,0.2607371271\C,0.4824547427,-1.256649436,-0.6349497363\H,0.8089058097,-2.0166660692,0.0707915348\C,-0.0491977038,-1.7704039548,-1.9524080654\H,-0.8762928462,-2.468983606,-1.7915595885\H,-0.4163104309,-0.9539384182,-2.5757921059\H,0.7287117522,-2.3054535581,-2.5043481892\N,-1.0153913933,0.7936675625,-0.6370931501\C,-0.8793827952,2.2108988481,-0.3162129072\H,-1.6187557195,2.7863305413,-0.8785486436\H,-1.0241825134,2.4249555247,0.7575226837\H,0.1135948643,2.5632607442,-0.6016168334\C,-2.3572239239,0.3030767045,-0.3291376854\H,-2.6093915786,0.3899152455,0.7424450225\H,-3.0952110915,0.8746406471,-0.8972710129\H,-2.4465315146,-0.7457281186,-0.6153950184\O,2.6075804106,-0.5241497,1.3557637513\H,3.4520928292,0.5420520954,-0.1302172901\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5955657\RMSD=5.306e-09\RMSF=1.153e-05\Thermal=0.\Dipole=-0.6796989,0.3800327,-0.9077168\PG=C01 [X(C7H13N1O1)]\

TS₁₀₋₁₁ (Me₂N/CHO)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\28-Jan-2011\0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight int=ultrafine\DA_N_CHO_TS_PhMe_PCM\0,1\C,-0.216847802,-0.0554010466,0.0174124529\C,0.5133470795,0.0556980552,2.2689867206\H,1.4846165512,-0.0911386595,2.7321998257\C,-0.3524956151,1.0605900414,2.6742319351\H,-0.0231958811,1.6329692873,3.5716127742\O,-1.4607867397,1.3574903446,2.1506533485\C,0.040646384,-0.92336708,1.2050196879\H,-0.952266512,-1.2984913234,1.48306014\C,0.9623597766,-2.1352179642

,1.0157371064\H,0.6489371578,-2.7641436295,0.1776041499\H,2.0075425549
 , -1.8601089312,0.8668309557\H,0.9178107233,-2.7404436147,1.9241335212\
 H,-1.2507486495,0.2215063295,-0.1568237556\N,0.6413384217,0.5331025344
 , -0.7745927278\C,2.0901999132,0.4214083794,-0.589678738\H,2.5788941962
 ,1.225492728,-1.1369995571\H,2.3065030291,0.5192026278,0.4774684811\H,
 2.4604746352,-0.534282435,-0.9607880986\C,0.1933752528,1.5039142164,-1
 .7788406964\H,0.6100890434,1.2423977105,-2.7533015389\H,-0.8927488133,
 1.4994788252,-1.8388658471\H,0.5336996984,2.5047149785,-1.5008277643\
 Version=AM64L-G03RevC.02\State=1-A\HF=-404.5596648\RMSD=7.696e-09\R
 MSF=1.332e-05\Thermal=0.\Dipole=1.7583391,-0.6417218,-3.040313\PG=C01 [
 X(C7H13N1O1)]\

11 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\28-Jan-2011\
 0\# opt freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=toluene) scf=tight\DA_
 N_CHO_2_PhMe_PCM\0,1\C,-0.0159915988,-0.3793594421,-0.0013665922\C,
 0.0732239955,-0.8172191588,2.5772307167\C,0.6515394891,-0.0614884027,1
 .3698949782\H,0.6075150791,1.0168855373,1.5554338279\C,2.0645739702,-0
 .530052759,1.0671724599\H,2.9293587396,-0.3443301795,1.6905526536\H,-0
 .9389268574,-0.4930076199,2.8282125075\H,0.7041169711,-0.6508724958,3.
 4554910058\C,2.0218815279,-1.3336870986,0.0080990532\O,0.7880257295,-1
 .4409335929,-0.5810375801\H,0.0397451217,-1.8907086602,2.3833225814\H,
 2.7963989986,-1.926934246,-0.4626907166\H,0.1273226128,0.4906883198,-0
 .6752401561\N,-1.4024192984,-0.7911136984,0.0396831104\C,-1.8466771678
 , -1.3925237029,-1.2178570104\H,-1.2444364679,-2.2688488675,-1.44509576
 75\H,-2.8880765814,-1.7036185685,-1.1101889355\H,-1.7835424052,-0.6938
 022898,-2.0718498094\C,-2.2552157891,0.343462761,0.3845720001\H,-3.287
 3988576,0.002079066,0.4849832266\H,-1.9553663332,0.7816582494,1.336931
 5895\H,-2.2324178783,1.1413126063,-0.3800866681\Version=AM64L-G03RevC
 .02\State=1-A\HF=-404.5944072\RMSD=2.384e-09\RMSF=1.318e-05\Thermal=0.
 \Dipole=-0.0487496,0.448993,0.1409978\PG=C01 [X(C7H13N1O1)]\

CH₂Cl₂ (Dichloromethane)

10 (MeO/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight\DA_O_CHO_1_DCM_PCM\0,1\C,0.0021304341,0.0047984348,0.0007684039\O,0.001178599,0.0072261438,1.3843448798\C,1.3109105224,-0.0028162614,1.9458177254\H,0.5472085347,-0.8190187943,-0.4645621356\C,0.1400455858,1.3673168379,-0.7365070983\H,0.1897198691,2.2405353155,-0.0912738565\C,0.9440859965,1.4014054895,-1.9607342586\H,1.8675272271,0.8977009519,1.6622907732\H,1.1890010717,-0.0297576946,3.0280596981\H,1.8719493679,-0.8870633805,1.6210013912\C,-1.168026944,0.5588381075,-0.7050642853\H,-1.3850367856,0.0762824751,-1.6563023823\C,-2.3623829014,1.1087364697,0.0388193083\H,-3.0758292736,0.3087602494,0.2589225207\H,-2.0709694355,1.5617053189,0.9873329344\H,-2.8794149464,1.8630698199,-0.5602296512\O,0.9474575199,0.5245149957,-2.809226461\H,1.5959149509,2.2923316115,-2.0828971216\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1533545\RM SD=7.139e-09\RMSF=1.368e-05\Thermal=0.\Dipole=0.1381955,0.59428,1.1240341\PG=C01 [X(C6H10O2)]\

TS₁₀₋₁₁ (MeO/CHO)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\28-Jan-2011\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight int=ultrafine\DA_O_CHO_TS_DCM_PCM\0,1\C,0.1052239537,-0.2916134368,-0.1311202509\C,-0.0032726713,0.0511281602,2.1636102639\H,0.7399792593,0.1546045699,2.9495631925\C,-1.0687727903,0.9097638986,2.0386037578\H,-1.2646896559,1.5558078826,2.9212210219\O,-1.8516811705,1.0135697338,1.0408906308\C,0.2215680851,-1.0541256283,1.1137699579\H,-0.5975639861,-1.7847365857,1.1327168243\C,1.5707354627,-1.7555070739,1.3105199175\H,1.7328590787,-2.5312717881,0.558609446\H,2.3984570445,-1.0457830356,1.2616940494\H,1.5858451798,-2.2263668375,2.2955564855\O,1.1093204994,0.364341362,-0.5953170833\C,0.9122192818,1.2798955846,-1.7044305149\H,1.7951790687,1.191349378,-2.3321796032\H,0.0099839148,1.0143927497,-2.2558295744\H,0.8331220354,2.2840759257,-1.2897398226\H,-0.8344860578,-0.2332176429,-0.6748617195\Version=AM64L-G03RevC.02\State=1-A\HF=-385.0989429\RM SD=4.461e-09\RMSF=1.012e-06\Thermal=0.\Dipole=1.873385,-0.6368319,-2.0691821\PG=C01 [X(C6H10O2)]\

11 (MeO/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight\DA_O_CHO_2_DCM_PCM\0,1\C,0.0000656905,0.0003263608,-0.0003003251\O,-0.0002876506,-0.0003567189,1.3918574599\C,1.3006964078,0.0002980774,1.9711778573\C,-2.4309888611,-0.8166254088,0.4182287747\C,-1.4417641698,-0.1598872965,-0.5478839717\H,-1.3835010986,-0.7805323122,-1.454076658\C,-1.767221558,1.2668101168,-0.9416600539\H,-2.7458032167,1.6207372529,-1.2421519991\H,-2.1143334225,-1.8278073378,0.6868851215\H,-3.416358674,-0.8888325897,-0.0506478698\H,1.1644895179,-0.0837066275,3.0488381635\H,1.8888653981,-0.8538962903,1.6126829786\C,-0.6531940996,1.

9887482521,-0.8945680871\O,0.4665621102,1.2895559953,-0.4966054262\H,1.8363313762,0.9260286226,1.7432400172\H,-2.5293380716,-0.2389627562,1.3378316777\H,-0.472270701,3.0322117118,-1.1279626323\H,0.710009064,-0.7417505052,-0.383964001\\Version=AM64L-G03RevC.02\State=1-A\HF=-385.162857\RMSD=4.948e-09\RMSF=8.395e-05\Thermal=0.\Dipole=0.0536497,-0.3254035,-0.1282084\PG=C01 [X(C6H10O2)]\\

10 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight\\DA_O_COOR_1_DCM_PCM\\0,1\C,0.0165715237,0.0145094188,0.0018596352\O,0.0200384577,0.0237744181,1.3966949322\C,1.339194224,-0.0152310891,1.9372194312\C,-0.0958159291,-2.6120694814,-0.0557577535\C,-0.0814226977,-1.2711692244,-0.7516654875\H,0.5632825503,0.8357637652,-0.4635029419\H,0.3740947237,-1.2513902222,-1.7389268542\C,-1.3121080705,-0.3552199214,-0.6325478893\H,-2.0613095847,-0.683779392,0.0753091433\O,-0.9520604524,0.781300254,-2.6822594715\H,0.9186101005,-3.0139207978,0.0248391637\H,-0.6955366397,-3.3374060343,-0.6125207023\H,1.2344060147,0.0125849384,3.0214492122\H,1.8650297031,-0.9308517734,1.6456608554\O,-3.0410720032,0.7060854262,-2.0052862547\C,-1.732334006,0.406584921,-1.8322934357\C,-4.0440384364,0.3381682765,-1.0431940777\H,-4.1356258832,-0.7468692685,-0.9620867472\H,-3.8351694605,0.7754648405,-0.0651030103\H,-4.973944186,0.7491191613,-1.4303016254\H,1.9242719909,0.8521310202,1.6085321759\H,-0.5051737593,-2.5352854866,0.953281717\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.7275854\RMSD=8.886e-09\RMSF=8.149e-05\Thermal=0.\Dipole=-0.2112828,-0.9801577,1.572324\PG=C01 [X(C7H12O3)]\\

TS₁₀₋₁₁ (MeO/COOMe)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) iop(1/7=900) scf=tight int=ultrafine\\DA_O_COOR_TS_DCM_PCM\\0,1\C,-0.0078533469,-0.0127085212,-0.0159954543\C,-0.0126225125,-0.0185240005,2.5046167168\C,0.8101645608,-0.0082682993,1.2094245172\H,1.435845046,0.8935018668,1.1732010447\C,1.6374226536,-1.2806618117,1.0508638903\H,1.589824436,-2.0057436472,1.8523576888\O,2.0933800982,-0.8141710044,-1.2106575759\H,-0.605141203,0.8929189296,2.6124067243\H,0.6696775259,-0.0849471217,3.3546334761\O,3.1470674624,-2.5564662732,-0.3293413968\C,2.255883617,-1.5078236127,-0.1717247268\C,3.5060077818,-3.3420994639,0.8023411202\H,3.8979982396,-2.7191983425,1.6118085467\H,2.6542808007,-3.9207963592,1.1754493903\H,4.2800871528,-4.0297331795,0.4618722933\H,-0.6846628738,-0.8779324194,2.5408482666\O,-1.0438171227,-0.7618278769,-0.1114966298\C,-1.7117691205,-0.9044523434,-1.3937744486\H,-2.778311488,-0.8989950025,-1.1837737063\H,-1.4351426181,-0.0831240389,-2.0549539285\H,-1.4052150377,-1.8618214259,-1.8126347004\H,0.2408653394,0.6113140385,-0.8717986723\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.6662566\RMSD=4.608e-09\RMSF=1.710e-05\Thermal=0.\Dipole=-2.8836632,0.6757163,0.6710955\PG=C01 [X(C7H12O3)]\\

11 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\03-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight\\DA_O_COOR_2_DCM_PCM\0,1\C,0.0012849551,0.0090065184,0.009301722\O,0.0025910939,0.0400269859,1.3977044096\C,1.3021676032,-0.015493739,1.9798597851\C,-2.4724719424,-0.6403008755,0.4362816279\C,-1.4484696262,-0.0558632029,-0.5395039857\H,0.6593094085,-0.7856140911,-0.3608746037\H,-1.4304263144,-0.6950269513,-1.4351295274\C,-1.6801350899,1.3875003059,-0.9362877752\H,-2.6345601332,1.8025876743,-1.2269228384\O,0.5613981457,1.2503527695,-0.5176194227\H,-2.2223347719,-1.6691564723,0.7096842309\H,-3.4625679244,-0.6507900406,-0.028285539\H,1.1595404753,-0.0676043647,3.0585966066\H,1.8437889826,-0.9078723399,1.6420247381\O,-0.1152286215,3.2677785563,-1.187050389\C,-0.5015542773,2.0187333756,-0.9033103373\C,-1.1482502737,4.1426907169,-1.6487862672\H,-1.5989330874,3.7554074725,-2.5668684667\H,-1.920350199,4.2634264006,-0.8837638667\H,-0.6674551595,5.0984007622,-1.8447418125\H,1.885631349,0.8752187249,1.7318357667\H,-2.5285662587,-0.0505777224,1.3518223358\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.7216705\RMSD=3.035e-09\RMSF=4.518e-06\Thermal=0.\Dipole=-0.3907879,-0.0645063,-0.2520124\PG=C01 [X(C7H12O3)]\\

10 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\26-Jan-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight\\DA_N_CHO_1_DCM_PCM\0,1\C,-0.0091566728,-0.0019974115,0.0012015897\H,0.009777673,0.0158027761,1.0980750504\C,1.3893575112,-0.017108203,-0.6296812461\H,1.4897714115,0.5048540771,-1.5771268572\C,2.5636843655,0.0046583027,0.254042218\C,0.48012948,-1.2573619696,-0.6326030915\H,0.8052956892,-2.017452396,0.0750848168\C,-0.0483543963,-1.7752974551,-1.9495758888\H,-0.8783966169,-2.4701882395,-1.78767951\H,-0.4102364771,-0.960668208,-2.5784512998\H,0.7300839206,-2.3153014466,-2.4959678869\N,-1.0145418592,0.7963315976,-0.6398336109\C,-0.8788989576,2.2118360213,-0.308505912\H,-1.6187327486,2.7910333307,-0.8664104981\H,-1.0244792768,2.4169888511,0.7668516631\H,0.1142334579,2.566340188,-0.5910760284\C,-2.3574903819,0.3044616377,-0.3357757259\H,-2.6095737488,0.3849875399,0.7362876641\H,-3.0945817945,0.8808993393,-0.9001954331\H,-2.4478823434,-0.7424357884,-0.6287686129\O,2.6118512939,-0.5161092612,1.3546349392\H,3.4508627274,0.5437789255,-0.1411100106\\Version=AM64L-G03RevC.02\State=1-A\HF=-404.598954\RMSD=4.065e-09\RMSF=2.055e-05\Thermal=0.\Dipole=-0.7165062,0.4192825,-1.0156705\PG=C01 [X(C7H13N1O1)]\\

TS₁₀₋₁₁ (Me₂N/CHO)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jan-2011\0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=dichloromethane) scf=tight int=ultrafine\\DA_N_CHO_TS_DCM_PCM\0,1\C,-0.2237439781,0.0670878432,-0.0864644342\C,0.5400449785,-0.0148739428,2.1978893336\H,1.5362715363,-0.1942334388,2.5934102872\C,-0.2955674313,0.93676747,2.7487364692\H,0.100635906,1.4328594566,3.6655843636\O,-1.4485791209,1.2734047038,2.3407365007\C,0.033620927,-0.8730461881,1.0493226381\H,-0.9644061211,-1.2506043147,1.3066182951\C,0.9224960997,-2.

0867778597,0.7376699322\H,0.5740457049,-2.6350622955,-0.142016926\H,1.9696054912,-1.8220756053,0.5834072002\H,0.8844664915,-2.7652420886,1.5932147269\H,-1.2626188832,0.3233333432,-0.2809700226\N,0.6350865576,0.7032598383,-0.8281915753\C,2.0875289716,0.5893221056,-0.649510679\H,2.470755239,-0.2919136927,-1.1652163844\H,2.5603634137,1.4770256374,-1.0666298685\H,2.3027845281,0.5295692147,0.4176520822\C,0.1927238731,1.6711479218,-1.8411626944\H,0.628360623,1.4074539814,-2.8065860604\H,-0.8924201552,1.6573190181,-1.9173307869\H,0.5282456781,2.6717928791,-1.5589688708\\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5700579\RMSE=6.373e-09\RMSEF=8.565e-06\Thermal=0.\Dipole=2.0125857,-0.5148266,-3.8487329\PG=C01 [X(C7H13N1O1)]\\

11 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jan-2011\0\# opt freq b3lyp/6-311g(d) scf=(iefpcm,solvent=dichloromethane) scf=tight\DA_N_CHO_2_DCM_PCM\0,1\C,-0.0187412134,-0.3907438788,-0.0017376714\C,0.0792020363,-0.8091704238,2.581275526\C,0.6499099873,-0.0614478045,1.3651079473\H,0.6027845036,1.0186155371,1.542925084\C,2.0640753441,-0.5286212296,1.063842757\H,2.9302166577,-0.3323779713,1.6841926104\H,-0.9314552251,-0.4836484428,2.8367204885\H,0.7153807809,-0.6351837596,3.4542234908\C,2.0232072213,-1.3431259573,0.0127610686\O,0.7859264499,-1.4602619408,-0.5724123494\H,0.0462376008,-1.8846785961,2.3964918066\H,2.7999445207,-1.9388504029,-0.454604244\H,0.1265386102,0.4729437364,-0.6836904219\N,-1.406161563,-0.8010187051,0.039536024\C,-1.8517893661,-1.3818097361,-1.228124249\H,-1.2573883559,-2.2611181787,-1.4660246993\H,-2.8964983589,-1.6846388067,-1.1291879226\H,-1.77895099,-0.6717331518,-2.0718134545\C,-2.2558713938,0.3351271685,0.3934585019\H,-3.2895613538,-0.0034494141,0.4884358332\H,-1.9558492252,0.7643879404,1.3495482333\H,-2.2279236673,1.1383897747,-0.3647578847\\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5967666\RMSE=3.594e-09\RMSEF=1.164e-05\Thermal=0.\Dipole=-0.0352999,0.5514677,0.1681543\PG=C01 [X(C7H13N1O1)]\\

DMSO (Dimethylsulfoxide)

10 (MeO/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dms) scf=tight\DA_O_CHO_1_DMSO_PCM\0,1\C,-0.0045416387,-0.0115075377,-0.0038486452\O,-0.033057626,-0.0197632868,1.3800202088\C,1.3083796713,0.0090419743,1.938557164\H,0.5596603366,-0.8191941679,-0.4755477038\C,0.1014731653,1.3599589693,-0.7302419244\H,0.1321582154,2.2291884858,-0.0778476638\C,0.9043238543,1.423342891,-1.9528812881\H,1.8334176004,0.9297179061,1.6603013236\H,1.1903975657,-0.0301297629,3.0209174298\H,1.8969335341,-0.8538025429,1.6051620865\C,-1.1877054729,0.5210911935,-0.7046118215\H,-1.3954191111,0.0402122499,-1.6591773321\C,-2.3933912791,1.0402590892,0.0430738333\H,-3.0889266196,0.2235893917,0.2596548269\H,-2.1110635477,1.4956404489,0.9932261819\H,-2.9275493464,1.7858454585,-0.5518971614\O,0.9283752778,0.5535921816,-2.8102729913\H,1.5354379061,2.3299920805,-2.0669003143\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1548664\RMSD=4.295e-09\RMSF=5.661e-06\Thermal=0.\Dipole=0.1371858,0.6346126,1.1597067\PG=C01 [X(C6H10O2)]\

TS₁₀₋₁₁ (MeO/CHO)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\01-Feb-2011\0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dms) scf=tight int=ultrafine\DA_O_CHO_TS_DMSO_PCM\0,1\C,-0.0028835838,0.0437429326,0.0004164843\C,-0.065317996,-0.0319497778,2.329743281\H,0.6947238319,-0.0483897252,3.1066321812\C,-1.1586557387,0.7959464345,2.3893359024\H,-1.3383160481,1.2744286789,3.3765263868\O,-1.9833887157,1.0435743943,1.449565637\C,0.165992383,-0.9197389511,1.0915601814\H,-0.6299816805,-1.6699091933,0.9930406783\C,1.540238281,-1.5995395942,1.1313311063\H,1.7065648766,-2.2187039529,0.246852804\H,2.3452357018,-0.8655376915,1.1983563673\H,1.5930627213,-2.2418868836,2.0127570721\O,0.9685546094,0.8018723977,-0.3570788466\C,0.7335952182,1.8758921947,-1.3075228948\H,1.5822438888,1.8720356026,-1.9869347451\H,-0.2006066327,1.7056579752,-1.8428800191\H,0.69712631,2.8058451575,-0.7417008512\H,-0.9563236445,0.161750566,-0.5111158485\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1018774\RMSD=9.624e-09\RMSF=1.772e-06\Thermal=0.\Dipole=1.9668182,-0.2298445,-2.3586017\PG=C01 [X(C6H10O2)]\

11 (MeO/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jan-2011\0\# opt freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=dms) scf=tight\DA_N_CHO_2_DMSO\0,1\C,-0.019041377,-0.398549523,-0.0014744559\C,0.0773929507,-0.8010904704,2.5845444974\C,0.6465346141,-0.0594341296,1.363896693\H,0.5965689635,1.0217232025,1.5350718839\C,2.0622757089,-0.5253628251,1.0674503616\H,2.927851456,-0.3206914228,1.686739232\H,-0.9332482089,-0.4750188532,2.839396356\H,0.7140666621,-0.6215021038,3.455967169\C,2.0248474571,-1.3487062703,0.0230607215\O,0.7868417086,-1.4742830467,-0.5615269234\H,0.0456811486,-1.8778874714,2.4061419643\H,2.804092232,-

1.9460615355,-0.4394390831\H,0.1298180831,0.4597000049,-0.6896742245\N
 ,-1.4071574873,-0.8071159044,0.0372781086\C,-1.8501527457,-1.379929763
 8,-1.2354095421\H,-1.2581183435,-2.2602974513,-1.4760295623\H,-2.89636
 75787,-1.6794765424,-1.1426379026\H,-1.7711991196,-0.6654194681,-2.074
 7261583\C,-2.2557684413,0.3306908062,0.3914523417\H,-3.2906473317,-0.0
 05823286,0.480714869\H,-1.9586735872,0.7564756661,1.3498444262\H,-2.22
 23637637,1.1356461453,-0.3644742971\\Version=AM64L-G03RevC.02\State=1
 -A\HF=-404.5977231\RMSD=9.038e-09\RMSF=3.851e-06\Thermal=0.\Dipole=-0
 .0287068,0.6026057,0.1774091\PG=C01 [X(C7H13N1O1)]\\

10 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\
 0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dms)\DA_O_COOR_1_DM
 SO_PCM\0,1\C,-0.0428270034,-0.012777242,-0.0413126113\O,0.0519861228,-
 0.0044840837,1.3442844138\C,1.3959591005,0.0930458863,1.8084181525\H,0.
 4977229706,-0.8230942275,-0.534948391\C,-0.0373906391,1.337411307,-0.778
 8232413\H,0.0040162271,2.2223503952,-0.1510237103\C,0.6571512629,1.4229
 539687,-2.0754879635\H,1.8593478292,1.0316164999,1.4836586569\H,1.35626
 75009,0.0658948713,2.8970418797\H,2.0002657354,-0.7475101867,1.4463991
 059\C,-1.29826674,0.4725369353,-0.6619168096\H,-1.5659031721,-0.0359427
 916,-1.5860117509\C,-2.4595805059,0.9676598804,0.1686931093\H,-3.11609
 01785,0.1362204755,0.4427527033\H,-2.1187783942,1.43873561,1.091611661
 7\H,-3.0554032305,1.6945338976,-0.3901213543\O,0.6971751747,0.53911245
 82,-2.9100829163\O,1.2700044592,2.6137596053,-2.2358914076\C,1.9930683
 21,2.7967073413,-3.4685718105\H,2.4084244444,3.8002413603,-3.414392321
 5\H,2.7907746565,2.0582015924,-3.5569178607\H,1.3208302861,2.707870754
 6,-4.3227815152\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.740275\RMS
 D=2.713e-09\RMSF=1.079e-05\Thermal=0.\Dipole=0.4824756,0.6391791,0.360
 0131\PG=C01 [X(C7H12O3)]\\

TS₁₀₋₁₁ (MeO/COOMe)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\04-Feb-2011\
 0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=d
 mso) scf=tight int=ultrafine\\DA_O_COOR_TS_DMSO_PCM\0,1\C,-0.019555
 802,-0.0240437879,-0.0334287235\C,-0.0499149252,-0.0682095756,2.484708
 7419\C,0.7888209071,-0.0253653353,1.199683226\H,1.3939890362,0.8912765
 473,1.1822002494\C,1.647794462,-1.2769097876,1.0401717589\H,1.60999863
 75,-2.007556474,1.8361226537\O,2.1454754447,-0.7706241769,-1.204836116
 6\H,-0.6654261045,0.827701338,2.5929954396\H,0.623487635,-0.1258677744
 ,3.3424636123\O,3.1944967491,-2.5198294048,-0.3293078752\C,2.290595624
 1,-1.4789149373,-0.1711465356\C,3.5257343939,-3.3323278597,0.792833060
 4\H,3.9023695,-2.7289839652,1.6241525394\H,2.6636790273,-3.9149707854,
 1.1341469925\H,4.3048457456,-4.0153501374,0.4546021818\H,-0.7012134751
 ,-0.9439696592,2.5046437547\O,-1.0341523642,-0.7934374365,-0.150706106
 8\C,-1.7127973302,-0.9095303717,-1.4322519351\H,-2.7777401437,-0.86268
 63982,-1.2184909312\H,-1.4052366354,-0.0996905289,-2.0936992704\H,-1.4
 447925095,-1.8797382717,-1.8476059981\H,0.2218146339,0.6237913807,-0.8
 754192939\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.6699278\RMSD=
 6.532e-09\RMSF=9.136e-06\Thermal=0.\Dipole=-3.1488128,0.6896489,0.68164

87\PG=C01 [X(C7H12O3)]\

11 (MeO/COOMe)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\03-Feb-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dmsol) scf=tight\DA_O_COOR_2_DMSO_PCM\0,1\C,0.0017920711,0.0122217707,0.011491043\O,0.0036738431,0.0503186884,1.399874136\C,1.3031005674,-0.0208523669,1.9819944422\C,-2.4706697674,-0.6426718491,0.4357218874\C,-1.4472874946,-0.0536515314,-0.5377655289\H,0.6597841783,-0.7837380259,-0.3560521932\H,-1.4271132456,-0.6911082598,-1.4347460991\C,-1.6819590586,1.3900844745,-0.9326914843\H,-2.6377715668,1.8038400804,-1.2223619723\O,0.561346371,1.2536589748,-0.5203000237\H,-2.2166085361,-1.6707378082,0.7084687341\H,-3.4598555146,-0.6566849416,-0.0306027121\H,1.160601372,-0.0686563482,3.0610032869\H,1.8327736222,-0.9206225911,1.6455969778\O,-0.117161444,3.2708613285,-1.188946317\C,-0.5036509871,2.0215498141,-0.903474902\C,-1.1505519587,4.1458513367,-1.6532688421\H,-1.6009538965,3.7561216832,-2.5702877516\H,-1.9225215827,4.2682179697,-0.8885163475\H,-0.6692904554,5.1009214483,-1.8512660583\H,1.8979584448,0.8619854701,1.7322029051\H,-2.5312266281,-0.0540788541,1.3518932109\Version=AM64L-G03RevC.02\State=1-A\HF=-499.722979\RMSD=3.355e-09\RMSF=5.350e-06\Thermal=0.\Dipole=-0.4201421,-0.111009,-0.2712469\PG=C01 [X(C7H12O3)]\

10 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jan-2011\0\# opt freq rb3lyp/6-311g(d) scrf=(iefpcm,solvent=dmsol) scf=tight\DA_N_CHO_1_DMSO_PCM\0,1\C,-0.0093505848,-0.0019861515,-0.000299841\H,0.0089394246,0.016773973,1.0968959343\C,1.3900451247,-0.0171474515,-0.6306066807\H,1.4925123833,0.5040474949,-1.5785469013\C,2.5624510601,0.0056682672,0.2539818651\C,0.4798042241,-1.257493931,-0.6329468284\H,0.8034477306,-2.0186257428,0.0746570587\C,-0.0477743363,-1.7757268803,-1.9501418192\H,-0.8788165782,-2.4694682722,-1.7883176869\H,-0.4079717898,-0.9611249294,-2.5800078283\H,0.7307841038,-2.3168592051,-2.495268987\N,-1.014701889,0.7964532404,-0.641246085\C,-0.87869149,2.211869099,-0.3084939308\H,-1.6201564694,2.7914361781,-0.8638650452\H,-1.022155441,2.4152822067,0.7674927084\H,0.1137355673,2.5669098881,-0.5928985035\C,-2.3573702162,0.3043896054,-0.3350325946\H,-2.6069228479,0.3839045459,0.7376969696\H,-3.0954606123,0.8818069696,-0.8971353053\H,-2.4485672397,-0.7422118196,-0.6289784254\O,2.6082633074,-0.5128876018,1.3572035221\H,3.4506788248,0.5430427248,-0.1407252663\Version=AM64L-G03RevC.02\State=1-A\HF=-404.6002239\RMSD=7.222e-09\RMSF=9.728e-06\Thermal=0.\Dipole=-0.7211278,0.4385765,-1.0621294\PG=C01 [X(C7H13N1O1)]\

TS₁₀₋₁₁ (Me₂N/CHO)

1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\28-Jan-2011\0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=dmsol) scf=tight int=ultrafine\DA_N_CHO_TS_DMSO_PCM\0,1\C,-0.1251108395,-0.0637894638,-0.1733732223\C,0.4485686539,0.0218728884,2.184090928\H,1.4253374138,-0.0990850374,2.645745913\C,-0.4413371817,0.97448665

65,2.6344413706\H,-0.1040519668,1.5363696967,3.5373339159\O,-1.5857037
603,1.2517077706,2.1550651637\C,0.0462036646,-0.9091091594,1.052152678
8\H,-0.9664256391,-1.2832005671,1.2508267775\C,0.966480815,-2.12991541
99,0.8906416398\H,0.6879652729,-2.7406743922,0.027465216\H,2.019414701
8,-1.8609727253,0.7932956678\H,0.8723445884,-2.7492648541,1.7858530512
\H,-1.1466876921,0.1303698631,-0.4965538619\N,0.7844167962,0.543353265
8,-0.8738441092\C,2.2170047852,0.4907847924,-0.5542554332\H,2.67493664
22,-0.392050803,-1.0023922501\H,2.6952496792,1.3816784488,-0.958739075
5\H,2.3347814235,0.4748159937,0.5284054762\C,0.4226287182,1.3977840866
,-2.0140912981\H,0.9612913836,1.0589983001,-2.900871365\H,-0.648537885
5,1.339309122,-2.1953319147\H,0.7056034199,2.4302341565,-1.7969664237\
\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5742113\RMSD=6.722e-09\R
MSF=1.066e-05\Thermal=0.\Dipole=2.4850747,-0.7670528,-3.939988\PG=C01 [X
(C7H13N1O1)]\

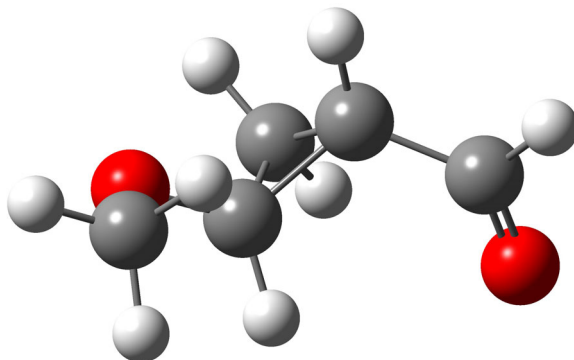
11 (Me₂N/CHO)

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\27-Jan-2011\
0\# opt freq b3lyp/6-311g(d) scrf=(iefpcm,solvent=dms) scf=tight\DA_N
_CHO_2_DMSO\0,1\C,-0.019041377,-0.398549523,-0.0014744559\C,0.0773929
507,-0.8010904704,2.5845444974\C,0.6465346141,-0.0594341296,1.36389669
3\H,0.5965689635,1.0217232025,1.5350718839\C,2.0622757089,-0.525362825
1,1.0674503616\H,2.927851456,-0.3206914228,1.686739232\H,-0.9332482089
,-0.4750188532,2.839396356\H,0.7140666621,-0.6215021038,3.455967169\C,
2.0248474571,-1.3487062703,0.0230607215\O,0.7868417086,-1.4742830467,-
0.5615269234\H,0.0456811486,-1.8778874714,2.4061419643\H,2.804092232,-
1.9460615355,-0.4394390831\H,0.1298180831,0.4597000049,-0.6896742245\N
,-1.4071574873,-0.8071159044,0.0372781086\C,-1.8501527457,-1.379929763
8,-1.2354095421\H,-1.2581183435,-2.2602974513,-1.4760295623\H,-2.89636
75787,-1.6794765424,-1.1426379026\H,-1.7711991196,-0.6654194681,-2.074
7261583\C,-2.2557684413,0.3306908062,0.3914523417\H,-3.2906473317,-0.0
05823286,0.480714869\H,-1.9586735872,0.7564756661,1.3498444262\H,-2.22
23637637,1.1356461453,-0.3644742971\Version=AM64L-G03RevC.02\State=1
-A\HF=-404.5977231\RMSD=9.038e-09\RMSF=3.851e-06\Thermal=0.\Dipole=-0
.0287068,0.6026057,0.1774091\PG=C01 [X(C7H13N1O1)]\

Methyl Substituents

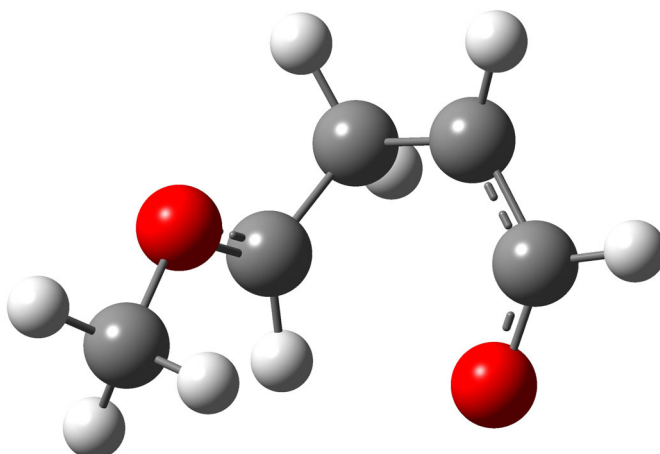
Without Methyl Substituent

12a (MeO/CHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H8O2\TSCHNEI\28-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHO_1_noMe\0,1\C,0.0165688429,0.0010
843174,-0.0009992965\O,0.0051344224,0.0039148979,1.3817418477\C,1.30471
80132,-0.000707212,1.9558259605\H,0.5933748189,-0.7953191365,-0.47070427
27\C,0.0775616982,1.3632237242,-0.739372317\H,0.0983574268,2.2390415989
,-0.1003607201\C,0.8585272719,1.4153230332,-1.9880809006\H,1.8677004218,
0.8981049012,1.675969556\H,1.17017822,-0.0216277526,3.0364668607\H,1.87
31628395,-0.8861269316,1.6454145523\C,-1.1824536646,0.4967283015,-0.692
1316322\H,-1.4643718042,0.0220581034,-1.6245613777\O,0.8595946428,0.540
7134393,-2.8274572987\H,1.4924832609,2.3187084069,-2.11977932\H,-1.9914
121087,0.8664558444,-0.0736328857\Version=AM64L-G03RevC.02\State=1-A\
HF=-345.8201064\RMSD=8.393e-09\RMSF=6.942e-06\Thermal=0.\Dipole=0.203
8016,0.4325532,0.8961635\PG=C01 [X(C5H8O2)]\
```

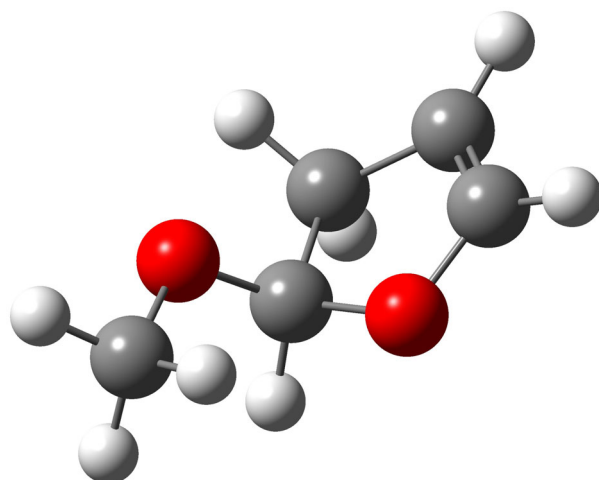
TS_{12a-12b} (MeO/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H8O2\TSCHNEI\28-Jun-2010\
0\# opt=(calcf,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultrafine\
DA_O_CHO_TS_noMe\0,1\C,-0.0004039613,0.0036825676,-0.0103338636\C,
-0.0067302679,0.0161908913,2.2835067002\H,0.7724719933,0.0385404945,3.
0368738015\C,-1.0880958515,0.882066376,2.3108979521\H,-1.2931910314,1.
```

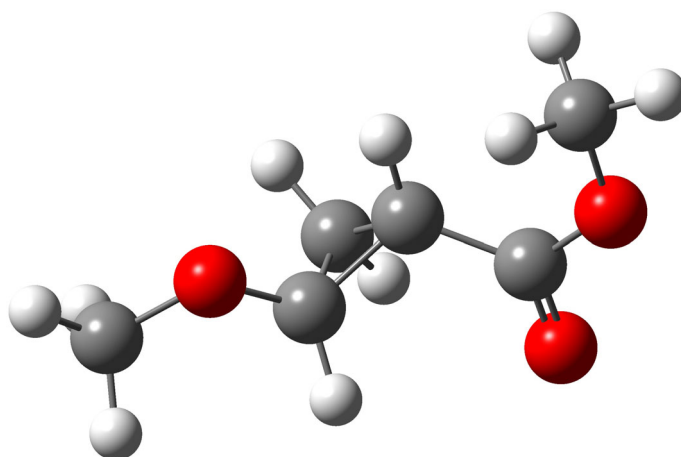
3429017815,3.2995845315\O,-1.8617286844,1.1583084589,1.3582019875\C,0.1651477804,-0.9328259189,1.0901194042\H,-0.5786369328,-1.7343256327,1.0500172048\O,0.9983004442,0.7304804934,-0.4248242129\C,0.6807296603,1.8811847573,-1.2382166405\H,1.6231007009,2.2176318443,-1.661466549\H,-0.0164550986,1.6031413301,-2.0310341728\H,0.2433462189,2.64965839,-0.6017088253\H,-0.9671131762,0.1744341102,-0.4675904902\H,1.1727841573,-1.3532913144,1.1050066487\\Version=AM64L-G03RevC.02\State=1-A\HF=-345.761007\RMSD=7.038e-09\RMSF=4.524e-07\Thermal=0.\Dipole=1.1877331,-0.1136394,-1.4341912\PG=C01 [X(C5H8O2)]\\

12b (MeO/CHO)



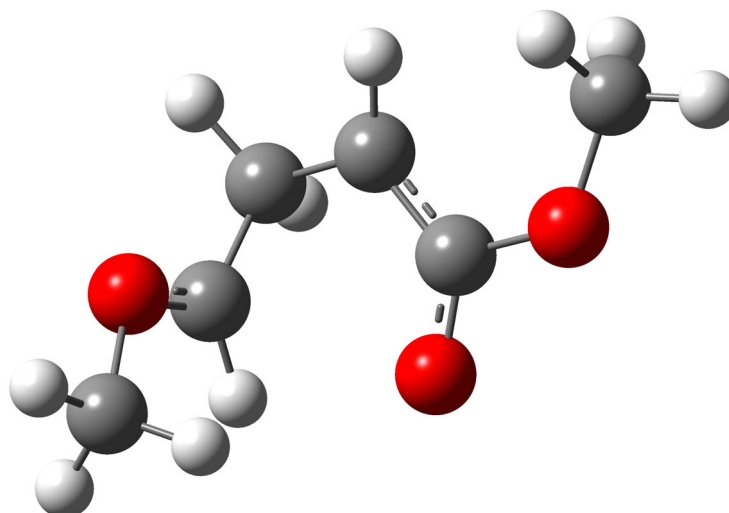
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H8O2\TSCHNEI\28-Jun-2010\0\\# opt freq rb3lyp/6-311g(d)\DA_O_CHO_2_noMe\\0,1\C,0.007143062,0.0088862714,-0.0132912419\O,-0.0038568901,-0.0274955684,1.3786877103\C,1.2883633548,-0.0120759862,1.9719846357\C,-1.4449939212,-0.0558115619,-0.5234873347\H,-1.5595049439,-0.7936802333,-1.3251614012\C,-1.6738057941,1.3569826617,-1.0036554094\H,-2.6176329088,1.7604941026,-1.3396086795\H,1.1382852119,-0.1085858752,3.0464982773\H,1.8952538943,-0.8553051295,1.6153456933\C,-0.5183159506,2.0104776292,-0.9461089049\O,0.5453162543,1.2706765817,-0.4914732433\H,1.8132792138,0.9222368501,1.7572269694\H,-0.2727705649,3.0303321768,-1.2097251892\H,0.6747914859,-0.7640937065,-0.410915715\H,-2.0987041002,-0.3531026974,0.3003381508\\Version=AM64L-G03RevC.02\State=1-A\HF=-345.835558\RMSD=7.721e-09\RMSF=1.454e-05\Thermal=0.\Dipole=0.0579887,-0.1924754,-0.0866319\PG=C01 [X(C5H8O2)]\\

12a (MeO/COOMe)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\14-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COOR_1_noMe\0,1\C,0.0810002639,0.02
45461459,0.0340258963\O,0.2195807239,0.035592103,1.4193414611\C,1.577
094,-0.0105322658,1.8349639617\C,0.0348087526,-1.2734330831,-0.6972743
236\H,0.5032277157,0.8826984006,-0.4864632292\H,0.4077808466,-1.302642
7511,-1.7135584572\C,-1.2527063739,-0.4782691322,-0.4730947706\H,-1.9042
754975,-0.8543846181,0.3027790261\O,-1.1541922249,0.6087487484,-2.5734
971583\H,1.5721729435,0.0022336669,2.9244198721\H,2.074041634,-0.92317
03351,1.48392023\O,-3.1695135511,0.4540795227,-1.6918494548\C,-1.83154
20959,0.2259929942,-1.6533564974\C,-4.0344735441,0.068297494,-0.620248
5587\H,-4.0586918215,-1.0169469143,-0.4923276804\H,-3.7523397485,0.548
9598278,0.3194419564\H,-5.0242516282,0.4124404431,-0.9133490413\H,2.13
64621614,0.8594199891,1.4679993191\H,0.1346188929,-2.1835456273,-0.117
3600392\Version=AM64L-G03RevC.02\State=1-A\HF=-460.3923172\RMSD=5.
475e-09\RMSF=4.779e-06\Thermal=0.\Dipole=-0.0449865,-0.6966525,1.298771
6\PG=C01 [X(C6H10O3)]\
```

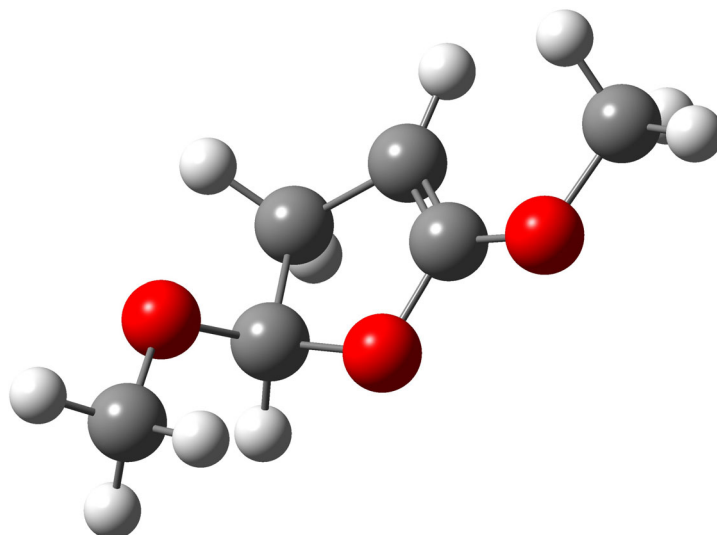
TS_{12a-12b} (MeO/COOMe)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\14-Jul-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultrafine
\DA_O_COOR_TS_noMe\0,1\C,0.0058990105,-0.0056525139,-0.0108483971
```

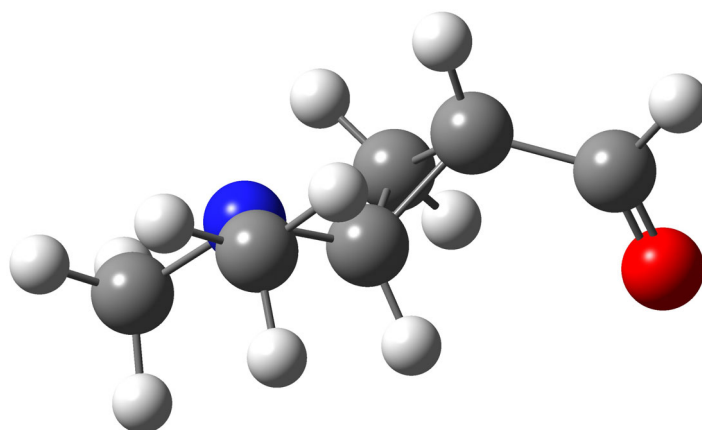
\C,-0.0044271095,-0.01689189,1.4501807532\H,1.0115255533,0.0656785681,
 1.8502489826\C,-0.6952115348,-1.3454058769,1.7174703596\H,-1.599459393
 1,-1.3263440145,2.3096161927\O,0.4807278088,-2.456952755,-0.0001599501
 \O,-0.7100007495,-3.7241496567,1.3678802298\C,-0.279970048,-2.47427740
 19,0.9895913659\C,-1.4290268844,-3.885150169,2.5821044967\H,-0.8995625
 539,-3.4311274035,3.4246689999\H,-2.4348307233,-3.4544752353,2.5161188
 47\H,-1.5176905789,-4.9600322849,2.7394631094\O,-1.046106086,0.3388830
 707,-0.6909398417\C,-1.0570574785,-0.0250385642,-2.0935736872\H,-2.0112
 041509,0.3205302086,-2.4807534786\H,-0.234585086,0.4713190324,-2.61219
 53689\H,-0.9683167446,-1.1071511347,-2.1748815689\H,0.8750864571,-0.322
 3546379,-0.5734018945\H,-0.6213705124,0.7948957329,1.8423572089\\Versio
 n=AM64L-G03RevC.02\State=1-A\HF=-460.3253448\RMSD=4.141e-09\RMSF=
 1.055e-06\Thermal=0.\Dipole=-0.589902,1.7306276,-0.5452829\PG=C01 [X(C6
 H10O3)]\

12b (MeO/COOMe)



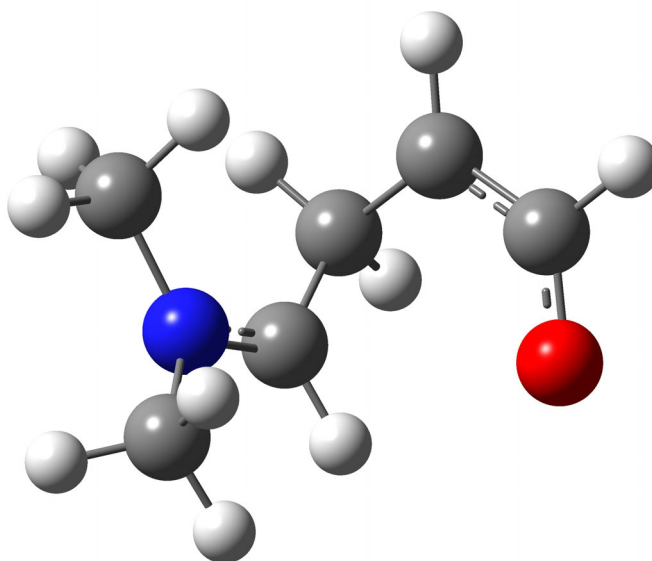
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O3\TSCHNEI\14-Jul-2010\
 0\\# opt freq rb3lyp/6-311g(d)\DA_O_COOR_2_noMe\0,1\C,0.0089650824,0.01
 59926937,-0.0079309967\O,0.0001708979,-0.0369874037,1.3815435991\C,1.2
 939660911,-0.0336124421,1.9732397856\C,-1.4431778762,-0.0321320728,-0.5
 215942119\H,0.6736704615,-0.7528516974,-0.4173536867\H,-1.5532982684,-
 0.7592207161,-1.3349385878\C,-1.6688152966,1.3907561571,-0.9664728914\
 H,-2.613997667,1.8036122821,-1.280402725\O,0.5583855551,1.2786876994,-
 0.4703468689\H,1.1444646551,-0.1435264089,3.0465095733\H,1.8968443282,
 -0.8744498597,1.6047098991\O,-0.1185054932,3.2835277107,-1.1728653344\
 C,-0.4956600172,2.0320279578,-0.8955370434\C,-1.1474454647,4.140339538
 8,-1.6570572804\H,-1.5697163735,3.752364732,-2.5892078086\H,-1.9434714
 942,4.2493620318,-0.9141081793\H,-0.6766332914,5.1040999814,-1.8376597
 427\H,1.8214667104,0.9015756809,1.7696712903\H,-2.0931105583,-0.350556
 4122,0.2977948557\\Version=AM64L-G03RevC.02\State=1-A\HF=-460.393116
 8\RMSD=6.029e-09\RMSF=4.541e-05\Thermal=0.\Dipole=-0.2856331,0.069856
 5,-0.2228385\PG=C01 [X(C6H10O3)]\

12a (Me₂N/CHO)



```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H11N1O1\TSCHNEI\15-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHO_1_noMe\0,1\C,0.0114031382,0.039
148045,0.0361403331\H,0.0633537649,0.0886043956,1.1286740173\C,1.3862
164054,-0.0341737206,-0.6381604086\H,1.4696253626,0.4712778328,-1.5934
71195\C,2.5835844453,-0.0304138556,0.2296445139\C,0.4487846352,-1.2379
030892,-0.5784817402\H,0.7524524858,-2.0428025898,0.0803775536\N,-1.00
1472652,0.8155007325,-0.616758719\C,-0.9013481006,2.2332983747,-0.2909
897946\H,-1.6311916025,2.7972768375,-0.8766988194\H,-1.0833711925,2.44
53510627,0.7775994506\H,0.094311776,2.602611648,-0.5449273292\C,-2.340
3608916,0.2934685903,-0.3584370108\H,-2.6391898168,0.3749467624,0.7016
800216\H,-3.0692468378,0.8442023579,-0.9580140699\H,-2.3902343728,-0.7
582480939,-0.6452638899\O,2.6460062318,-0.5715595905,1.3109209466\H,3.
4603567491,0.5246450335,-0.1688676151\H,-0.0058913138,-1.5289113644,-1
.5179314123\Version=AM64L-G03RevC.02\State=1-A\HF=-365.2677379\RMSD
=4.617e-09\RMSF=1.569e-05\Thermal=0.\Dipole=-0.6214326,0.3964126,-0.7309
653\PG=C01 [X(C6H11N1O1)]\
```

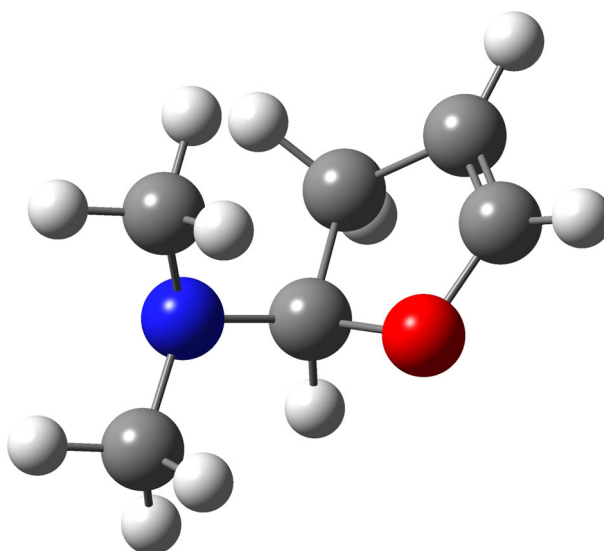
TS_{12a-12b} (Me₂N/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H11N1O1\TSCHNEI\15-Jul-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra
```

fine\\DA_N_CHO_TS_noMe\\0,1\\C,0.1820165019,-0.1362520602,0.0360181\\C,-
 0.3951040505,0.4045831337,2.2317188278\\H,0.093451839,0.8675361506,3.08
 17435315\\C,-1.7331127047,0.6384494525,1.9276771613\\H,-2.2847838057,1.2
 377256574,2.6860491561\\O,-2.3615798213,0.2270338558,0.9224742144\\C,0.3
 634194393,-0.6349753976,1.4148088555\\H,-0.0567774408,-1.6433348414,1.4
 96123386\\H,-0.6751835851,-0.4956512674,-0.5164620695\\N,0.865978771,0.8
 327876861,-0.5301801278\\C,0.3717155092,1.4795255178,-1.7465481192\\H,-0
 .0354225951,2.4658457018,-1.5053080406\\H,1.1847884814,1.5921036329,-2.
 4661818951\\H,-0.4189536603,0.8754507243,-2.1861227483\\C,1.9146734132,1
 .5345077876,0.2052322532\\H,1.4650806825,2.0075038478,1.0870452509\\H,2.
 6875280544,0.8392783767,0.5341756516\\H,2.3682159002,2.2858645488,-0.43
 79598917\\H,1.4130870815,-0.6703686851,1.7164698862\\Version=AM64L-G03
 RevC.02\\State=1-A\\HF=-365.2313411\\RMSD=8.956e-09\\RMSF=6.469e-06\\Ther
 mal=0.\\Dipole=2.4330246,0.5482608,-1.4294766\\PG=C01 [X(C6H11N1O1)]\\

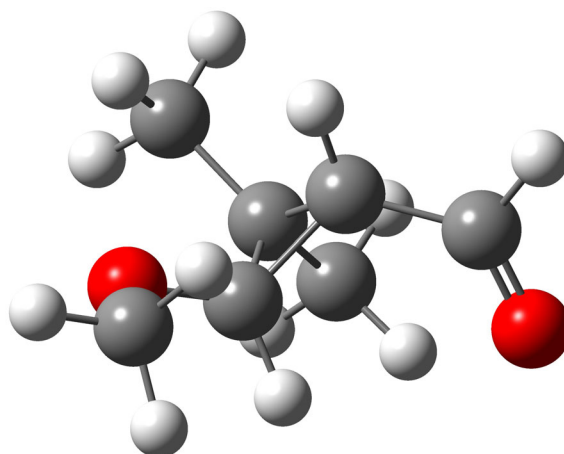
12b (Me₂N/CHO)



1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C6H11N1O1\\TSCHNEI\\15-Jul-2010\\
 0\\# opt freq b3lyp/6-311g(d)\\DA_N_CHO_2_noMe\\0,1\\C,-0.214039241,-0.15
 35818845,-0.0343305429\\C,0.1539375781,-0.0881723941,1.4719511898\\H,1.2
 306977681,0.0723481559,1.5940702463\\C,-0.2852929629,-1.4358935387,1.98
 73255078\\H,-0.2626650749,-1.7511632545,3.0204983496\\C,-0.6963654433,-2
 .1698791687,0.9551120434\\O,-0.6360995551,-1.5658265343,-0.2645507517\\H
 ,-1.0767772771,-3.1836852656,0.9352628036\\H,0.6588899991,-0.0198702483
 ,-0.6732313206\\N,-1.2077454792,0.7810192456,-0.4560972378\\C,-2.5086811
 015,0.6520090212,0.1953181825\\H,-3.1172983543,1.5271191329,-0.04475286
 36\\H,-3.0558770882,-0.2470495037,-0.1237579488\\H,-2.3948719579,0.61124
 63132,1.2786797702\\C,-1.3421466136,0.8762948233,-1.9071133257\\H,-1.786
 8256243,-0.0228785207,-2.3593946566\\H,-1.9732535209,1.7329594449,-2.15
 66716521\\H,-0.3616892301,1.0403053595,-2.3601682525\\H,-0.3414261673,0.
 7578454426,1.9573777015\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-365.27
 73976\\RMSD=3.681e-09\\RMSF=7.850e-06\\Thermal=0.\\Dipole=-0.0705277,0.215
 455,0.1288721\\PG=C01 [X(C6H11N1O1)]\\

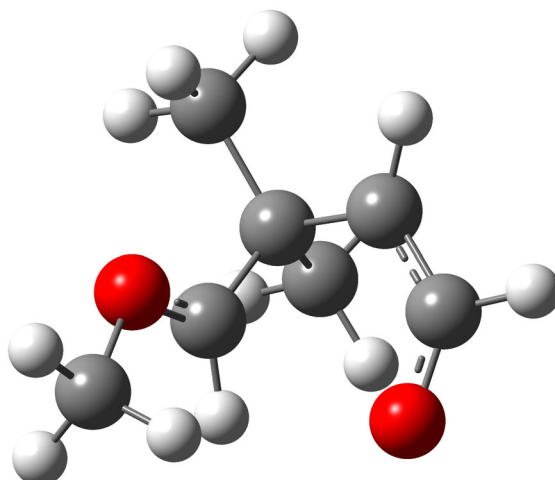
Two Methyl Substituents

12a (MeO/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\28-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHO_1_2Me\0,1\C,0.0053986349,-0.0141
312695,0.0127004966\O,0.0228106754,0.0051721156,1.3983444431\C,1.33440
74085,0.0204551989,1.9425696031\H,0.5639533787,-0.8314778375,-0.445966
5577\C,0.1175634859,1.3195351806,-0.7533038418\H,0.0897628758,2.213784
6186,-0.1383877382\C,0.9842087802,1.3991496444,-1.9404599482\H,1.88558
77482,0.9164131156,1.631450443\H,1.2250840139,0.0207670024,3.026453892
4\H,1.9018272092,-0.8673228833,1.6368739726\C,-1.1951597645,0.47633123
77,-0.6971749918\O,1.2587854282,0.4760853402,-2.679313767\H,1.41878490
57,2.4050337403,-2.1310357251\C,-2.3156113174,1.0864662292,0.123694309
3\H,-2.8668259311,1.8246584444,-0.4661349202\H,-3.0216144652,0.3080907
192,0.4297474291\H,-1.9464004221,1.5666044394,1.0294779694\C,-1.65430
05077,-0.2554913726,-1.943090951\H,-2.3029304039,-1.0913353014,-1.66201
44118\H,-2.2311116315,0.4099626837,-2.5928282397\H,-0.8180753167,-0.64
47968588,-2.5220977094\Version=AM64L-G03RevC.02\State=1-A\HF=-424.46
77529\RMSD=5.822e-09\RMSF=1.901e-05\Thermal=0.\Dipole=-0.1226457,0.42
68614,0.7843346\PG=C01 [X(C7H12O2)]\

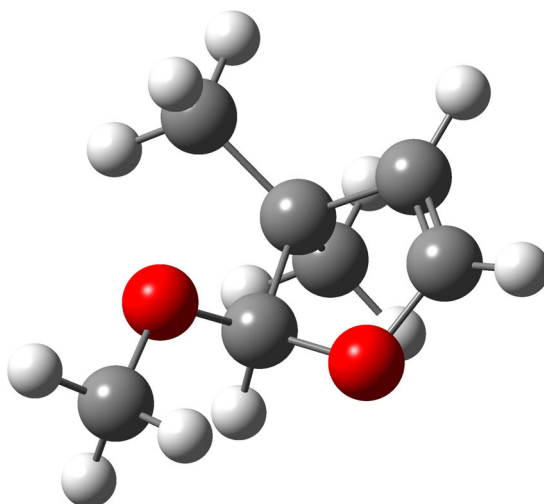
TS_{12a-12b} (MeO/CHO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O2\TSCHNEI\28-Jun-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHO_1_2Me\0,1\C,0.0053986349,-0.0141
312695,0.0127004966\O,0.0228106754,0.0051721156,1.3983444431\C,1.33440
74085,0.0204551989,1.9425696031\H,0.5639533787,-0.8314778375,-0.445966
5577\C,0.1175634859,1.3195351806,-0.7533038418\H,0.0897628758,2.213784
6186,-0.1383877382\C,0.9842087802,1.3991496444,-1.9404599482\H,1.88558
77482,0.9164131156,1.631450443\H,1.2250840139,0.0207670024,3.026453892
4\H,1.9018272092,-0.8673228833,1.6368739726\C,-1.1951597645,0.47633123
77,-0.6971749918\O,1.2587854282,0.4760853402,-2.679313767\H,1.41878490
57,2.4050337403,-2.1310357251\C,-2.3156113174,1.0864662292,0.123694309
3\H,-2.8668259311,1.8246584444,-0.4661349202\H,-3.0216144652,0.3080907
192,0.4297474291\H,-1.9464004221,1.5666044394,1.0294779694\C,-1.65430
05077,-0.2554913726,-1.943090951\H,-2.3029304039,-1.0913353014,-1.66201
44118\H,-2.2311116315,0.4099626837,-2.5928282397\H,-0.8180753167,-0.64
47968588,-2.5220977094\Version=AM64L-G03RevC.02\State=1-A\HF=-424.46
77529\RMSD=5.822e-09\RMSF=1.901e-05\Thermal=0.\Dipole=-0.1226457,0.42
68614,0.7843346\PG=C01 [X(C7H12O2)]\

0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tigh
t\\DA_O_CHO_TS_2Me\\0,1\\C,0.008096879,0.0118070737,-0.0003862843\\C,-
0.0078572904,-0.0031117324,2.271769843\\H,0.7628792018,-0.0203708685,3.
036509754\\C,-1.0328156524,0.9286387657,2.3005503896\\H,-1.2344052597,1.
3767063131,3.2952338317\\O,-1.7611779455,1.2835788864,1.3355975186\\C,0.
1607236867,-0.9656654119,1.0793117789\\O,0.9968783595,0.7509853355,-0.4
164833702\\C,0.6468183199,1.8847665071,-1.2453041301\\H,1.5777843385,2.4
110392007,-1.4362734514\\H,0.209514793,1.5372663135,-2.1834640552\\H,-0.
0555372147,2.5153833208,-0.7023081835\\H,-0.9581137068,0.1750095426,-0.
4622727431\\C,1.557106479,-1.6044023091,1.1278360459\\H,1.6506384455,-2.
1852373902,2.048065541\\H,1.7121819079,-2.2785729726,0.2816324906\\H,2.3
446769085,-0.8498117303,1.1200953313\\C,-0.9512657277,-2.022461199,1.00
93048198\\H,-0.8574655665,-2.6502487296,0.1147647592\\H,-0.901495446,-2.
6639133827,1.8912518595\\H,-1.9320415897,-1.5430122475,0.9999539636\\Ve
rsion=AM64L-G03RevC.02\\State=1-A\\HF=-424.4095627\\RMSD=4.879e-09\\RMS
F=1.046e-06\\Thermal=0.\\Dipole=1.0926586,-0.1885294,-1.3206194\\PG=C01 [X(
C7H12O2)]\\

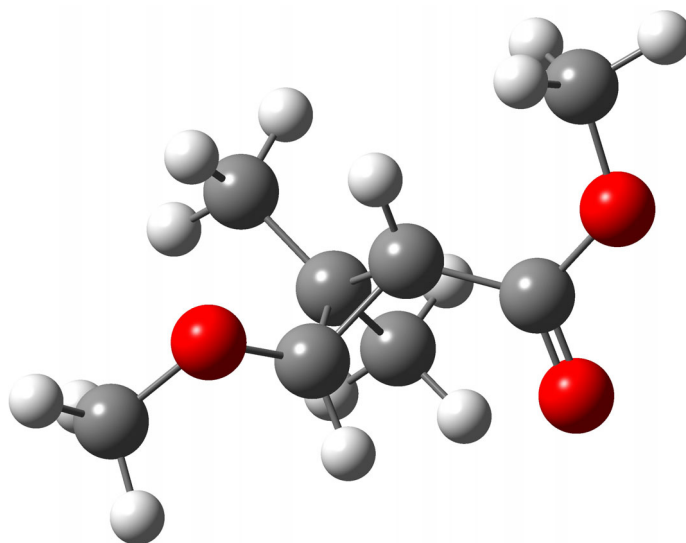
12b (MeO/CHO)



1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H12O2\\TSCHEI\\28-Jun-2010\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_O_CHO_2_2Me\\0,1\\C,-0.003680693,0.00955
78362,0.0208815481\\O,0.0216642513,0.0320706932,1.4106138943\\C,1.329394
9317,0.0320540924,1.967957472\\C,-1.4701803045,-0.0709140035,-0.5103531
102\\C,-1.6724477599,1.3637295028,-0.9667171004\\H,-2.6196308784,1.77765
34063,-1.2832822691\\H,1.2069932022,-0.02098988,3.0490435534\\H,1.902101
6898,-0.8405339557,1.6260216805\\C,-0.5056066879,1.9960748136,-0.948673
7359\\O,0.5538645992,1.2379980785,-0.5120813908\\H,1.873527976,0.942430
4646,1.7040887477\\H,-0.2447542818,3.0071271977,-1.2316224563\\H,0.63999
42334,-0.7948711428,-0.3560375703\\C,-2.4775267024,-0.5040345372,0.5634
855404\\H,-3.4873310852,-0.5046880863,0.1421348131\\H,-2.2652496761,-1.51
3105446,0.9262724097\\H,-2.4596637956,0.1703828257,1.4185629574\\C,-1.52
95787093,-1.0333401763,-1.713890544\\H,-1.3404447983,-2.0666367756,-1.40
30147331\\H,-2.516151548,-1.0024387306,-2.1842480284\\H,-0.7915285857,-0.
7643942638,-2.4741211863\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-424
.4798061\\RMSD=9.473e-09\\RMSF=1.379e-05\\Thermal=0.\\Dipole=0.0687763,-

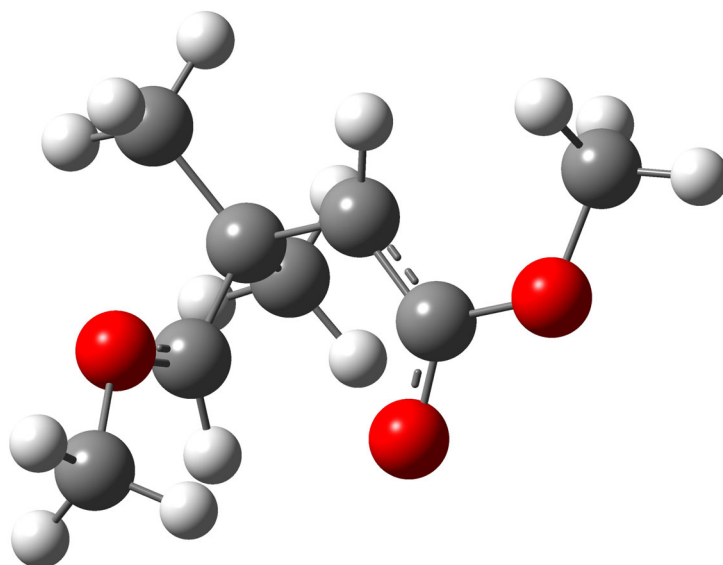
0.1722704,-0.0521925\PG=C01 [X(C7H12O2)]\

12a (MeO/COOMe)



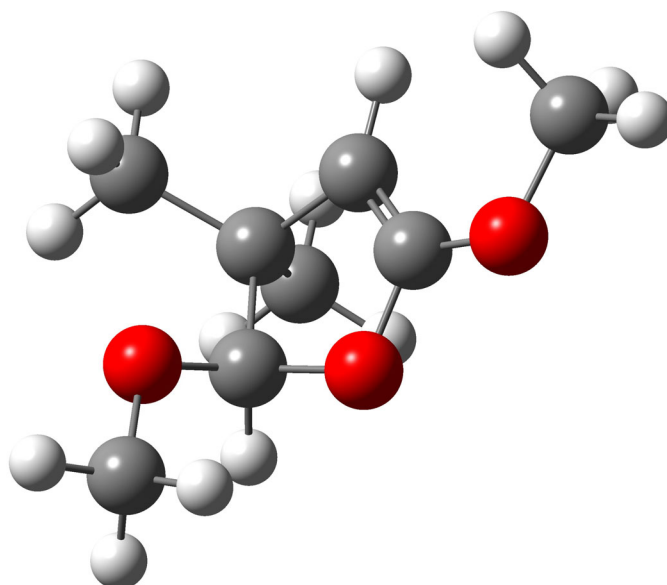
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H14O3\TSCHNEI\06-Jan-2011\
0\# opt freq rb3lyp/6-311g(d) iop(1/7=600)\DA_O_COOR_1_2Me\0,1\C,0.2586
085946,0.0919770942,0.0122088642\O,0.4731643071,0.0450325475,1.3899547
927\C,1.8521743965,0.038871181,1.7292700474\C,0.0814796104,-1.16435884
18,-0.7919218916\H,0.7129895084,0.9437492716,-0.4931326095\C,-1.135312
7316,-0.2580809983,-0.4366793375\H,-1.7559870014,-0.666407338,0.350235
0813\O,-1.1838733962,1.3431354955,-2.1967568704\H,1.9083043549,0.02461
63139,2.8174160286\H,2.3641153008,-0.8441830969,1.3284228363\O,-3.1428
904613,0.5445421085,-1.5868217354\C,-1.7889982756,0.6027204633,-1.4620
000391\C,-3.9418928681,-0.3378041324,-0.7964775474\H,-3.6255458846,-1.
3781907061,-0.9041720756\H,-3.9321974263,-0.0535773659,0.2590835945\H,
-4.9541148802,-0.2313913634,-1.1818775581\H,2.3565180355,0.9393089257,
1.3561349325\C,0.1149984672,-2.4984490025,-0.0711720805\H,-0.555444248
,-3.2184222279,-0.550771699\H,1.1236563401,-2.9234588978,-0.1001632812
\H,-0.1747357438,-2.4015608257,0.9758885611\C,0.5938304521,-1.20042821
39,-2.2176786271\H,0.016249537,-1.9068195227,-2.8233590955\H,0.5362982
189,-0.224960634,-2.6982378675\H,1.6374630597,-1.5313486622,-2.2298785
997\Version=AM64L-G03RevC.02\State=1-A\HF=-539.0393459\RMSD=6.116e
-09\RMSF=1.485e-05\Thermal=0.\Dipole=0.1024753,-1.230394,0.9110357\PG=
C01 [X(C8H14O3)]\

TS_{12a-12b} (MeO/CHO)



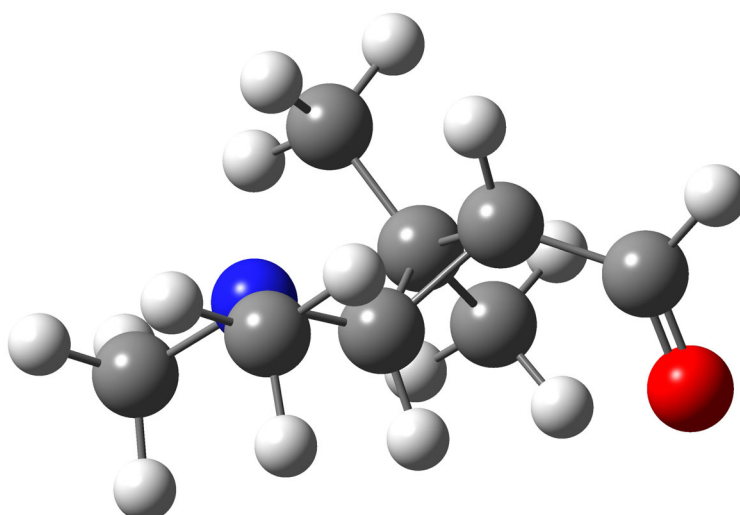
```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H14O3\TSCHNE\14-Jul-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_O_COOR_TS_2Me\0,1\C,0.0122853014,-0.0037480786,-0.004655210
7\C,0.0029757569,-0.0008158044,1.4672581619\C,1.5097844991,-0.00119531
73,1.7170503226\H,1.9036306273,-0.8035126238,2.3281117839\O,1.99391979
28,1.462928791,-0.0690653174\O,3.6465838876,1.0377356935,1.337620827\C
,2.3412715421,0.8408122674,0.9583959448\C,4.1013075981,0.533810635,2.5
855456957\H,3.4446240507,0.8413853932,3.404326558\H,4.1749191072,-0.55
96497275,2.5761911589\H,5.0970971071,0.9511456455,2.7344056493\O,0.199
1711077,-1.0844510175,-0.7004859264\C,0.5129174208,-0.8997146308,-2.103
9159856\H,0.7302258289,-1.8912419418,-2.4907329576\H,-0.3481551761,-0.4
718713841,-2.6209508119\H,1.380164701,-0.2466837179,-2.1838789493\H,-0
.1328886805,0.9151842835,-0.5600417202\C,-0.619296723,-1.2751193645,2.
0600819961\H,-0.4437275015,-1.2845039803,3.1382135756\H,-1.6983947437,
-1.3056641526,1.8894603264\H,-0.173194982,-2.175105616,1.6346220384\C,
-0.7024418223,1.262832588,1.982237708\H,-1.7656394208,1.2736699339,1.7
101748862\H,-0.620973429,1.3080541854,3.0699424502\H,-0.228191739,2.15
68897451,1.5727478257\Version=AM64L-G03RevC.02\State=1-A\HF=-538.974
5143\RMSD=8.503e-09\RMSF=2.197e-06\Thermal=0.\Dipole=-1.1870441,-1.209
287,-0.4341241\PG=C01 [X(C8H14O3)]\
```

12b (MeO/COOMe)



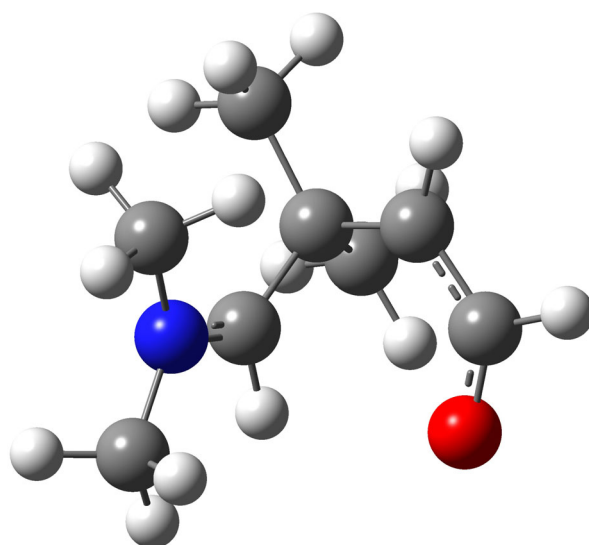
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H14O3\TSCHNEI\14-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COOR_2_2Me\0,1\C,-0.007912455,0.016
4803133,0.0227526499\O,0.0169181137,0.0265605642,1.4103299364\C,1.324
9556346,0.0198781703,1.9687389645\C,-1.4729353583,-0.0481725221,-0.514
8526658\H,0.6356428365,-0.7829529392,-0.3637922991\C,-1.6782543671,1.3
998986864,-0.9200090702\H,-2.628298458,1.8228453097,-1.2077426988\O,0.
558286408,1.2474412187,-0.4978795484\H,1.2010817444,-0.0403772486,3.04
92083762\H,1.89541468,-0.8518184218,1.6211742378\O,-0.10020564,3.26303
74918,-1.187697575\C,-0.4937316187,2.020583316,-0.8918233128\C,-1.12410
71837,4.1333721217,-1.658512223\H,-1.5755533205,3.7417044292,-2.575295
0278\H,-1.9002479823,4.2662878118,-0.8986298811\H,-0.6398593088,5.0858
766837,-1.8619245143\H,1.8702157011,0.9311319717,1.711045019\C,-2.4766
533209,-0.5215197025,0.5458509759\H,-3.4871572847,-0.5083055866,0.1259
032529\H,-2.2647650789,-1.5433773232,0.8724557791\H,-2.4593158161,0.12
33296171,1.4233907168\C,-1.5254309961,-0.98273983,-1.740846806\H,-1.33
45266817,-2.0239066541,-1.4572960299\H,-2.511365798,-0.9408124918,-2.21
16815514\H,-0.7870326789,-0.6911768844,-2.4923743528\\Version=AM64L-G
03RevC.02\State=1-A\HF=-539.0378963\RMSD=6.981e-09\RMSF=8.597e-06\T
hermal=0.\Dipole=-0.2681594,0.1142711,-0.179525\PG=C01 [X(C8H14O3)]\

12a (Me₂N/CHO)



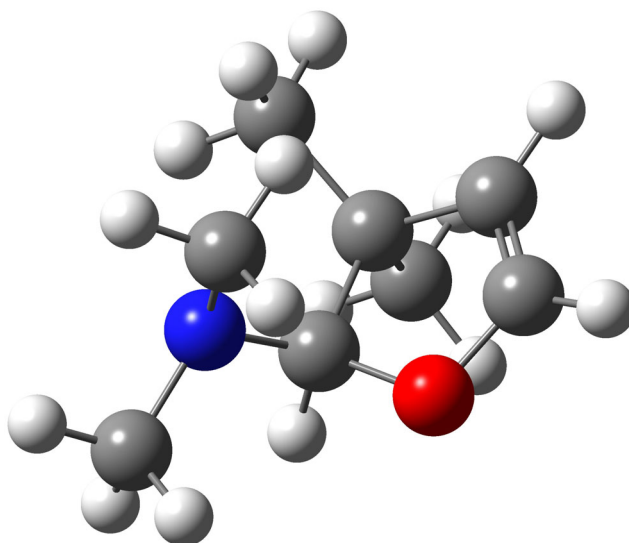
```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNEI\15-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHO_1_2Me\0,1\C,-0.019374005,0.005
3141443,0.0120627788\H,-0.0110064693,0.0086794568,1.1082384533\C,1.382
5079236,0.00770991,-0.5881854\H,1.4810374983,0.495772054,-1.5529117303
\C,2.5650030671,0.1196429548,0.2884102979\C,0.4776160621,-1.2564663542
,-0.618712659\N,-1.0242954875,0.811339493,-0.6223857786\C,-0.881935774
9,2.2249277668,-0.2908278009\H,-1.6124522275,2.8090532597,-0.855813982
8\H,-1.0332977906,2.433195536,0.783081789\H,0.1156076813,2.5726245967,
-0.5654556529\C,-2.3675128083,0.3236247102,-0.3225639588\H,-2.61995789
73,0.393446451,0.7504897721\H,-3.1034828048,0.9069435587,-0.8812662315
\H,-2.4619928426,-0.7200202195,-0.6261789959\O,2.607476008,-0.18095311
06,1.4620224604\H,3.474236187,0.5215554924,-0.2103686622\C,-0.0213795
973,-1.64952344,-1.9968225235\H,0.7624438062,-2.1686267112,-2.55678950
39\H,-0.8708265046,-2.3358776055,-1.9150538622\H,-0.345949414,-0.781356
3042,-2.5703180454\C,0.8166213662,-2.4284809256,0.2816062938\H,1.55367
45347,-3.0848655941,-0.1919191092\H,1.2214863694,-2.1074265065,1.24043
73031\H,-0.0831158041,-3.0235943333,0.4694170801\\Version=AM64L-G03Re
vC.02\State=1-AHF=-443.9144521\RMSD=5.106e-09\RMSF=4.050e-06\Therma
l=0.\Dipole=-0.6107658,0.1287757,-0.804118\PG=C01 [X(C8H15N1O1)]\\
```

TS_{12a-12b} (MeO/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNEI\15-Jul-2010\
0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_N_CHO_TS_2Me\0,1\C,0.0635725948,-0.1264957513,-0.128334089\C
,-0.3658564551,0.1908612382,2.1188808245\H,0.2450396408,0.4654053319,2
.974063647\C,-1.6231405116,0.7676759524,1.9263476283\H,-1.9942651882,1
.3600974779,2.7929366836\O,-2.3585474359,0.6703063744,0.9158372009\C,
0.168606826,-0.8724593758,1.1627980488\H,-0.8390899199,-0.3199375819,-0
.6930827068\N,0.7996879209,0.843782792,-0.6309807284\C,0.3001279927,1.
6141061916,-1.7743652358\H,-0.032921193,2.6013633745,-1.4420706023\H,1
.0922104594,1.7319594362,-2.5164952953\H,-0.5423966865,1.0977522507,-2
.2281904831\C,1.9285632217,1.4325282959,0.0858512348\H,1.6100834431,1.
6470027309,1.1123005846\H,2.7851984881,0.7599097522,0.0995212616\H,2.2
193037055,2.3577462838,-0.408465524\C,1.5711440068,-1.3460918006,1.579
3037697\H,1.473603816,-1.9251010036,2.5004855777\H,2.0203262217,-1.995
7543961,0.8223858275\H,2.2606276902,-0.5298959187,1.7924249373\C,-0.76
18264063,-2.1003038146,1.073051638\H,-0.4166648418,-2.8120451115,0.312
1284635\H,-0.7853245562,-2.6090930147,2.0384234828\H,-1.7774268535,-1.
7851112428,0.8323694543\Version=AM64L-G03RevC.02\State=1-A\HF=-443.
8722399\RMSD=8.463e-09\RMSF=6.888e-06\Thermal=0.\Dipole=2.2661708,0.
3210804,-1.3688467\PG=C01 [X(C8H15N1O1)]\
```

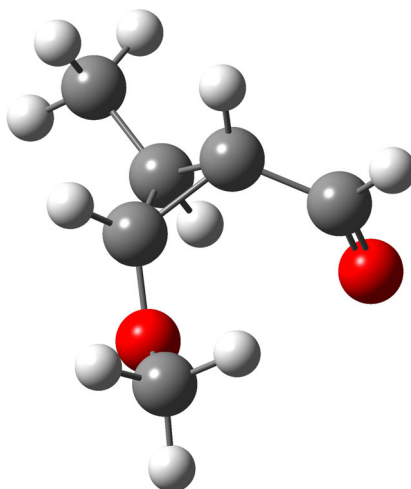
12b (Me₂N/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C8H15N1O1\TSCHNE\15-Jul-2010\
0\# opt freq b3lyp/6-311g(d)\DA_N_CHO_2_2Me\0,1\C,0.2455474209,-0.2188
477738,0.0822293347\C,-0.0057218504,0.0288338096,1.6163511898\C,1.419
1324077,0.1098708351,2.13288972\H,1.6962670272,0.1369112638,3.1778445
859\C,2.246397964,0.234082863,1.098101375\O,1.6568712957,0.181439531,-
0.1330517192\H,3.3206449761,0.3682094371,1.0746823445\H,-0.3446134415,
0.4818537794,-0.5081852163\N,-0.018551102,-1.5299313191,-0.429223834\C,
0.9383020501,-2.5700740046,-0.0545026234\H,0.5008053613,-3.5509855703,
-0.2582346673\H,1.8825942982,-2.4911024337,-0.6122286855\H,1.176191326
5,-2.5162503797,1.0056994744\C,-0.284229104,-1.560762809,-1.8652120663
\H,0.6082356899,-1.3502398925,-2.4757117136\H,-0.6568365903,-2.5506542
613,-2.1411746719\H,-1.057333184,-0.8329113367,-2.1199960832\C,-0.8759
436531,-1.0352416983,2.2987717442\H,-1.8500203333,-1.1172841507,1.8110
043454\H,-0.4207135853,-2.0249032153,2.2925975352\H,-1.0465895536,-0.7
561561458,3.3432325462\C,-0.6906220391,1.4055642041,1.77874447\H,-1.70
95810793,1.3894212214,1.3757230613\H,-0.7531303023,1.6844429731,2.8342
819503\H,-0.128783209,2.1869392791,1.2610511164\\Version=AM64L-G03Rev
C.02\State=1-A\HF=-443.9173265\RMSD=9.651e-09\RMSF=8.765e-06\Thermal
=0.\Dipole=-0.123832,-0.1672192,0.0734119\PG=C01 [X(C8H15N1O1)]\

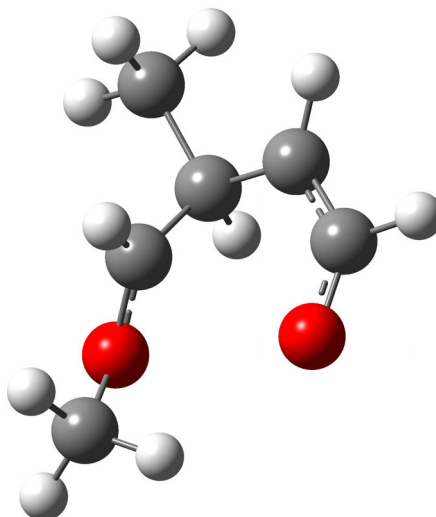
cis-Configured Cyclopropanes

13a (MeO/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\12-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_O_CHOx_1\0,1\C,0.2208833899,0.1384811263,-0.1749220243\C,-0.0077293464,0.0478094322,1.3655724328\C,1.3802076695,0.009618764,0.7265506499\O,-0.0898025523,-0.9231633125,-0.9974148292\C,-0.5672226551,-1.1871971731,1.9534375561\H,-0.0087695679,1.1210587033,-0.592717281\O,-0.169063849,-2.3088728432,1.7380738324\H,-1.4306062099,-1.0225182652,2.6361046997\H,-0.3301140042,0.9733594636,1.8345413675\C,-1.4559042519,-0.9704530116,-1.378141497\H,-2.1082882354,-1.0973561292,-0.5059834069\H,-1.7521570841,-0.0598024211,-1.9154033761\H,-1.567278316,-1.8299068662,-2.0374702967\C,2.3594712221,1.139468652,0.9433277821\H,2.8498638748,1.0534535931,1.9169148014\H,3.1376700581,1.1326931526,0.1744758069\H,1.866346603,2.1152748137,0.9062143375\H,1.7920472751,-0.996206259,0.7405758404\Version=AM64L-G03RevC.02\State=1-A\HF=-385.1411103\RMSD=5.496e-09\RMSF=1.368e-05\Thermal=0.\Dipole=-0.3712349,1.3180723,-0.1434568\PG=C01 [X(C6H10O2)]\

TS_{13a-13b} (MeO/CHO)



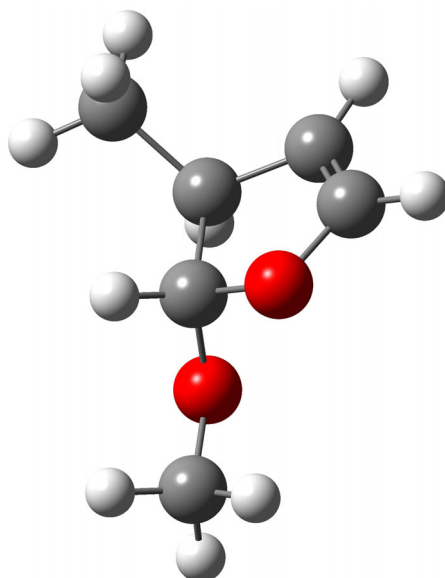
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\12-Jul-2010\

```

0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_O_CHOx_TS\0,1\C,0.1241070246,-0.0777127963,-0.0828419159\C,0.
0128868799,0.0096942502,2.1934502852\H,0.7505551665,-0.0358455113,2.98
92178835\C,-0.933237444,1.0333770628,2.1647610763\H,-1.089420076,1.550
8783551,3.1353982087\O,-1.6208204534,1.3984245518,1.1841024438\C,0.140
4536294,-0.9897721333,1.0577709682\H,-0.7068393149,-1.678351997,0.9727
497428\C,1.4545627278,-1.779771032,1.1764649061\H,1.565662764,-2.50151
41312,0.3647533976\H,2.3213776208,-1.1133048479,1.1748113215\H,1.45527
81331,-2.3216118235,2.1251647411\O,-0.7608797744,-0.1792863375,-1.0229
004735\C,-1.0710252376,0.9931564001,-1.8062783251\H,-1.7450790009,1.59
81299381,-1.2029803516\H,-0.1581397719,1.5460203371,-2.0407766903\H,-1
.546905622,0.63356417,-2.7146536147\H,0.8512587348,0.7309777591,-0.140
5138393\Version=AM64L-G03RevC.02\State=1-A\HF=-385.0888499\RMSD=3.
390e-09\RMSF=1.862e-05\Thermal=0.\Dipole=1.0571546,-0.4068655,-1.309688
6\PG=C01 [X(C6H10O2)]\

```

13b (MeO/CHO)

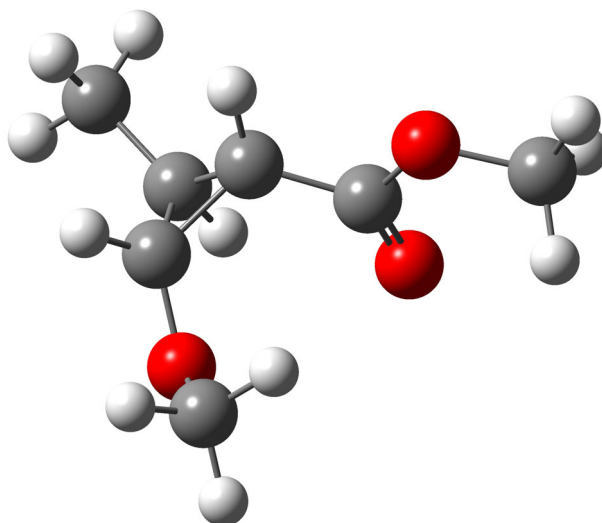


```

1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C6H10O2\TSCHNEI\12-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_CHOx_2\0,1\C,-0.2971289469,0.1125731
207,0.3244787765\C,0.1741001204,-0.2702195706,2.8266011364\C,0.7576000
206,0.0973619161,1.4557044847\H,1.192133676,1.1010604121,1.5040956858\
C,1.7458915713,-0.9162115948,0.9241298717\H,2.7030044079,-1.1443242317
,1.3710711239\H,-0.5613803094,0.470824971,3.1555148818\H,0.9606530001,
-0.3153859794,3.5844576974\C,1.2319729553,-1.4881643859,-0.1596760085\
O,-0.0087248156,-1.027976705,-0.5248065762\H,-0.3140452019,-1.24841629
06,2.7983777588\H,1.625648041,-2.2661667908,-0.8000891382\O,-0.1803872
504,1.3013586746,-0.3900031813\C,-1.1381527858,1.452802908,-1.43029783
07\H,-0.978064323,2.441366004,-1.8587978177\H,-1.0080648761,0.69206578
85,-2.20424416\H,-2.1611935668,1.3921160814,-1.0351256167\H,-1.3299664
3,-0.0290494894,0.6669770883\Version=AM64L-G03RevC.02\State=1-A\HF=-
385.1589015\RMSD=8.686e-09\RMSF=3.492e-06\Thermal=0.\Dipole=-0.15854
27,-0.0023346,0.1410587\PG=C01 [X(C6H10O2)]\

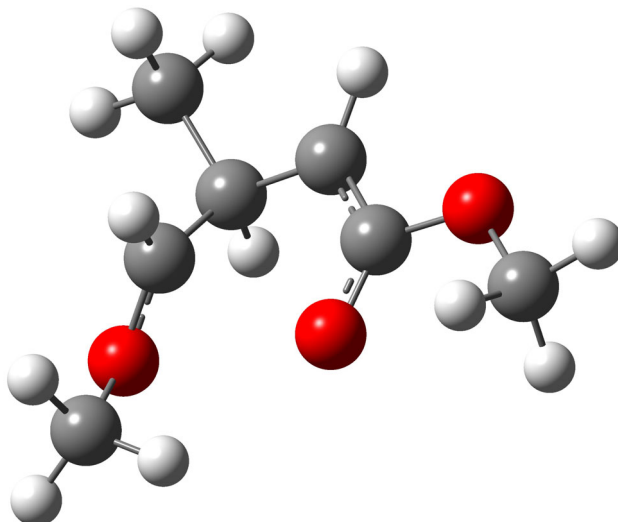
```

13a (MeO/COOMe)



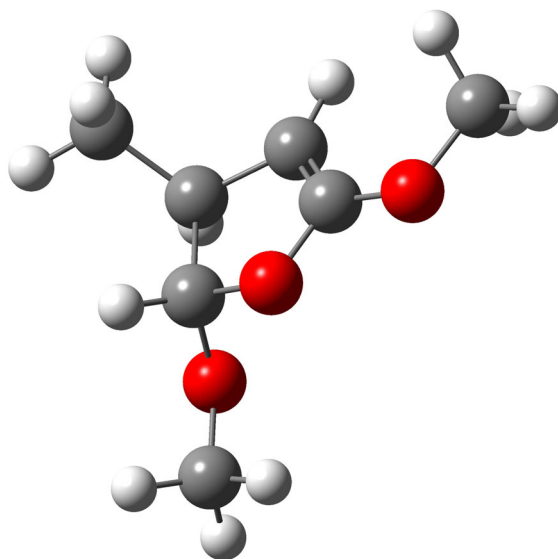
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\15-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_COORx_1\0,1\C,0.024017854,0.01219695
79,0.0550125647\C,0.1665212755,0.1179355657,1.5906706573\C,1.372600812
,0.0976066493,0.6566735304\O,-0.3496856863,-1.173336109,-0.5498542492\
C,-0.0836568878,-1.0677164267,2.4444726057\H,-0.3903994688,0.908464355
3,-0.411910288\O,0.3670183792,-2.1756367283,2.2825812957\H,-0.13397837
67,1.0644441497,2.025202512\C,-1.7541705222,-1.3710901301,-0.584690519
\H,-2.1825213045,-1.3881403244,0.424349216\H,-2.2534436528,-0.58532157
02,-1.1675287586\H,-1.9227305601,-2.3348203847,-1.063294747\C,2.2483292
509,1.318523811,0.4983002032\H,2.9602342044,1.4026135416,1.3243094668
\H,2.8198837424,1.2701820983,-0.4332676242\H,1.6576659183,2.2389745103
,0.4766438648\H,1.8826045752,-0.8613850619,0.679902581\O,-0.9166169736
, -0.7477968723,3.4685320532\C,-1.2238855815,-1.8216887449,4.3698435945
\H,-1.8764595174,-1.3901183655,5.1256594649\H,-1.7305800801,-2.63288286
56,3.8448726084\H,-0.3140503943,-2.2128231865,4.82729016\Version=AM64
L-G03RevC.02\State=1-A\HF=-499.7270509\RMSD=2.736e-09\RMSF=1.795e-0
5\Thermal=0.\Dipole=-0.5803968,0.7401341,0.1882246\PG=C01 [X(C7H12O3)]\

TS_{13a-13b} (MeO/COOMe)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\15-Jul-2010\0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=tight\DA_O_COORx_TS\0,1\C,-0.0523422527,0.0000591721,0.1267161275\C,0.021626062,-0.4185696151,2.386444081\H,0.7435186214,-0.4934650228,3.1890572182\C,-1.142294699,0.3445331212,2.5179570732\O,-1.8904431959,0.6999398504,1.5758254839\C,0.3072826869,-1.0699617677,1.0617647278\H,-0.3079429423,-1.9506190067,0.8355099008\C,1.7971901725,-1.4472516614,0.9428793167\H,2.020173179,-1.922001484,-0.0148642955\H,2.4397553271,-0.5713960458,1.0655192951\H,2.0416150616,-2.1505238048,1.7423380901\O,-0.8769330894,-0.1950213027,-0.8507574123\C,-1.50176775,0.9588946628,-1.4525384405\H,-2.2928490547,1.2776787563,-0.7766691949\H,-0.768997327,1.7566643192,-1.5943432835\H,-1.8963655321,0.6258237848,-2.4086029516\H,0.402135912,0.9830138511,0.2368262295\O,-1.4469877891,0.7058722071,3.8038913849\C,-2.5955428617,1.5353932055,3.960443747\H,-2.6166877581,1.8110119076,5.0143612084\H,-2.5273805173,2.430340276,3.3374119887\H,-3.5109050754,1.0000369698,3.6981600548\Version=AM64L-G03RevC.02\State=1-A\HF=-499.6619296\RMSD=6.479e-09\RMSF=2.106e-06\Thermal=0.\Dipole=0.4824587,0.4440663,-1.6032359\PG=C01 [X(C7H12O3)]\

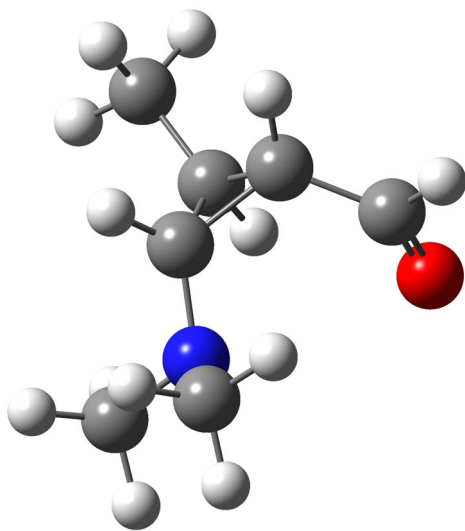
13b (MeO/COOMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\15-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_O_COORx_2\0,1\C,-0.0196907958,-0.0027388779,0.0419162434\C,-0.0744231428,0.1238674495,2.6091092424\C,0.7991955042,-0.0123368272,1.3548360638\H,1.4873885115,0.8381144715,1.3036970631\C,1.5243436019,-1.3324760555,1.2443672577\H,2.3016521176,-1.6678064653,1.9128971747\H,-0.6059558044,1.0813366674,2.6229086811\H,0.5374741806,0.0719837754,3.5136297548\C,1.03100302,-1.9942886044,0.1898038426\O,0.0483224196,-1.3483077852,-0.4987796181\H,-0.8132281324,-0.6807706176,2.6643280667\O,0.5421311125,0.9102132158,-0.8420196545\C,-0.1619661952,1.0424385918,-2.0714346759\H,0.3428508613,1.8257388263,-2.6353224808\H,-0.1442341374,0.1101057809,-2.6413057014\H,-1.2051244331,1.3382424704,-1.8970226921\H,-1.0894777822,0.1991398247,0.1767313415\O,1.2900034337,-3.1922122797,-0.3422355688\C,2.2783226941,-3.9625799717,0.3342388216\H,2.3589868478,-4.8978972989,-0.2151200087\H,3.2429237085,-3.44

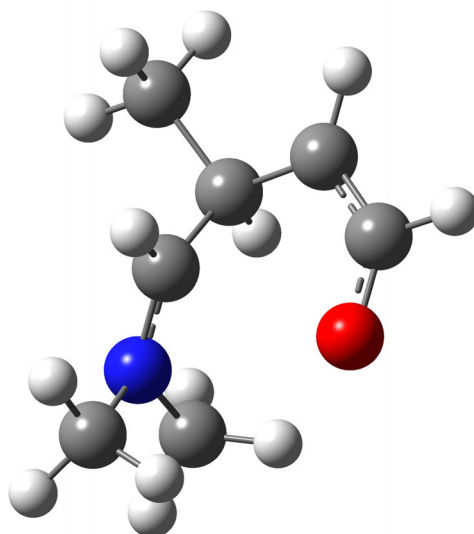
59032488,0.3312050897\H,1.9752513296,-4.1622059614,1.3667011761\\Version=AM64L-G03RevC.02\State=1-A\HF=-499.7168875\RMSD=5.747e-09\RMSF=1.391e-05\Thermal=0.\Dipole=0.167632,-0.1565745,0.3051258\PG=C01 [X(C7H12O3)]\\

13a (Me₂N/CHO)



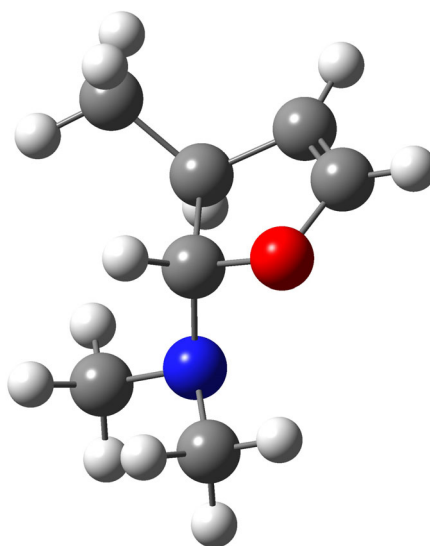
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\16-Jul-2010\0\# opt freq rb3lyp/6-311g(d)\DA_N_CHOx_1\0,1\C,0.2495850755,0.0188783245,-0.1675851621\C,-0.0442475039,0.09950367,1.3482978143\C,1.3714918865,-0.0207265531,0.8110641103\C,-0.6513907172,-1.0505985653,2.0632518227\H,0.0921811093,0.9793883302,-0.6765869071\O,-0.2171899854,-2.1771223483,2.0789098183\H,-0.3818991273,1.0742635951,1.6899047034\C,0.8145642388,-1.436995661,-1.9886344186\H,0.7993850529,-0.6722414524,-2.7869938298\H,1.8321684911,-1.5047108837,-1.6005694141\H,0.5615317746,-2.3996417151,-2.4393972327\C,2.3492919083,1.122471031,0.9532575167\H,2.7873992265,1.1445106702,1.9551564077\H,3.1686993569,1.0309876425,0.2336034173\H,1.8669447403,2.0891827416,0.7815914189\H,1.7718205055,-1.017995379,0.973478735\N,-0.1119464615,-1.1506741485,-0.9016783472\C,-1.4972241462,-1.1280090599,-1.3441974063\H,-1.7464569139,-2.0786198906,-1.8211257608\H,-2.1600886012,-0.9998824743,-0.4856438274\H,-1.7108675092,-0.3170165551,-2.065245972\H,-1.5843630996,-0.805199007,2.6187960438\\Version=AM64L-G03RevC.02\State=1-A\HF=-404.5875855\RMSD=7.820e-09\RMSF=4.648e-06\Thermal=0.\Dipole=-0.0205938,1.0594267,-0.5272915\PG=C01[X(C7H13N1O1)]\\

TS_{13a-13b} (Me₂N/CHO)



```
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\16-Jul-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=
tight\DA_N_CHOx_TS\0,1\C,0.3046993192,-0.1272463875,-0.1058989943\C,
-0.0279473915,-0.1494544847,2.2361075604\H,0.5383758927,-0.1543272531,
3.1609479186\C,-1.1891761865,0.5693236065,2.06936625\O,-1.8373367486,0
.6800621849,0.9809364726\C,0.4416376477,-1.0080169245,1.0762169017\H,-
0.1671963639,-1.9127004596,0.959555474\C,1.9145216726,-1.429526337,1.2
458180339\H,2.2642490353,-2.0570921846,0.4214357864\H,2.5687338072,-0.
5566426679,1.3242435458\H,2.0157019607,-1.9992509654,2.1726088633\H,0
.892625303,0.7851937743,-0.0678498539\N,-0.3706639679,-0.3181125636,-1.
2122908443\C,-0.5584347055,0.8053496874,-2.1336652288\H,-1.4984191408,
1.3077594521,-1.8920800897\H,0.2612289146,1.5133915062,-2.0252583297\H
,-0.5835027595,0.4405832349,-3.1611508147\C,-1.4129502256,-1.3441815209
,-1.2822716569\H,-1.7786977496,-1.4142273133,-2.3054528571\H,-1.02554165
98,-2.3142758105,-0.9807158247\H,-2.2097026153,-1.029872959,-0.597829995
6\H,-1.596449795,1.0755803442,2.9676560464\\Version=AM64L-G03RevC.02\S
tate=1-A\HF=-404.5588909\RMSD=5.607e-09\RMSF=4.386e-06\Thermal=0.\Dipo
le=0.9627136,-0.622005,-1.9617471\PG=C01 [X(C7H13N1O1)]\\
```

13b (Me₂N/CHO)

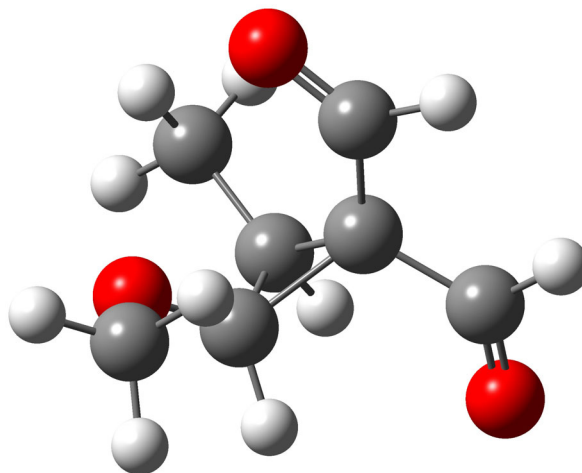


1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O1\TSCHNEI\16-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_N_CHOx_2\0,1\C,0.0641522779,0.018196
5228,0.0211461488\C,0.1025005191,0.0279231064,2.6104002096\C,0.9296039
472,-0.0346521404,1.3197099578\H,1.6378315717,0.8006792106,1.305690678
1\C,1.6695674607,-1.3397439516,1.1330433263\H,2.4249343486,-1.72245301
74,1.8047466903\H,-0.4458246757,0.9722344841,2.689271266\H,0.744732551
2,-0.056726175,3.4914932506\C,1.2469976806,-1.9219859352,0.017667797\O
,0.2850654903,-1.234201113,-0.6702740354\H,-0.6237463428,-0.7885449271
,2.6505713779\H,-1.0162350365,0.0377804032,0.2558246416\N,0.4247747036
,1.1156145985,-0.8661809473\C,-0.2017676559,0.9886455158,-2.1814665176
\H,0.1528693013,1.7982162454,-2.8230843188\H,0.0761450042,0.0400557274
, -2.6338457635\H,-1.305283982,1.0446838398,-2.1365976322\C,0.083854196
9,2.4031214,-0.2704920221\H,-1.0021025095,2.5215718773,-0.0953735847\H
,0.5966391659,2.5454580158,0.6816495758\H,0.4042296612,3.2041527085,-0
.9393554003\H,1.5319807932,-2.8599871559,-0.4398384632\\Version=AM64L-
G03RevC.02\State=1-A\HF=-404.5953858\RMSD=7.294e-09\RMSF=6.226e-06\
Thermal=0.\Dipole=-0.0311378,0.2630392,0.3035823\PG=C01 [X(C7H13N1O1)]\

Two Acceptors/Donors

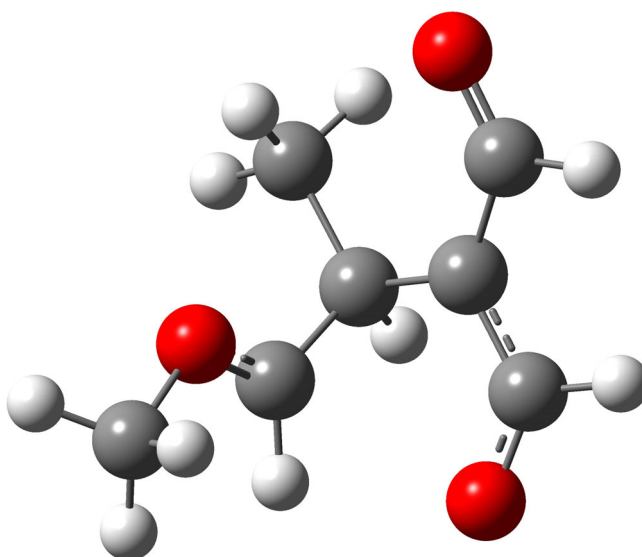
Two Acceptors

14a (MeO/2xCHO)



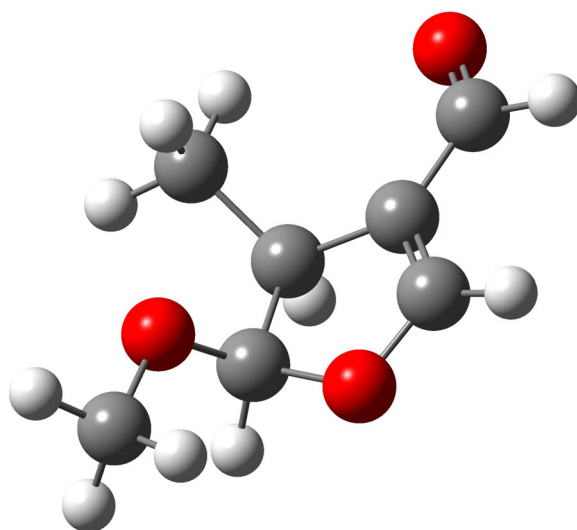
```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H10O3\TSCHNEI\12-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_2CHO_1\0,1\C,0.004028314,0.031848959
9,-0.0304917117\O,-0.0263086457,-0.0215155303,1.3269099294\C,1.2558633
943,-0.060328363,1.9473618874\H,0.6671797463,-0.6740684763,-0.53077805
46\C,0.0794029867,1.4782504923,-0.769596478\C,0.887609163,1.4569523891
,-2.0026603556\H,1.8080247771,0.866037937,1.7599424949\H,1.0780608258,
-0.1658108509,3.0155016353\H,1.8404377532,-0.9136498894,1.5848334154\C
,-1.1602633977,0.5309126139,-0.7505394323\H,-1.2801273826,0.087601483,
-1.7359652872\C,-2.4369222102,0.9260785212,-0.0465923299\H,-3.05592781
41,0.0361755073,0.0994758001\H,-2.2425133402,1.37815117,0.9222991456\H
,-3.0052940497,1.6349564416,-0.6532046763\O,0.9044804874,0.5421186584,
-2.7986946801\H,1.5266826678,2.3514431164,-2.1675043158\C,0.1664628597
,2.6925648943,0.0616617849\O,-0.4256135747,2.9203305754,1.0926302415\H
,0.8819773426,3.4466683527,-0.3402858665\\Version=AM64L-G03RevC.02\Sta
te=1-A\HF=-498.4930802\RMSE=6.799e-09\RMSE=6.993e-06\Thermal=0.\Dipol
e=0.4418418,-0.2759303,0.2537409\PG=C01 [X(C7H10O3)]\
```

TS_{14a-14b} (MeO/2xCHO)



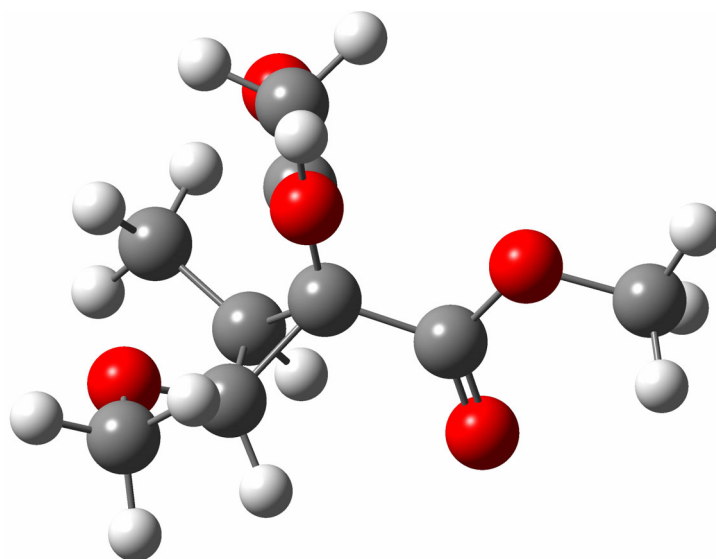
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H10O3\TSCHNE\12-Jul-2010\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) int=ultrafine scf=ti
ght\DA_O_2CHO_TS\0,1C,-0.0011072752,-0.0469770166,0.0215042795\C,-0
.054135937,-0.043371842,2.341079038\C,1.3347620106,0.1896389039,2.3977
393054\H,1.821271558,-0.0009462157,3.3733397424\O,2.0398542963,0.59376
8449,1.452323171\C,-0.7696947299,0.5659296953,1.1049035575\H,-0.543710
107,1.6368576638,1.0832974236\C,-2.2880607011,0.342379511,1.0225885741
\H,-2.6816740141,0.8187376698,0.1198699961\H,-2.5478982431,-0.71210989
02,1.0248259087\H,-2.7684727157,0.7920801454,1.8894269754\O,-0.2546170
782,-1.2499471309,-0.3609936058\C,0.6687710869,-1.92221578,-1.24916634
35\H,0.0633996843,-2.5285031768,-1.9177148207\H,1.2595259349,-1.194345
792,-1.8062820924\H,1.312994785,-2.5524556431,-0.6376975534\H,0.827503
2805,0.4675080844,-0.4528837253\C,-0.6973202244,-0.8472229968,3.338234
2849\H,-0.014321972,-1.0744277279,4.1905206774\O,-1.8412236417,-1.2880
182324,3.3620167698\\Version=AM64L-G03RevC.02\State=1-A\HF=-498.4564
825\RMSD=4.808e-09\RMSF=2.540e-05\Thermal=0.\Dipole=0.4616965,-0.2425
967,-2.5260653\PG=C01 [X(C7H10O3)]\
```

14b (MeO/2xCHO)



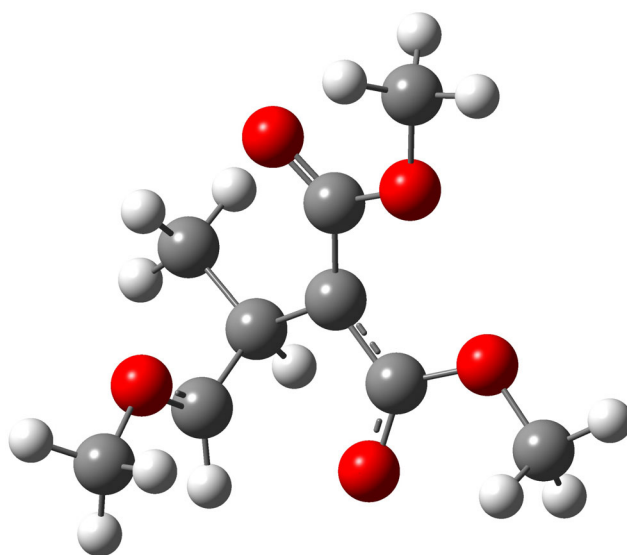
```
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H10O3\TSCHNEI\12-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_2CHO_2\0,1\C,0.013261256,0.191859803
9,0.1040502577\O,0.1857686294,-0.3123127,1.3750569416\C,1.5430928012,-
0.4068419437,1.7974678044\C,-2.3450925639,-0.8262238012,0.489675867\C,
-1.4774831869,0.1373663426,-0.3262945376\H,-1.5159978271,-0.1690909592
,-1.3786732761\C,-1.8732507997,1.6003503633,-0.2334233204\H,-1.9885848
447,-1.8543280966,0.3919812247\H,-3.3713225974,-0.7743120376,0.1271433
859\H,1.5298251664,-0.8917438438,2.7720260011\H,2.1283916907,-1.015504
3681,1.096864799\C,-0.7631031934,2.3263193805,-0.0100517706\O,0.378740
3579,1.6254008118,0.0894675624\H,1.9991364759,0.5823234216,1.88505247
36\H,-2.3343909078,-0.5659650819,1.5480971367\H,-0.6517701845,3.400009
7438,0.0836718656\H,0.7062421828,-0.2766543661,-0.6027068674\C,-3.19104
14127,2.1638184509,-0.4402477812\H,-3.2423246499,3.2706410818,-0.33266
93165\O,-4.1919484331,1.5314908339,-0.7210855626\\Version=AM64L-G03Re
vC.02\State=1-A\HF=-498.5191429\RMSD=3.533e-09\RMSF=1.860e-05\Therma
l=0.\Dipole=1.6239994,0.0028199,0.2199136\PG=C01 [X(C7H10O3)]\\
```

14a (MeO/2xCOOMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C9H14O5\TSCHEI\13-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_2COOR_1\0,1\C,0.0715994224,0.2468303
877,-0.0481665926\O,0.2255857733,0.2968967281,1.3252976961\C,1.5825229
394,0.2033608672,1.7494989422\H,0.657170634,-0.5160916182,-0.558805072
\C,-0.0775767097,1.5781721719,-0.8318601832\C,0.5017134494,1.568032735
8,-2.2038372066\H,2.1778434435,1.029342682,1.352297579\H,1.5689865164,
0.2496863663,2.8378275904\H,2.0235550228,-0.7508787818,1.436064568\C,-
1.2527948763,0.608752245,-0.6054366983\H,-1.5075157032,0.0700689034,-1
.5130253242\C,-2.4258176006,0.9517721919,0.2855302939\H,-2.9860599564,
0.0382360736,0.5053744025\H,-2.1109891646,1.3863897628,1.2318485097\H,
-3.0969194501,1.6583650737,-0.2052349852\O,0.5759247086,0.5816488142,-
2.9003502843\O,0.9259666255,2.7869190146,-2.5915601897\C,1.4937256643,
2.8613291501,-3.9101176658\H,1.76116821,3.9058129305,-4.0507245464\H,2
.3767156244,2.2254185155,-3.98186347\H,0.7651379723,2.5466909548,-4.657
7201607\C,-0.0326940446,2.8825754927,-0.0804705308\O,1.2205971709,3.15
41921543,0.3428192359\O,-0.9698433166,3.6120651674,0.1175673948\C,1.38
78937798,4.4208090937,1.0008273561\H,0.7724099221,4.4697226987,1.89969
53054\H,2.4438494199,4.47996626,1.2544816591\H,1.1079753708,5.23521810
8,0.3318669609\Version=AM64L-G03RevC.02\State=1-A\HF=-727.658217\RMS
D=3.638e-09\RMSF=8.507e-06\Thermal=0.\Dipole=1.033556,0.3240235,0.13094
24\PG=C01 [X(C9H14O5)]\

TS_{14a-14b} (MeO/2xCHO)

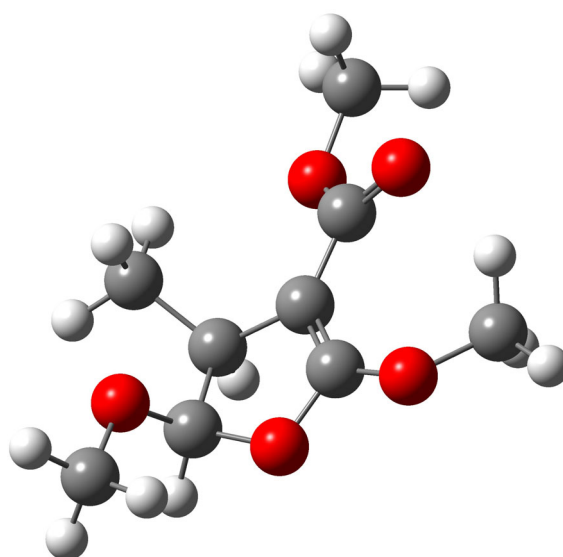


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C9H14O5\TSCHNE\14-Jul-2010\
0\# opt=(calcfc,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\DA_O_2COOR_TS\0,1\C,-0.0520947044,-0.008646315,0.1270287298\C,-0
.2642690341,0.0587411755,2.4448780614\C,1.110948694,0.4515986712,2.536
5271769\O,1.7704579269,0.8092236591,1.5388869545\C,-0.9108113866,0.600
3975218,1.1570579377\H,-0.718147553,1.6762540724,1.1062924086\C,-2.412
8208161,0.3675459276,0.9237251962\H,-2.7185809168,0.8733784979,0.00202
15421\H,-2.6621448933,-0.6871441811,0.866013539\H,-2.9766108155,0.7895
549619,1.7544109778\O,-0.1514335385,-1.2649141477,-0.1518903497\C,0.86
39630455,-1.8842744069,-0.9701966822\H,0.3720421631,-2.6906319344,-1.5
074370122\H,1.2910254343,-1.1584561958,-1.6639443616\H,1.6340849094,-2
.2785127268,-0.3079015742\H,0.6749302159,0.5630197291,-0.4398586023\O,
1.6784634558,0.4707239063,3.7584013568\C,3.0692461265,0.8009278613,3.7
991723345\H,3.3673876299,0.6584120041,4.8363281793\H,3.6476990876,0.14
78784913,3.1429570658\H,3.2355170989,1.836536008,3.4972594875\C,-0.951
4042198,-0.8825771811,3.2936139833\O,-2.0645202904,-1.3538650213,3.096
7842859\O,-0.2263963702,-1.2577591046,4.3920490082\C,-0.8845123982,-2.
1731795176,5.2661171346\H,-0.1880483905,-2.3403810731,6.0867198705\H,-
1.8205473384,-1.756925484,5.6442051583\H,-1.1066168732,-3.1154807815,4
.7601254266\Version=AM64L-G03RevC.02\State=1-A\HF=-727.6005063\RMS
D=5.619e-09\RMSF=8.995e-07\Thermal=0.\Dipole=0.9997813,-0.3471796,-2.00
93279\PG=C01 [X(C9H14O5)]\

```

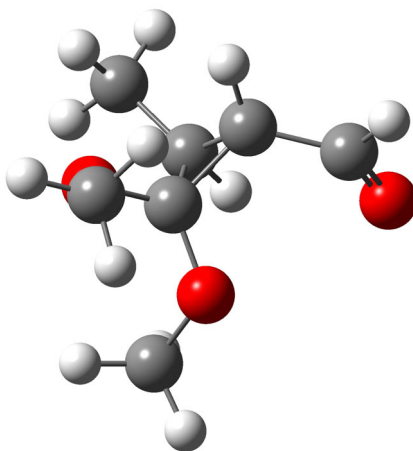
14b (MeO/2xCOOMe)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C9H14O5\TSCHNEI\13-Jul-2010\
0\# opt freq rb3lyp/6-311g(d)\DA_O_2COOR_2\0,1\C,-0.0613160596,0.139737
7904,0.0569112105\O,0.3037270541,-0.2982525194,1.3189132608\C,1.709087
5198,-0.4039712714,1.5178688533\C,-2.2969854407,-0.8731174538,0.797186
2714\C,-1.5984084906,0.1476508014,-0.1058052345\H,-1.8229768722,-0.106
9461997,-1.1499507799\C,-1.9115469668,1.6236465322,0.1383435843\H,-1.9
025186824,-1.8766877184,0.6164257469\H,-3.3660548014,-0.8834259912,0.5
942009701\H,1.8500090564,-0.8198635329,2.5142358425\H,2.1594220125,-1.
0774784395,0.7770956224\C,-0.7329220601,2.3074549153,0.0651163317\O,0.
3509497642,1.5210221632,-0.1299210456\H,2.1928512054,0.5739792327,1.45
63138933\H,-2.1396795019,-0.6391014534,1.8502737766\H,0.4708306539,-0.
4222004753,-0.7183514345\O,-0.3686175428,3.5749542376,0.0968463536\C,-
1.2572098714,4.6240586738,-0.33123857\H,-2.0275864287,4.8044483682,0.4
116700053\H,-0.6143099872,5.4916221346,-0.4638324112\H,-1.7198314738,4.
.35278763,-1.2827546616\C,-3.2259808141,2.1775428539,0.4092854412\O,-3
.4844683974,3.2591981377,0.9043695872\O,-4.2144456989,1.3125582956,0.0
412617633\C,-5.5503106865,1.750026495,0.3190286497\H,-6.1961365044,0.9
374689071,-0.0077406809\H,-5.6834722843,1.9395863912,1.3851141936\H,-5
.780768522,2.6636318997,-0.2310320482\Version=AM64L-G03RevC.02\State
=1-A\HF=-727.6566209\RMSE=4.974e-09\RMSE=1.092e-05\Thermal=0.\Dipole
=0.1205811,-0.4273039,-0.5999443\PG=C01 [X(C9H14O5)]\

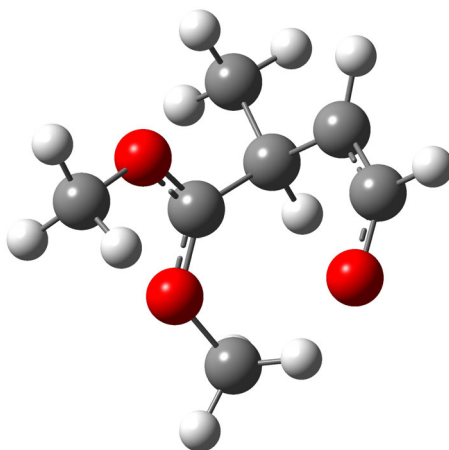
Two Donors

14a (2xMeO/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\28-Jan-2011\
0\# opt freq rb3lyp/6-311g(d)\DA_2O_CHO_1\0,1\C,-0.0053941374,-0.032819
5822,0.0548358803\O,0.06057244,0.0738530646,1.4356247485\C,1.385103626
9,0.2024996834,1.9526873949\C,0.0941958517,1.2688810652,-0.7530424549\
C,0.7612285281,1.2851615651,-2.0794337065\H,1.8641165281,1.1146132039,
1.5781885853\H,1.2856902188,0.2631389624,3.0353392062\H,2.0009594216,-
0.6586886281,1.68410258\C,-1.22938515,0.5078843882,-0.5885798506\H,-1.
4936953617,-0.0074691332,-1.5084442125\C,-2.3733623561,1.1052426956,0.
1962359666\H,-3.0987507116,0.3344285327,0.4726021334\H,-2.023115703,1.
5710955128,1.1181087054\H,-2.8977107963,1.8603292112,-0.3961600306\O,0
.4403164797,0.6100887853,-3.0277422418\H,1.6199836294,1.9874005383,-2.
1575551838\H,0.2396791071,2.1555213358,-0.1423130577\O,0.6533289487,-1
.1260826274,-0.4763852317\C,-0.0249043272,-2.366180308,-0.272390622\H,
0.6107042402,-3.1358170936,-0.7071966977\H,-0.1719299838,-2.5672023694
,0.7928212702\H,-0.995626397,-2.3694361513,-0.7789354256\\Version=AM64
L-G03RevC.02\State=1-A\HF=-499.695866\RMSD=3.885e-09\RMSF=5.678e-06\
Thermal=0.\Dipole=0.0107056,0.108995,1.1048156\PG=C01 [X(C7H12O3)]\\

TS_{14a-14b} (2xMeO/CHO)



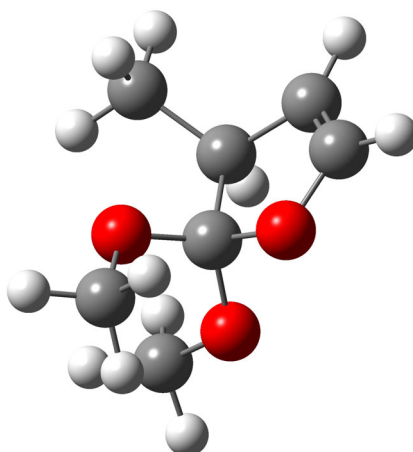
1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H12O3\TSCHNEI\29-Jan-2011\
0\# opt freq rb3lyp/6-311g(d)\DA_2O_CHO_1\0,1\C,-0.0053941374,-0.032819
5822,0.0548358803\O,0.06057244,0.0738530646,1.4356247485\C,1.385103626
9,0.2024996834,1.9526873949\C,0.0941958517,1.2688810652,-0.7530424549\
C,0.7612285281,1.2851615651,-2.0794337065\H,1.8641165281,1.1146132039,
1.5781885853\H,1.2856902188,0.2631389624,3.0353392062\H,2.0009594216,-
0.6586886281,1.68410258\C,-1.22938515,0.5078843882,-0.5885798506\H,-1.
4936953617,-0.0074691332,-1.5084442125\C,-2.3733623561,1.1052426956,0.
1962359666\H,-3.0987507116,0.3344285327,0.4726021334\H,-2.023115703,1.
5710955128,1.1181087054\H,-2.8977107963,1.8603292112,-0.3961600306\O,0
.4403164797,0.6100887853,-3.0277422418\H,1.6199836294,1.9874005383,-2.
1575551838\H,0.2396791071,2.1555213358,-0.1423130577\O,0.6533289487,-1
.1260826274,-0.4763852317\C,-0.0249043272,-2.366180308,-0.272390622\H,
0.6107042402,-3.1358170936,-0.7071966977\H,-0.1719299838,-2.5672023694
,0.7928212702\H,-0.995626397,-2.3694361513,-0.7789354256\\Version=AM64
L-G03RevC.02\State=1-A\HF=-499.695866\RMSD=3.885e-09\RMSF=5.678e-06\
Thermal=0.\Dipole=0.0107056,0.108995,1.1048156\PG=C01 [X(C7H12O3)]\\

```

0\\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultraf
ine\\DA_2O_CHO_TS\\0,1\\C,-0.4195411597,-0.1967696996,-0.2991837248\\C,-
0.0270196731,0.283699759,2.0309735373\\C,1.3364097343,0.4218120226,1.89
46595661\\H,1.9371843849,0.2422593629,2.8103239312\\O,1.9517210769,0.745
893015,0.8332012197\\C,-0.917320039,0.6165346114,0.8507112787\\H,-0.8202
087367,1.670287908,0.5688116581\\C,-2.3990026934,0.3159503156,1.1350905
572\\H,-3.0465936073,0.5745298317,0.292588276\\H,-2.5447123758,-0.737936
0297,1.3765265786\\H,-2.7086776726,0.9070999163,1.9990075414\\O,-0.59038
04622,-1.4868781661,-0.2489139178\\C,0.1028932105,-2.3342416003,-1.1953
16846\\H,-0.1042567725,-3.3464840684,-0.861282603\\H,-0.2813606751,-2.17
17952879,-2.2017606047\\H,1.1696967582,-2.120874268,-1.1569829123\\H,-0.
4835691532,-0.152016535,2.9127511961\\O,0.1455291785,0.228626308,-1.383
1120967\\C,0.5750668037,1.6101930168,-1.5436020998\\H,1.2504438847,1.815
5934037,-0.7096834882\\H,1.08296494,1.6210558048,-2.5040845363\\H,-0.292
8119456,2.2677243381,-1.5671714614\\Version=AM64L-G03RevC.02\\State=1-A
\\HF=-499.6635563\\RMSD=9.154e-09\\RMSF=1.464e-05\\Thermal=0.\\Dipole=-1.36
73168,-0.6140549,-1.8579404\\PG=C01 [X(C7H12O3)]\\

```

14b (2xMeO/CHO)



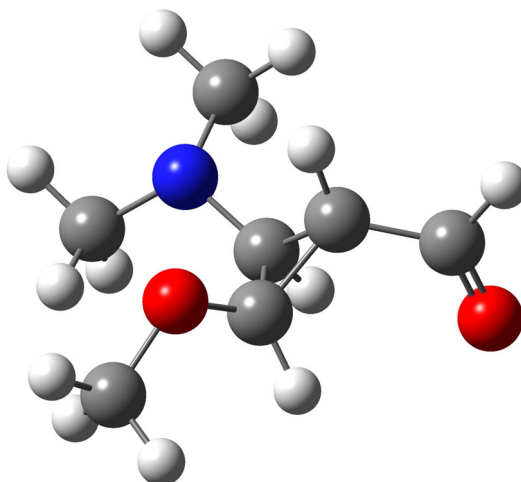
```

1\\1\\GINC-WERZ01\\FOpt\\RB3LYP\\6-311G(d)\\C7H12O3\\TSCHNEI\\28-Jan-2011\\
0\\# opt freq rb3lyp/6-311g(d)\\DA_2O_CHO_2\\0,1\\C,-0.083918269,-0.0640234
481,0.1416473864\\O,-0.0685489406,-0.3286165147,1.5045308188\\C,1.202739
9684,-0.1943237624,2.1479063843\\C,-2.6409923547,-0.3215823527,0.664254
6282\\C,-1.5637748242,0.0179200022,-0.371489247\\H,-1.6554603301,-0.6763
628948,-1.214744672\\C,-1.6202952277,1.4403415198,-0.8753611702\\H,-2.54
54589218,-1.3483277227,1.0241074998\\H,-3.6327153455,-0.2122351683,0.21
55537143\\H,1.0627509665,-0.5658735811,3.1618676592\\H,1.969589641,-0.78
25229118,1.6386247085\\C,-0.438429172,2.0149914412,-0.6905722483\\O,0.51
49658135,1.2143156002,-0.1175227611\\H,1.5117260946,0.8519070001,2.1745
289247\\H,-2.5800381021,0.3417048035,1.5274014633\\H,-0.0941502354,3.014
2507154,-0.9190427231\\H,-2.491437287,1.904257535,-1.3157674836\\O,0.728
0269674,-0.9545870441,-0.5798460492\\C,0.4074119935,-2.3326091254,-0.43
25781175\\H,-0.5992648569,-2.5607225625,-0.8016823022\\H,1.1333158327,-2
.8744104175,-1.0371078774\\H,0.4823799188,-2.6582413213,0.608569209\\Ve
rsion=AM64L-G03RevC.02\\State=1-A\\HF=-499.7137862\\RMSD=6.354e-09\\RMSF
=6.730e-06\\Thermal=0.\\Dipole=-0.2303461,-0.311369,0.1135275\\PG=C01 [X(C7
H12O3)]\\

```

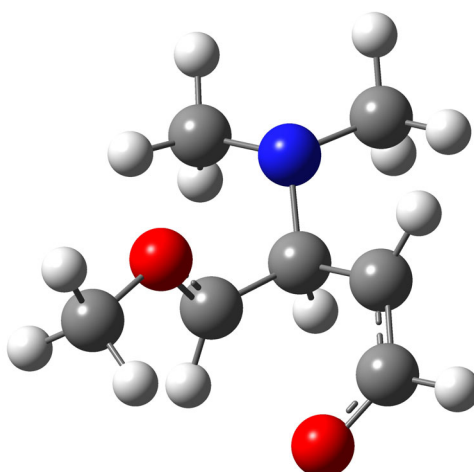
Vincinal Donors

15a (MeO,Me₂N/CHO)



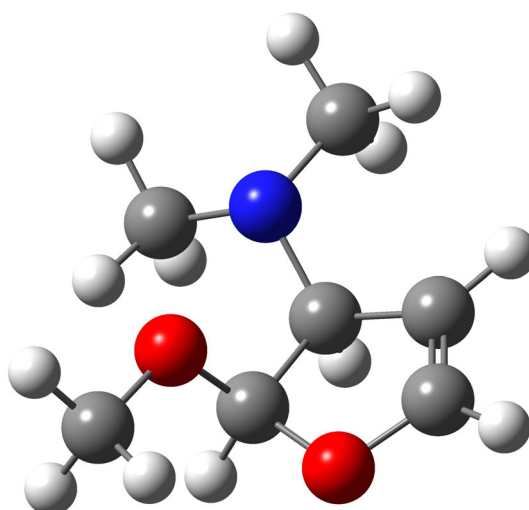
1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\16-Feb-2011\0\# opt freq rb3lyp/6-311g(d)\DA_2ON_CHO_1\0,1\C,0.0267081182,0.1165957943,-0.0327285185\C,0.0046399039,0.0024822096,1.5054329962\C,1.3110619964,0.0515459564,0.7310362249\H,-0.2434805497,1.1159492849,-0.3939071097\H,-0.2560254412,-0.9814688277,1.8787242143\H,1.8588125471,0.9882277874,0.8264451778\C,-0.3845319864,1.1781737816,2.3076535172\O,-0.1616061564,2.3247919029,1.9841983024\H,-0.9149475048,0.9585695155,3.2588033778\O,2.0895910325,-1.0982663844,0.7673842987\C,3.3622494868,-0.9412094446,0.158862841\H,3.943140518,-0.1493774524,0.6485391826\H,3.882150633,-1.8908371039,0.2790577631\H,3.2816160597,-0.7089233909,-0.9100838251\N,-0.4533801429,-1.0118450956,-0.7646938223\C,-1.9055800597,-1.0052487911,-0.8870677825\H,-2.2373859581,-1.9296913573,-1.3658702522\H,-2.3609695089,-0.9557508879,0.1040571892\H,-2.2869258115,-0.1557854292,-1.4818521201\C,0.2043423216,-1.1649241123,-2.0569736589\H,-0.1460798213,-2.0825927142,-2.5356359136\H,0.0082083143,-0.3247640895,-2.7471758771\H,1.2811409541,-1.2521081417,-1.9151813015\\Version=AM64L-G03RevC.02\\State=1-A\HF=-479.8062194\RMSD=8.541e-09\RMSF=1.598e-05\Thermal=0.\Dipole=0.2266616,-0.6951338,-0.5202332\PG=C01 [X(C7H13N1O2)]\\

TS_1_{15a-15b} (MeO,Me₂N/CHO)



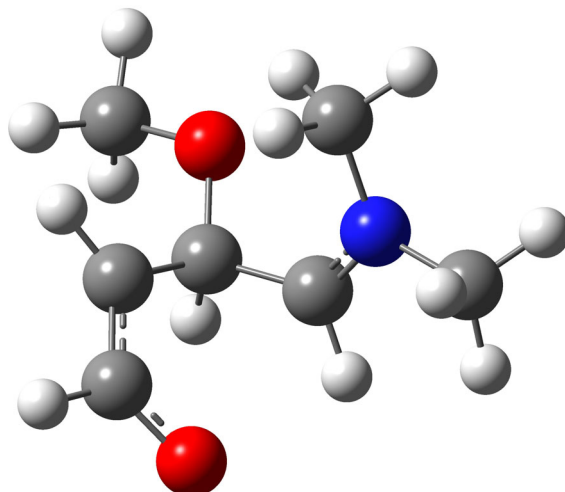
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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\16-Feb-2011\
0\# opt=(calcf,ts,noeigentest) freq rb3lyp/6-311g(d) scf=tight int=ultrafine
\DA_2ON_CHO_TSa\0,1\C,0.0927388032,-0.3306454726,-0.1015324544\C,
0.1964040617,0.1835392872,2.1265340119\H,1.0606554941,0.3424400871,2.
7606100922\C,-0.7719077148,1.1480024855,1.9409951921\H,-0.9062447054,
1.8696935191,2.7702461652\O,-1.5314157768,1.2562892804,0.9354014085\C,
0.226858574,-1.0320307761,1.1835651003\H,-0.6839345252,-1.6484190893,1
.3106427374\O,1.0950136021,0.2637452163,-0.6755214773\C,0.766187476,1.
1763286516,-1.7506020613\H,1.7012174251,1.653974117,-2.0288646099\H,0.
3584204065,0.6204480485,-2.5972599416\H,0.0473412424,1.9068334591,-1.3
827016245\H,-0.8738365014,-0.2613633693,-0.5821967718\N,1.4481580046,-
1.8149635535,1.343358121\C,1.4912311374,-2.4613949617,2.6521989049\H,2
.4612039854,-2.946439583,2.7815360705\H,1.3674197318,-1.7272258955,3.4
463423991\H,0.703331543,-3.2271950588,2.7729844499\C,1.6064008081,-2.8
037498169,0.282759973\H,2.5163498341,-3.3807025636,0.4603680966\H,0.76
11943388,-3.5149017971,0.2250954394\H,1.7149870927,-2.3122603261,-0.68
54957158\Version=AM64L-G03RevC.02\State=1-A\HF=-479.7437745\RMSE=6.94
1e-09\RMSE=2.235e-06\Thermal=0.\Dipole=0.8982593,-0.6650393,-1.3091114
\PG=C01 [X(C7H13N1O2)]\
```

15_1b (MeO,Me₂N/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\16-Feb-2011\0\# opt freq rb3lyp/6-311g(d)\DA_2ON_CHO_2a\0,1\C,0.2463263812,0.1732971801,0.105817371\C,-0.1181059061,0.0492105096,1.5713437252\C,1.3002362713,-0.1108256067,2.210097261\C,1.5180141047,-0.1762651199,-0.043195755\H,-0.653463791,-0.9140948986,1.7207910391\H,1.3659098996,-0.9289431325,2.9363192829\O,2.1731255273,-0.4996630708,1.1163998562\O,1.7333462923,1.0801776511,2.7698043416\C,2.9922293084,0.9818162971,3.4238268613\H,3.1857247921,1.956254891,3.8700800223\H,2.9681120326,0.2196805194,4.2148127162\H,3.7887479434,0.7371503066,2.7166824493\N,-0.9067743728,1.1396818462,2.139163441\C,-2.1207094576,1.3960504416,1.3766680004\H,-2.7874686465,0.5148425591,1.3030779629\H,-2.6820008129,2.1986512015,1.8599732279\H,-1.8797963644,1.7300564752,0.3672769529\C,-1.2281919235,0.8867746241,3.5383543776\H,-1.8036926441,1.7253958605,3.9363309091\H,-1.8247182662,-0.0349607174,3.6837904611\H,-0.3134023586,0.8082878885,4.1243541829\H,-0.433814973,0.4110956267,-0.696739317\H,2.1200814152,-0.2647946677,-0.9375506415\\Version=AM64L-G03RevC.02\State=1-A\HF=-479.8159736\RMSD=1.984e-09\RMSF=2.059e-05\Thermal=0.\Dipole=-0.109432,-0.2305166,0.1520173\PG=C01 [X(C7H13N1O2)]\

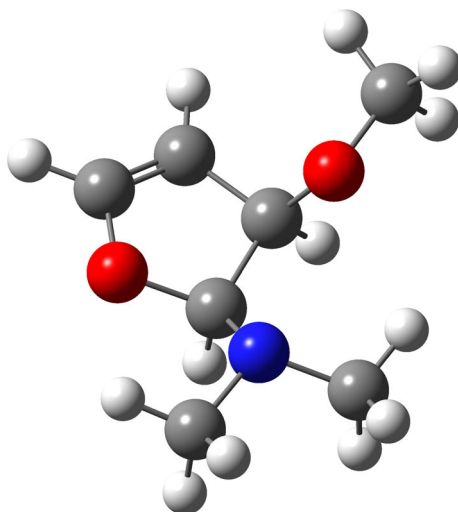
TS_2_{15a-15b} (MeO,Me₂N/CHO)



1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\17-Feb-2011\0\# opt=(calcfc,ts,noeigentest) freq b3lyp/6-311g(d) scf=tight int=ultra fine\DA_2ON_CHO_TSb\0,1\C,-0.2431376577,-0.2721351598,-0.0049739704\C,-0.2453764102,-0.3033023918,1.4922149856\C,2.188482196,0.0888703993,1.3236060183\H,0.2103014167,-1.121372427,-0.4943612158\H,-0.1437710396,-1.364388214,1.7722974041\O,-1.4650795892,0.2068452649,2.0215984353\C,-1.6070843784,-0.0410239202,3.4119704003\H,-2.5732319703,0.370591971,3.7038427342\H,-1.5975798434,-1.1190464387,3.6195280691\H,-0.8141573616,0.4349438605,3.9965884253\N,-0.5689300652,0.7278344454,-0.7782244167\C,-0.2209997833,0.7064330981,-2.2007144468\H,-1.101017156,0.9435122209,-2.8017808515\H,0.5570542855,1.4493643961,-2.3962703089\H,0.1558963953,-0.2758098325,-2.4756422159\C,-1.0071166094,2.0257592782,-0.2565329116\H,-1.6264932297,2.5176978182,-1.0066120772\H,-1.5665686053,1.8797238293,0.6604656759\H,-0.1220269664,2.6340657542,-0.0449961486\H,3.1089707694,0.5482771404,1.7412965352\O,2.3122373617,-0.7653216488,0.399449

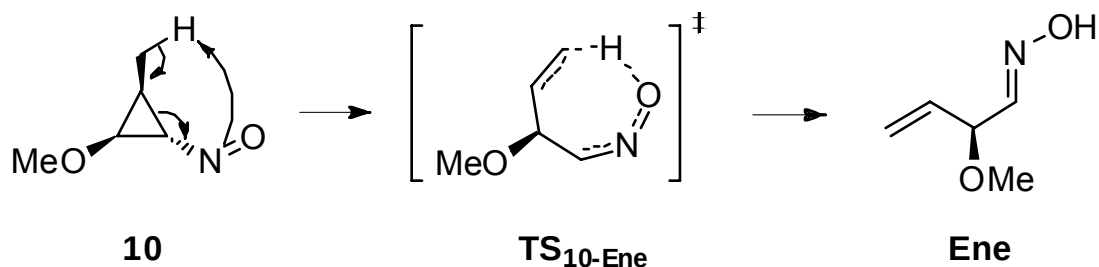
9922\C,0.9903101169,0.4894337251,1.8820154215\H,0.8817707077,1.3356374
942,2.5510367599\\Version=AM64L-G03RevC.02\State=1-A\HF=-479.7733025\R
MSD=4.000e-09\RMSF=2.116e-06\Thermal=0.\Dipole=-1.9896723,0.944517,-1.
0214868\PG=C01 [X(C7H13N1O2)]\\

15_2b (MeO,Me₂N/CHO)



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C7H13N1O2\TSCHNEI\16-Feb-2011\
0\# opt freq rb3lyp/6-311g(d)\DA_2ON_CHO_2b\0,1\C,-0.0362362821,0.133
6698841,-0.008929164\C,-0.2240972693,-0.0643741828,1.5228178523\C,2.00
09311686,0.0794858816,0.9386592367\H,-0.1404096862,-0.8650199435,-0.48
0908041\H,-0.8855438116,-0.9212868052,1.7134912899\O,-0.7919457867,1.0
934346169,2.1285525687\C,-1.074375299,0.9280515599,3.502521623\H,-1.57
61679119,1.8374115463,3.833349407\H,-1.739106359,0.0690142788,3.679134
8959\H,-0.1631273256,0.7934777491,4.0985810883\N,-0.8543852018,1.12545
81526,-0.6479347572\C,-0.4938448393,1.2994515934,-2.0527779837\H,-0.66
51060384,0.3879170266,-2.6558780311\H,-1.0973536096,2.1052635663,-2.47
55635752\H,0.5552258971,1.5752049171,-2.1358219469\C,-2.2751704997,0.8
284944913,-0.5011417911\H,-2.8526600655,1.6195806366,-0.9835313849\H,-
2.5656715262,-0.1319655359,-0.9676412399\H,-2.5442924255,0.8123975366,
0.5527339441\H,3.0810152527,0.1284949815,0.8842897867\O,1.3655853824,0
.4770894348,-0.1928998815\C,1.2093686287,-0.3148275867,1.9359320664\H,
1.5370456955,-0.6504654721,2.9083869433\\Version=AM64L-G03RevC.02\Stat
e=1-A\HF=-479.8134671\RMSD=5.628e-09\RMSF=5.644e-06\Thermal=0.\Dipole
=-0.1716049,-0.5558295,0.3691658\PG=C01 [X(C7H13N1O2)]\\

Retro-Ene Reaction vs. Ring-Enlargement

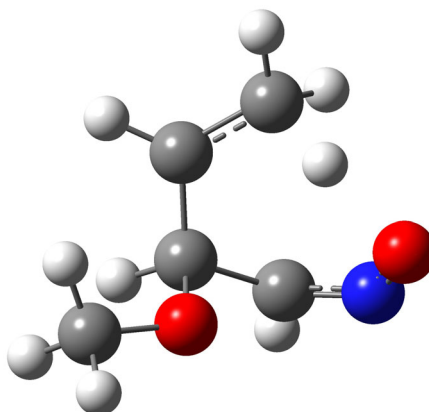


Reaction Type	10 ^a	product ^a	TS ^a	$\Delta G^\ddagger$ [kJ/mol]	ΔG_R [kJ/mol]
Retro-Ene	-400.974647	-400.995964	-400.902595	189.17	-55.97
Ring-Enlargement		-401.030545	-400.948303	69.16	-146.76

10 (MeO/NO)

see page 25

TS_{10-Ene} (MeO/NO)

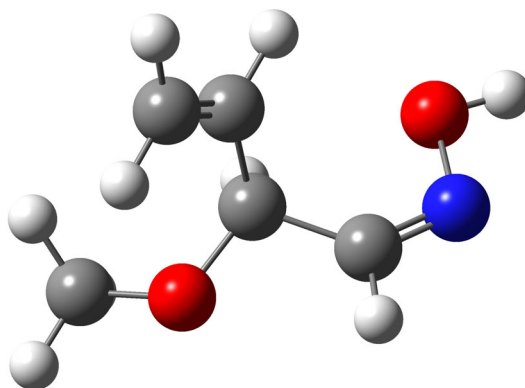


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1\1\GINC-WERZ01\FTS\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\18-Feb-2011\
0\# opt=(calcf,ts,modredundant,noeigentest) freq rb3lyp/6-311g(d) scf=ti
ght int=ultrafine\RetroEN_O_NO_TS2\0,1\C,-0.0404546862,-0.2207529607
,0.2007491211\H,-0.2267554122,0.109193605,1.2317174981\C,1.4676604156,
-0.3485523474,-0.0416468034\H,2.1418299809,-0.0703885576,0.759844264\C
,-0.8353536436,-1.4232430843,-0.1312410189\H,-1.7990761648,-1.55502021
86,0.3546434979\C,-0.4406480904,-2.258336873,-1.2062053624\N,2.0071241
279,-0.4871946764,-1.2010875863\O,1.4867733802,-0.8336502164,-2.298135
2935\O,-0.4360227167,0.8607771777,-0.6915278666\C,-1.68464589,1.452915
0698,-0.3787880431\H,-1.726209314,1.7697797311,0.672851467\H,-1.770747
3064,2.3329213144,-1.0162257871\H,-2.5332304214,0.7886437124,-0.581480
832\H,0.0580681365,-1.5405246797,-2.0179997072\H,-1.1956616188,-2.9496
779327,-1.5779177586\H,0.5070551176,-2.7854524341,-1.032384161\Versio
n=AM64L-G03RevC.02\State=1-A\HF=-401.0366942\RMSE=9.038e-09\RMSEF=
9.479e-06\Thermal=0.\Dipole=-1.421339,-0.3294601,1.2832085\PG=C01 [X(C5
H9N1O2)]\

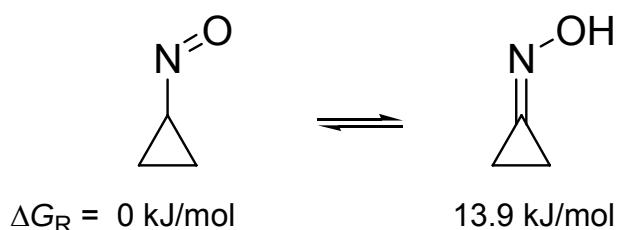
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Ene (MeO/NO)

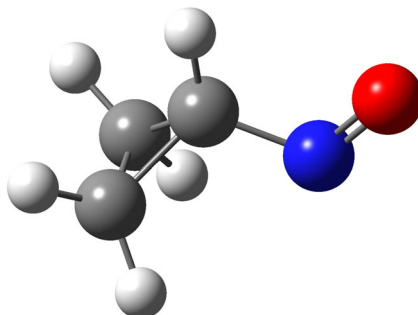


1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C5H9N1O2\TSCHNEI\16-Feb-2011\
0\# opt freq b3lyp/6-311g(d)\RetroEN_O_NO_2\0,1\C,0.1941991046,-0.0035
350369,-0.037578251\C,-0.0976063969,0.0716170248,1.4486248064\C,1.1913
580614,-0.0412867962,2.2315143474\H,0.4998367415,-0.9862790837,-0.3869
486734\H,-0.7366155104,-0.7786621239,1.7265013052\O,-0.6976071823,1.29
35780901,1.84780756\H,1.6262399019,0.8818616329,2.6041686295\C,-2.1078
771166,1.3128206956,1.7048595631\H,-2.5788411755,0.5431052113,2.330490
9569\H,-2.4427246839,2.2946681571,2.0393573142\H,-2.4175763187,1.16289
99673,0.6645916314\N,1.8373363505,-1.1009057918,2.5019359456\O,1.20476
33708,-2.242749823,1.9631248085\C,0.1299326432,1.0313000246,-0.8676517
926\H,1.7693072556,-2.9630663075,2.2627458728\H,-0.1573666671,2.017743
7779,-0.5200689144\H,0.3653135539,0.9251610422,-1.921141776\Version=A
M64L-G03RevC.02\State=1-A\HF=-401.1352403\RMSD=5.552e-09\RMSF=3.25
5e-06\Thermal=0.\Dipole=-0.4281412,-0.3032767,-0.1659206\PG=C01 [X(C5H9
N1O2)]\

NO vs. NOH

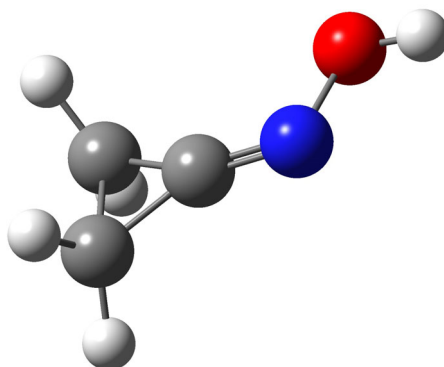


Nitrosocyclopropane



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C3H5N1O1\TSCHNEI\16-Dec-2010\0\# opt freq b3lyp/6-311g(d)\NO\0,1\C,-0.0214737286,-0.0074162332,0.029001656\C,0.0184771631,0.0076976367,1.513450931\C,1.329223335,-0.0056723387,0.7354624207\H,-0.2823922798,-0.9227494421,-0.4881087845\H,-0.2871311933,0.9082890926,-0.4851546171\H,-0.2137439788,-0.8962594777,2.0632587003\H,-0.2194193655,0.9340924258,2.0220350822\H,1.9649970392,-0.8863267714,0.7269291154\N,2.003744534,1.2602322582,0.7045282787\O,3.2116016339,1.1825184065,0.6727599823\\Version=AM64L-G03RevC.02\State=1-A\HF=-247.2467713\RMSD=4.472e-09\RMSF=5.102e-05\Thermal=0.\Dipole=-0.9880892,-0.7800644,0.0344915\PG=C01 [X(C3H5N1O1)]\\

Cyclopropanone Oxim



1\1\GINC-WERZ01\FOpt\RB3LYP\6-311G(d)\C3H5N1O1\TSCHNEI\16-Dec-2010\0\# opt freq b3lyp/6-311g(d)\NOH\0,1\C,0.0693651927,-0.0111460849,-0.0300831836\C,0.0702509627,0.0052513399,1.5209103059\C,1.3064136794,0.0504123311,0.7454068173\H,-0.1833758652,-0.9409423851,-0.5316859225\H,-0.2624566655,0.8831401439,-0.549896642\H,-0.1891654632,-0.9145771901,2.0376514045\H,-0.2685737317,0.9099331428,2.0180519556\N,2.5603693745,0.1028531694,0.8261792344\O,3.1563064607,0.1139624283,-0.4578426662\H,4.

0962811759,0.1558832344,-0.2490506048\\Version=AM64L-G03RevC.02\\State=1-A\\HF=-247.2412696\\RMSD=8.609e-09\\RMSF=3.272e-05\\Thermal=0.\\Dipole=-0.3268775,-0.0134018,0.0308977\\PG=C01 [X(C3H5N1O1)]\\

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