CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

The DMAP-Catalyzed Acetylation of Alcohols - A Mechanistic Study

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Experimental Details

Solvent: Dichloromethane was vigorously stirred over concentrated H_2SO_4 to remove traces of olefins (3 days), and then washed with water, 5% aqueous K_2CO_3 solution and water. After drying over $CaCl_2$ for 2 days it was distilled from CaH_2.

Chemicals: 4-dimethylaminopyridine (DMAP) was purchased from Acros Corporation and used without further purification. Cyclohexanol and nonane (used as internal standard) were purchased from Acros Corporation and distilled from sodium before use. Triethylamine was distilled from CaH_2; acetic anhydride was refluxed with MgC_2 at 80-90 °C for 5 days and distilled.

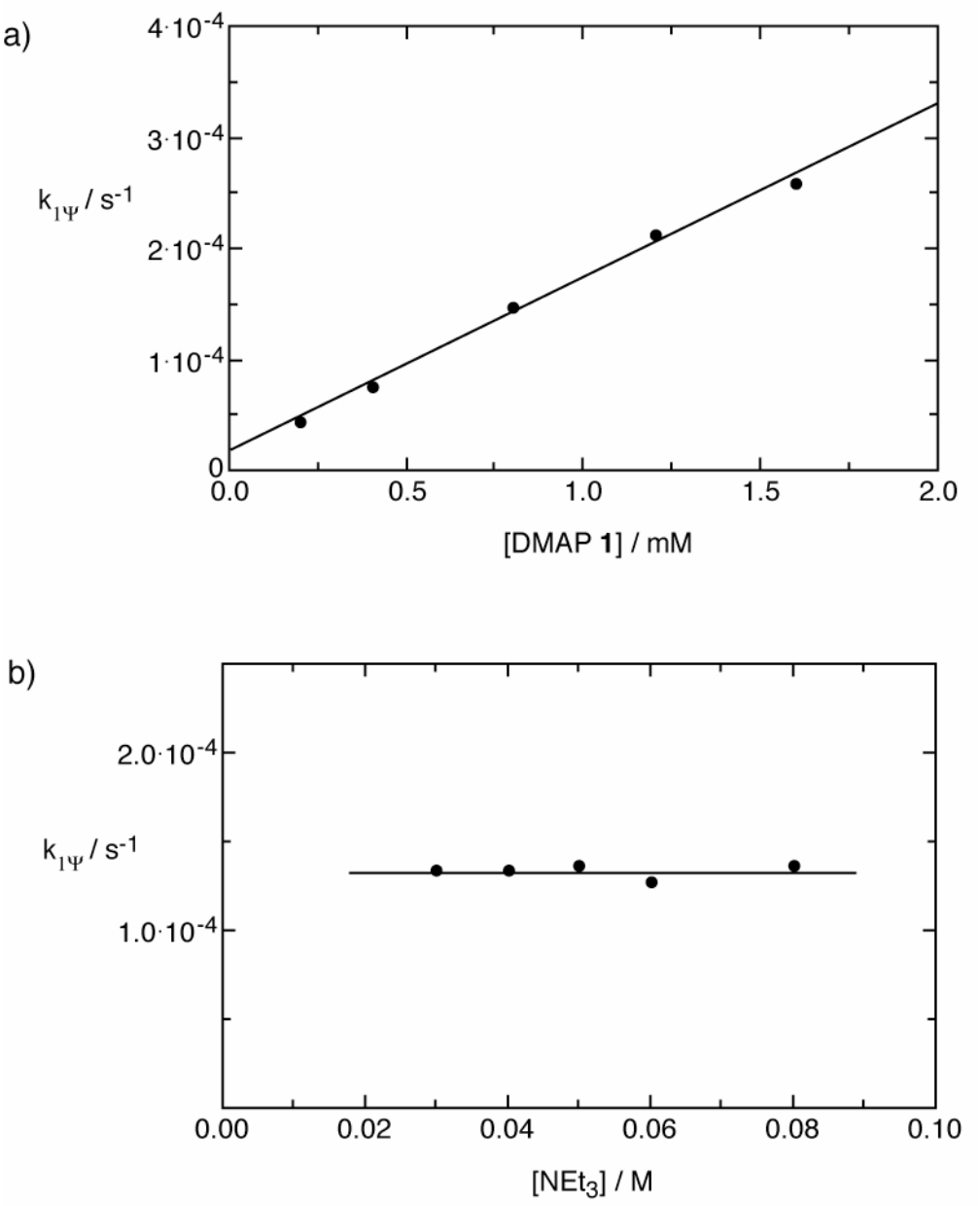
Kinetic Measurements: Reaction solutions were prepared through mixing stock solutions of DMAP with a calibrated solution containing cyclohexanol, acetic anhydride, and triethylamine. Reactions have been performed under a nitrogen atmosphere at 20 °C. All kinetic measurements have been performed using gas chromatography (FISONS 8130, Column: SE30) with nonane as internal standard. Rate measurements have been performed through following the disappearance of the minor reaction component under pseudo-first order conditions. For concentrations of cyclohexanol exceeding 0.320 M the rate of reaction is too fast to be measured directly with the GC technique. Small samples (0.2 ml) of the reaction mixture have therefore been removed at regular time intervals, quenched through injection into a small volume (2 ml) of methylene chloride held at -78 °C, and analyzed by GC after completion of the reaction.

Supplemetal Table 1a: Rate Data for the Acetylation of Cyclohexanol in CH_2Cl_2 at 20 ^{o}C in the Presence of DMAP as the Catalyst, Triethylamine as the Auxiliary Base, and Cyclohexanol as the Excess Reagent.

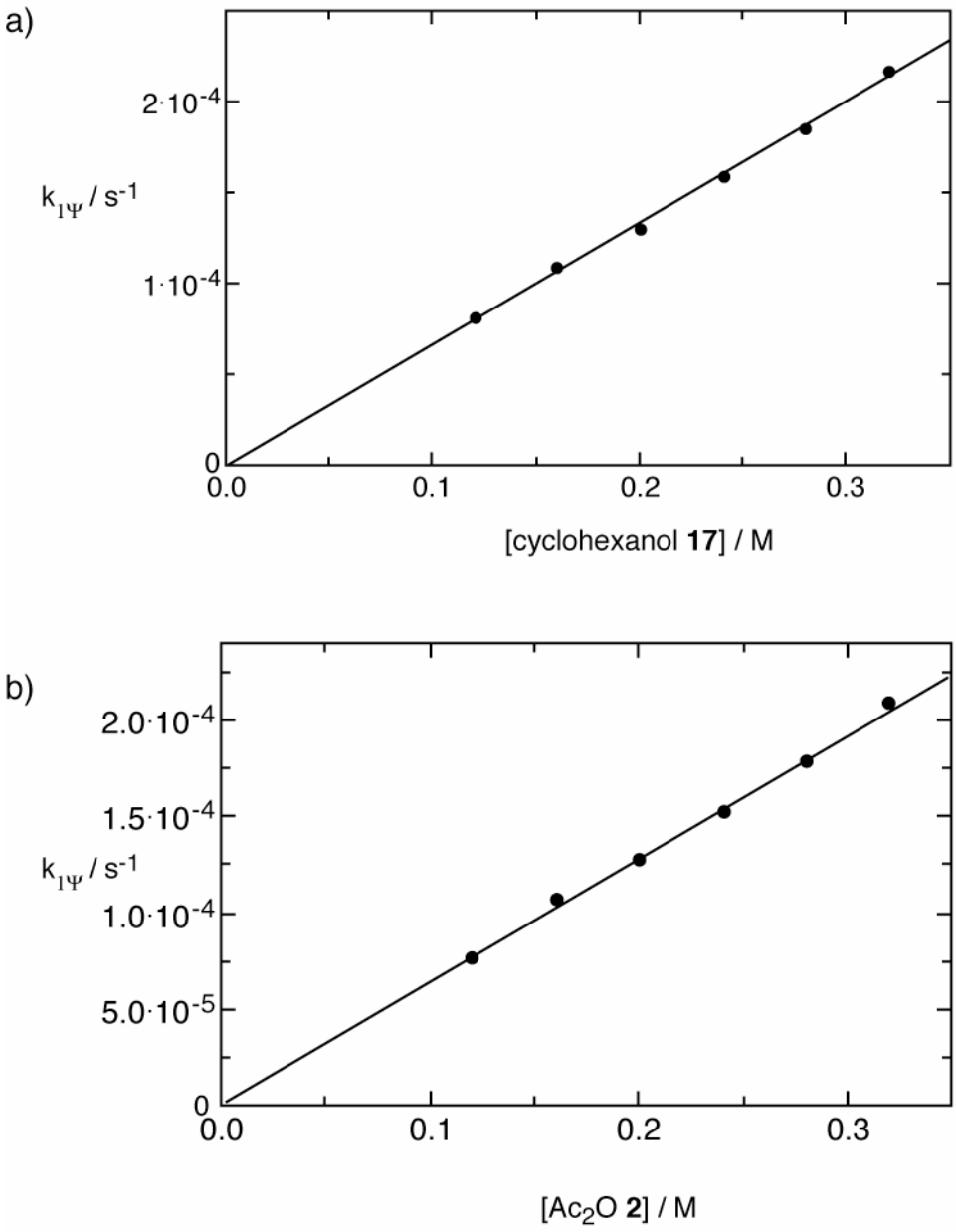
$[Ac_2O]$/M	$[C_6H_{11}OH]$/M	$[NEt_3]$/M	[DMAP]/M	Conv/%	$k_{1\Psi}$ / s^{-1}
0.020	**0.120**	0.060	0.00040	45.0	$8.208x10^{-5}$
0.020	**0.160**	0.060	0.00040	47.9	$1.088x10^{-4}$
0.020	**0.200**	0.060	0.00040	69.2	$1.300x10^{-4}$
0.020	**0.240**	0.060	0.00040	61.4	$1.586x10^{-4}$
0.020	**0.280**	0.060	0.00040	68.4	$1.853x10^{-4}$
0.020	**0.320**	0.060	0.00040	81.3	$2.172x10^{-4}$
for cyclohexanol concentrations above 0.320 M the quenching method was used					
0.020	**0.400**	0.060	0.00040	74.9	$2.371x10^{-4}$
0.020	**0.600**	0.060	0.00040	77.3	$3.422x10^{-4}$
0.020	**0.800**	0.060	0.00040	67.8	$4.512x10^{-4}$
0.020	**1.000**	0.060	0.00040	73.1	$5.305x10^{-4}$
0.020	**1.200**	0.060	0.00040	72.6	$6.243x10^{-4}$
0.020	**1.400**	0.060	0.00040	80.2	$6.942x10^{-4}$

Supplemetal Table 1b: Rate Data for the Acetylation of Cyclohexanol in CH_2Cl_2 at 20 ^oC in the Presence of DMAP as the Catalyst, Triethylamine as the Auxiliary Base, and Acetic Anhydride as the Excess Reagent.

$[Ac_2O]$/M	$[C_6H_{11}OH]$/M	$[NEt_3]$/M	[DMAP]/M	Conv/%	$k_{1\Psi}$ / s^{-1}
0.120	0.020	0.060	0.00040	41.1	$7.689x10^{-5}$
0.160	0.020	0.060	0.00040	71.5	$1.082x10^{-4}$
0.200	0.020	0.060	0.00040	63.5	$1.284x10^{-4}$
0.240	0.020	0.060	0.00040	77.3	$1.535x10^{-4}$
0.280	0.020	0.060	0.00040	83.5	$1.798x10^{-4}$
0.320	0.020	0.060	0.00040	83.5	$2.099x10^{-4}$
0.120	0.020	0.060	**0.00020**	50.8	$4.520x10^{-5}$
0.120	0.020	0.060	**0.00040**	41.1	$7.689x10^{-5}$
0.120	0.020	0.060	**0.00080**	55.5	$1.478x10^{-4}$
0.120	0.020	0.060	**0.00120**	52.2	$2.125x10^{-4}$
0.120	0.020	0.060	**0.00160**	66.0	$2.598x10^{-4}$
0.200	0.020	**0.030**	0.00040	67.4	$1.349x10^{-4}$
0.200	0.020	**0.040**	0.00040	62.0	$1.337x10^{-4}$
0.200	0.020	**0.050**	0.00040	73.4	$1.370x10^{-4}$
0.200	0.020	**0.060**	0.00040	63.5	$1.284x10^{-4}$
0.200	0.020	**0.080**	0.00040	66.1	$1.364x10^{-4}$



Supplemental Figure 1. Variation of the pseudo-first order rate constant $k_{1\Psi}$ as a function of the reaction conditions (20 ^{o}C, CH_2Cl_2): (a) dependence of $k_{1\Psi}$ on the concentration of DMAP with $[Ac_2O]_0$ = 0.12 M, $[cyclohexanol]_0$ = 0.02 M, $[NEt_3]_0$ = 0.06 M. (b) dependence of $k_{1\Psi}$ on the concentration of NEt_3 with $[cyclohexanol]_0$ = 0.02 M, $[Ac_2O]_0$ = 0.20 M, $[DMAP]_0$ = 0.0004 M.



Supplemental Figure 2. Variation of the pseudo-first order rate constant $k_{1\Psi}$ as a function of the reaction conditions (20 ^{o}C, CH_2Cl_2): (a) dependence of $k_{1\Psi}$ on the concentration of cyclohexanol with $[Ac_2O]_0$ = 0.02 M, $[NEt_3]_0$ = 0.06 M, $[DMAP]_0$ = 0.0004 M. (b) dependence of $k_{1\Psi}$ on the concentration of Ac_2O with $[cyclohexanol]_0$ = 0.02 M, $[NEt_3]_0$ = 0.06 M, $[DMAP]_0$ = 0.0004 M.

Computational Details

All stationary points have been optimized at the Becke3LYP/6-31G(d) level of theory. For all stationary points a number of conformational isomers exist. Only the energetically most favorable conformer has been used to generate the enthalpy profile discussed in the text. An overview of all isomers is available in the supplemental material. The nature of all stationary points has been verified through calculation of the vibrational frequency spectrum. Thermochemical corrections to calculate enthalpies at 298 K have been obtained using the rigid rotor/harmonic oscillator model and the force constants calculated at Becke3LYP/6-31G(d) level. Single point calculations have subsequently been performed at the Becke3LYP/6-311+G(d,p) level of theory. Combination of the single point energies with thermochemical corrections calculated at Becke3LYP/6-31G(d) level yields the "H_{298}" values cited in the text. Solvent effects have been estimated through single point calculations for the Becke3LYP/6-31G(d) gas phase structures. The PCM/UAHF model was used for this purpose, again in combination with the Becke3LYP/6-31G(d) method.[24] Solvent effect calculations have been performed for carbontetrachloride (CCl_4, ε=2.23), chloroform ($CHCl_3$, ε=4.90), and methylenechloride (CH_2Cl_2, ε=8.93) using Gaussian 03, Rev. B.03. All other calculations have been performed with Gaussian 98, Rev. A.11.[25]

Supplemental Table 3a. Energies for all Stationary Points Located on the Potential Energy Surface of DMAP (**1**) + Acetic Anhydride (**2**) + tert-Butanol (**3**) as Optimized at the Becke3LYP/6-31G(d) Level of Theory. Total Energies are in Hartree, Relative Enthalpies in kJ/mol.

reactants and products

stationary point	Etot (B3LYP/6-31G(d))	H298 (B3LYP/6-31G(d))	Etot (B3LYP/6-311+G(d.p)// B3LYP/6-31G(d))	"H298" (B3LYP/6-311+G(d,p)// B3LYP/6-31G(d))	"ΔH298" (B3LYP/6-311+G(d,p)// B3LYP/6-31G(d))
DMAP (**1**)	-382.257304	-382.085088	-382.359977	-382.187761	-
acetic anhydride (**2**)	-381.727898	-381.620018	-381.847722	-381.739842	-
tert-butanol (**3**)	-233.670958	-233.527102	-233.752240	-233.608384	-
tert-butyl acetate (**4**)	-386.338979	-386.153421	-386.4554585	-386.269901	-
acetic acid (**5**)	-229.081787	-229.014236	-229.164574	-229.097023	-
1 + **2** + **3**	-997.656160	-997.232208	-997.959939	-997.535987	0.0
1 + 4 + 5	-997.678070	-997.252745	-997.9800095	-997.554685	-49.1

nucleophilic catalysis

stationary points	Etot (B3LYP/6-31G(d))	H298 (B3LYP/6-31G(d))	Etot (B3LYP/6-311+G(d,p)// B3LYP/6-31G(d))	"H298" (B3LYP/6-311+G(d,p)// B3LYP/6-31G(d))	
reactant complex **6h**	-997.676353	-997.247266	-997.971967	-997.542880	-18.1
reactant complex **6g**	-997.678223	-997.249206	-997.972873	-997.543856	-20.7
reactant complex **6f**	-997.679327	-997.250059	-997.974113	-997.544845	-23.3
reactant complex **6e**	-997.682074	-997.253235	-997.977603	-997.548764	-33.5
reactant complex **6d**	-997.682213	-997.253287	-997.977263	-997.548337	-32.4
reactant complex **6c**	-997.682511	-997.253432	-997.976768	-997.547689	-30.7
reactant complex **6b**	-997.682694	-997.253687	-997.977310	-997.548303	-32.3
reactant complex **6a**	-997.683450	-997.254361	-997.978436	-997.549347	**-35.1**
transition state **7d**	-997.653500	-997.226247	-997.951434	-997.524181	+31.0
transition state **7c**	-997.655556	-997.227094	-997.952063	-997.523601	+32.5
transition state **7b**	-997.656032	-997.227481	-997.952349	-997.523798	+32.0
transition state **7a**	-997.657357	-997.229181	-997.954276	-997.526100	**+26.0**

intermediate complex **8d**	-997.662401	-997.232634	-997.961050	-997.531283	+12.4
intermediate complex **8c**	-997.662173	-997.232665	-997.962515	-997.533007	+7.8
intermediate complex **8b**	-997.662812	-997.233233	-997.962232	-997.532653	+8.8
intermediate complex **8a**	-997.662739	-997.233351	-997.962770	-997.533382	**+6.8**
transition state **9b**	-997.643185	-997.217925	-997.939429	-997.514169	+57.3
transition state **9a**	-997.651435	-997.226854	-997.947324	-997.522743	**+34.8**
product complex **10g**	-997.695018	-997.265630	-997.991462	-997.562074	-68.5
product complex **10f**	-997.697292	-997.267346	-997.991063	-997.561117	-66.0
product complex **10e**	-997.706687	-997.277120	-998.001383	-997.571816	-94.1
product complex **10d**	-997.707223	-997.277553	-998.001749	-997.572079	-94.8
product complex **10c**	-997.708754	-997.279340	-998.0036404	-997.574226	-100.4
product complex **10b**	-997.708612	-997.279233	-998.003851	-997.574472	-101.0
product complex **10a**	-997.709346	-997.279757	-998.004185	-997.574596	**-101.4**

concerted base catalysis
(direct reaction from reactant complex**6** to product complex **10**)

stationary point	Etot (B3LYP/6-31G(d))	H298 (B3LYP/6-31G(d))	Etot (B3LYP/6-311+G(d.p)//B3LYP/6-31G(d))	"H298" (B3LYP/6-311+G(d,p)//B3LYP/6-31G(d))	
transition state **11c**	-997.636012	-997.210699	-997.929491	-997.504178	+83.5
transition state **11b**	-997.637600	-997.211376	-997.932821	-997.506597	+77.2
transition state **11a**	-997.641238	-997.215934	-997.933609	-997.508305	**+72.7**

stepwise base catalysis
(stepwise reaction from reactant complex **6** to product complex **10**)

stationary point	Etot (B3LYP/6-31G(d))	H298 (B3LYP/6-31G(d))	Etot (B3LYP/6-311+G(d.p)//B3LYP/6-31G(d))	"H298" (B3LYP/6-311+G(d,p)//B3LYP/6-31G(d))	
product complex **10c**	-997.708754	-997.279340	-998.0036404	-997.574226	-100.4
product complex **10a**	-997.709346	-997.279757	-998.004185	-997.574596	-101.4

transition state **12c**	-997.622295	-997.195901	-997.913144	-997.486750	+129.3
transition state **12b**	-997.659047	-997.234171	-997.951832	-997.526956	+23.7
transition state **12a**	-997.665620	-997.240402	-997.959545	-997.534327	**+4.4**
tetrahedral int. **13c**	-997.662454	-997.232604	-997.952754	-997.522904	+34.3
tetrahedral int. **13b**	-997.670674	-997.241134	-997.960750	-997.531210	+12.5
tetrahedral int. **13a**	-997.679348	-997.249912	-997.969728	-997.540292	**-11.3**
transition state **14**	-997.609819	-997.182967	-997.903909	-997.477057	**+154.7**
tetrahedral int. **15**	-997.624674	-997.197744	-997.919783	-997.492853	**+113.2**
transition state **16**	-997.621892	-997.195653	-997.91699	-997.490751	**+120.5**
reactant complex **6b**	-997.682694	-997.253687	-997.977310	-997.548303	-32.3

Supplemental Table 3b. Solvation Free Energies (in kJ/mol) Calculated Using the PCM/UAHF/Becke3LYP/6-31G(d) Level of Theory for all Stationary Points Located on the Potential Energy Surface of DMAP (**1**) + Acetic Anhydride (**2**) + tert-Butanol (**3**) as Optimized at the Becke3LYP/6-31G(d) Level of Theory.

reactants and products

stationary point	ΔGsolv(CCl4) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CHCl3) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CH2Cl2) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))
DMAP (**1**)	-6.8	-12.4	-18.4
acetic anhydride (**2**)	+1.0	-4.6	-9.6
tert-butanol (**3**)	-3.0	-6.6	-10.7
tert-butyl acetate (**4**)	+2.7	-0.9	-5.6
acetic acid (**5**)	-3.0	-7.7	-11.5
1 + **2** + **3**	-8.8	-23.6	-38.7
1 + **4** + **5**	-7.1	-21.0	-35.5

nucleophilic catalysis

stationary points	ΔGsolv(CCl4) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CHCl3) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CH2Cl2) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))
reactant complex **6h**	+26.8	+17.1	+7.0
reactant complex **6g**	+30.8	+22.1	+12.6
reactant complex **6f**	+29.4	+20.6	+11.0
reactant complex **6e**	+30.8	+21.5	+11.8
reactant complex **6d**	+28.9	+19.7	+10.1
reactant complex **6c**	+30.7	+21.8	+12.2
reactant complex **6b**	+31.2	+22.2	+13.0
reactant complex **6a**	+29.0	+19.3	+9.7
transition state **7d**	+12.4	-3.3	-16.2
transition state **7c**	+12.4	-1.8	-13.8
transition state **7b**	+13.6	-0.4	-12.3

transition state **7a**	+17.4	+5.6	-5.6
intermediate complex **8d**	+15.6	+0.5	-12.1
intermediate complex **8c**	+16.1	+0.6	-11.9
intermediate complex **8b**	+21.5	+7.4	-4.2
intermediate complex **8a**	+17.9	+3.0	-9.0
transition state **9b**	+8.1	-6.9	-19.3
transition state **9a**	+11.5	-1.3	-12.6
product complex **10g**	+25.7	+16.0	+5.8
product complex **10f**	+29.7	+20.9	+11.4
product complex **10e**	+28.6	+16.5	+6.2
product complex **10d**	+27.4	+17.0	+7.0
product complex **10c**	+26.3	+16.9	+6.7
product complex **10b**	+25.8	+16.4	+6.2
product complex **10a**	+29.4	+21.3	+11.6

concerted base catalysis
(direct reaction from reactant complex **6** to product complex **10**)

stationary point	ΔGsolv(CCl4) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CHCl3) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CH2Cl2) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))
transition state **11c**	+9.4	-3.8	-15.6
transition state **11b**	+9.6	-4.5	-16.8
transition state **11a**	+10.2	-2.8	-14.4
stepwise base catalysis			
stationary point	ΔGsolv(CCl4) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CHCl3) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))	ΔGsolv(CH2Cl2) (PCM/UAHF/ B3LYP/6-31G(d)// B3LYP/6-31G(d))
product complex **10c**	+26.3	+16.9	+6.7
product complex **10a**	+29.4	+21.3	+11.6

transition state **12c**	+9.0	-4.9	-16.7
transition state **12b**	+12.2	+0.17	-10.9
transition state **12a**	+10.3	-2.0	-13.6
tetrahedral int. **13c**	+10.4	-2.2	-13.8
tetrahedral int. **13b**	+16.9	+7.7	-2.6
tetrahedral int. **13a**	+7.7	+8.1	-2.1
transition state **14**	+5.5	-11.4	-24.7
tetrahedral int. **15**	+21.6	+8.7	-2.1
transition state **16**	+21.5	+8.8	-1.9
reactant complex **6b**	+31.2	+22.2	+13.0

Structures of all Stationary Points

reactants and products

1

1\1\GINC-TEA\SP\RB3LYP\6-311+G(d,p)\C7H10N2\ZIPSE\26-Apr-2002\0\\#BECK
E3LYP/6-311+G(D,P) SCF=TIGHT GEOM=CHECK GUESS=READ\\py3xsp1 b3lyp/6-31
1+G(d,p)//b3lyp/6-31G(d) sp\\0,1\N,-1.558388251,0.0010918068,-0.088479
8196\C,-0.1804786331,0.0001586869,-0.0415745535\C,0.5713144855,1.19724
90519,-0.0175188823\C,0.5697770802,-1.1979428202,-0.0199908207\H,0.090
2643562,2.1679109837,-0.0158740267\H,0.0874814051,-2.167987799,-0.0203
48458\N,2.6763963076,-0.0017354266,0.0169819053\C,1.9579590435,-1.1330
662654,0.0046572702\C,1.9594119074,1.1305398402,0.0069933982\H,2.53034
02867,-2.0602778335,0.0186212473\H,2.5329829458,2.0569850649,0.0228702
917\C,-2.2831292582,1.254522891,0.0423794643\C,-2.2847384205,-1.251675
7807,0.0397845157\H,-3.3525027352,1.0613018039,-0.0600812665\H,-3.3538
623086,-1.0568706889,-0.0622808274\H,-2.1151454241,-1.7412562829,1.011
0658071\H,-1.9979590679,-1.9561729793,-0.7502956893\H,-1.995449008,1.9
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sion=SGI-G98RevA.6\HF=-382.3599769\RMSD=4.053e-09\Dipole=-1.9087024,0.
001184,0.039729\PG=C01 [X(C7H10N2)]\\@

2

1\1\GINC-TERMINUS\SP\RB3LYP\6-311+G(d,p)\C4H6O3\ZIPSE\03-Jul-2003\0\\#
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\cpy2cxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\X\O,1,1.\X,2,1.,
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0163,2,182.93620837,0\C,5,1.5065014938,7,126.87330163,2,182.93620837,0
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67,5,109.58255241,11,-120.47036079,0\H,9,1.0945955034,5,110.35036728,1
1,121.53064502,0\\Version=x86-Linux-G98RevA.7\State=1-A\HF=-381.847721
9\RMSD=3.138e-09\Dipole=0.,0.,-1.6249639\PG=C02 [C2(O1),X(C4H6O2)]\\@

3

1\1\GINC-TERMINUS\SP\RB3LYP\6-311+G(d,p)\C4H10O1\ZIPSE\04-Jul-2003\0\\
#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECK GUESS=READ\\cp
y5xsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp t-butanol, cs\\0,1\H\O,1,
0.9706274355\C,2,1.4367285413,1,107.59813921\C,3,1.5308171375,2,104.69
493632,1,180.,0\C,3,1.5365615579,2,109.64765305,4,-118.98967248,0\C,3,
1.5365615579,2,109.64765305,4,118.98967248,0\H,4,1.0953155854,3,111.09
540887,2,180.,0\H,4,1.0948935968,3,110.16012821,7,120.40555813,0\H,4,1
.0948935968,3,110.16012821,7,-120.40555813,0\H,5,1.0981951369,3,110.77
926483,2,-63.20965647,0\H,6,1.0981951369,3,110.77926483,2,63.20965647,
0\H,5,1.0963458175,3,111.60130631,10,-119.79902054,0\H,6,1.0963458175,
3,111.60130631,11,119.79902054,0\H,5,1.0949740599,3,110.1716607,10,119
.59142636,0\H,6,1.0949740599,3,110.1716607,11,-119.59142636,0\\Version
=x86-Linux-G98RevA.7\State=1-A'\HF=-233.7522469\RMSD=9.195e-09\Dipole=
0.5920408,0.,-0.333045\PG=CS [SG(C2H2O1),X(C2H8)]\\@

4

1\1\GINC-CICUM81\SP\RB3LYP\6-311+G(d,p)\C6H12O2\ZIPSE\24-Sep-2003\0\\#
BECKE3LYP/6-311+G(D,P) INT=FINEGRID SCF=(DIRECT,TIGHT) GEOM=CHECK GUES
S=READ\\cpy9axsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,1.41918
90476,-0.0671669736,0.1106224621\O,1.4341990194,-0.1231314493,1.322563
7032\C,2.6579444593,-0.0815157378,-0.7613052045\O,0.313945488,0.016288
0674,-0.6591191287\C,-1.0400998914,0.0488859899,-0.0739668073\C,-1.199
8705646,1.291178986,0.8091115413\C,-1.9354996645,0.1445185278,-1.31178

66968\C,-1.311092911,-1.2498066786,0.6932587969\H,2.7019435162,0.82797
58107,-1.369466885\H,3.5445044206,-0.1492754085,-0.1297665051\H,2.6248
421996,-0.9320723064,-1.4500885976\H,-1.1438728358,-2.1168891077,0.044
6355907\H,-0.666635357,-1.3341443113,1.5696415111\H,-2.3562830769,-1.2
698714899,1.0223908756\H,-0.9553772959,2.1957390007,0.2412191861\H,-2.
2405786035,1.3721482154,1.143070225\H,-0.5538380273,1.2391559903,1.686
8465272\H,-1.708473982,1.0500098754,-1.8837197836\H,-1.7861273956,-0.7
216809208,-1.9644342787\H,-2.9886824734,0.1770870251,-1.0134890116\\Ve
rsion=x86-Linux-G98RevA.7\HF=-386.4554585\RMSD=6.269e-09\Dipole=-0.403
98,0.0487927,-0.6806792\PG=C01 [X(C6H12O2)]\\@

5

1\1\GINC-TERMINUS\SP\RB3LYP\6-311+G(d,p)\C2H4O2\ZIPSE\24-Sep-2003\0\\#
P BECKE3LYP/6-311+G(D,P) SCF=TIGHT GEOM=CHECK GUESS=READ INT=FINEGRID\
\cpy3dxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp acetic acid\\0,1\C,0.
1145251349,0.,-0.1060380379\C,0.050049472,0.,1.4007392685\O,1.12075467
91,0.,-0.7781383217\O,-1.128750808,0.,-0.6544195254\H,-0.9940626434,0.
,-1.6207891038\H,1.0610667379,0.,1.8083579894\H,-0.4952413526,-0.88203
71815,1.7523432537\H,-0.4952413526,0.8820371815,1.7523432537\\Version=
x86-Linux-G98RevA.7\State=1-A'\HF=-229.1645742\RMSD=3.298e-09\Dipole=-
0.5702992,0.,0.3852158\PG=CS [SG(C2H2O2),X(H2)]\\@

nucleophilic catalysis

6g

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\23-Sep-2003\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK
GUESS=READ\\cpy7nsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp min\\0,1\C,
1.4754658045,0.7003519182,-0.8594921082\N,0.8363598318,0.7638642646,0.
3198662803\C,1.5404396044,1.2995621096,1.3307810586\C,2.8408344549,1.7
734031456,1.2286464612\C,3.5117869932,1.7019202504,-0.015398068\C,2.77
24447521,1.1403328206,-1.0837606218\C,-2.3065732743,1.5077410098,2.312
1305681\O,-2.550698404,2.0549206074,3.3502439406\N,4.8005306697,2.1476
162282,-0.175325822\C,5.4272058681,2.105188778,-1.487304552\C,5.497677
3824,2.7708163601,0.939136141\O,-1.7618806923,0.2075286409,2.398032849
\C,-1.9423834431,-0.7643540331,1.4544933943\C,-1.0051910319,-1.9152921
396,1.6849719875\C,-2.4231010074,2.113226217,0.9411815219\O,-2.7829308
001,-0.6940118176,0.5808113107\O,-2.8105750352,-3.217452664,-0.8697231
453\C,-2.566092807,-3.0497156543,-2.2723362367\C,-1.3127363802,-2.1829
819803,-2.4857082869\C,-2.3448339588,-4.4642056995,-2.8152700771\C,-3.
7927192066,-2.398944817,-2.9326345082\H,3.3191033097,2.1908158756,2.10
62462181\H,3.1961460316,1.0456687275,-2.0760983805\H,0.9109314374,0.26
64743898,-1.6834108659\H,1.0276700142,1.3521153291,2.2899033429\H,6.50
71983084,3.039638789,0.624741459\H,6.4475662644,2.4831102744,-1.408779
1669\H,4.8899218585,2.7223573672,-2.2214640201\H,5.4769374135,1.079442
9739,-1.875293364\H,5.5817911171,2.0859321747,1.7929086134\H,4.9919926
964,3.6843755634,1.2827063747\H,-3.2740150603,1.6770521898,0.412710642
1\H,-2.5666693986,3.1886349993,1.0590068306\H,-1.5223596353,1.89757587
74,0.3579698571\H,-1.029053123,-2.2204886425,2.7352413\H,-1.2763826248
,-2.7445486715,1.0300396233\H,0.0083640393,-1.5716643497,1.4528534786\
H,-2.9569371187,-2.3326489227,-0.4820809031\H,-1.4940056599,-4.9346127
59,-2.3106386119\H,-3.2309194552,-5.0814184188,-2.6330136452\H,-2.1459
834317,-4.4476884955,-3.8927530314\H,-3.9665642201,-1.3971222351,-2.52
05124864\H,-3.6618549719,-2.2988408038,-4.0169425934\H,-4.6863479638,-
3.0034112182,-2.7444582411\H,-1.4531239901,-1.1899464444,-2.0415386477
\H,-0.4440480469,-2.6501362833,-2.0085145284\H,-1.0922543503,-2.051198
5833,-3.5521521436\\Version=x86-Linux-G98RevA.7\HF=-997.971967\RMSD=2.
217e-09\Dipole=3.086138,1.0929353,-1.1740649\PG=C01 [X(C15H26N2O4)]\\@

6f

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\07-Aug-2003\0\\#P

B3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GUESS=R
EAD\\cpy7esp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,0.219006471
1,1.4632766848,-2.2883350464\N,-0.2165843984,0.6676787225,-1.299211537
2\C,0.7332841576,-0.0188359213,-0.6375702431\C,2.0917574739,0.05892011
13,-0.9163467453\C,2.5493855765,0.9069874866,-1.9517216982\C,1.5490903
798,1.6204048143,-2.6535969894\C,-2.6854063964,0.7849625235,0.99977169
11\O,-2.3427958037,0.3535543542,2.0786385015\N,3.8848366533,1.03154761
87,-2.2573468147\C,4.2952806903,1.8320556003,-3.3995221313\C,4.8643766
909,0.2001856977,-1.5755422569\O,-2.9357196763,-0.1595940586,0.0270398
727\C,-3.2078935334,0.0986616325,-1.3132974501\C,-3.031878911,-1.17253
81065,-2.0950320122\C,-2.8295824139,2.2486112141,0.6960473897\O,-3.562
2139518,1.1631739693,-1.7459974906\O,-0.5475408282,-1.9463496632,1.999
4841045\C,0.0511871814,-1.9891235626,3.303655738\C,-1.0117563787,-2.39
26622282,4.3389467518\C,1.1470906656,-3.0543540522,3.2098905198\C,0.65
1721924,-0.6165017733,3.6504055874\H,2.7790529331,-0.5401881695,-0.331
51613\H,1.796027339,2.2854954435,-3.4721414966\H,-0.5518088591,2.01094
21704,-2.8294592745\H,0.3880763847,-0.6727821382,0.1626814681\H,5.8635
323566,0.4646359408,-1.9255799273\H,5.3845371234,1.8307547241,-3.46470
52138\H,3.9676143178,2.8740412337,-3.2938769623\H,3.8947718848,1.44349
37743,-4.3476361791\H,4.7061756288,-0.8717913393,-1.7647416492\H,4.835
5989866,0.3615848102,-0.4907537388\H,-3.8323740798,2.48373695,0.334220
1893\H,-2.6048315402,2.7991209763,1.6107277236\H,-2.1295715115,2.52332
53541,-0.097558958\H,-3.5698045354,-1.9960011629,-1.615883318\H,-3.388
4887729,-1.0245219613,-3.1151200165\H,-1.9671664162,-1.4247784915,-2.1
027314282\H,-1.2754259805,-1.2949677959,2.0299275528\H,0.7137156338,-4
.0212172951,2.9325751839\H,1.8802056533,-2.7789424751,2.4435777814\H,1
.6703090996,-3.1669269547,4.1660827907\H,-0.1285232907,0.1526732002,3.
6581660331\H,1.1321439885,-0.6270305338,4.6364936724\H,1.4022018773,-0
.3314750259,2.9044326361\H,-1.8136495092,-1.6456096813,4.3769570852\H,
-1.4559609477,-3.3564952725,4.067625993\H,-0.581942934,-2.4782382096,5
.3443061108\\Version=x86-Linux-G98RevA.11.3\HF=-997.9728726\RMSD=2.595
e-09\Dipole=1.7042639,0.5696904,-1.0774642\PG=C01 [X(C15H26N2O4)]\\@

6e

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\06-Jul-2004\0\
\#P BECKE3LYP/6-311+G(D,P) GEOM=CHECKPOINT GUESS=READ SCF=TIGHT INT=FI
NEGRID\\b3lyp/6-311+G(d,p) nuc26ircr3optsp singlepoint\\0,1\C,0,-0.766
9729536,1.3520313338,-0.1936983763\N,0,-0.5461106565,2.4583286361,-0.9
27177811\C,0,-1.6314049708,3.1359002706,-1.3324729501\C,0,-2.934198846
7,2.7606937445,-1.0436257255\C,0,-3.1701297023,1.5922522201,-0.2765713
577\C,0,-2.0222204636,0.8851999058,0.1546117296\C,0,2.8577555984,2.123
0251257,-0.8755125451\O,0,2.0554161826,3.0407476818,-1.3937921804\N,0,
-4.4363814039,1.1661645896,0.0311590434\C,0,-4.6208484365,-0.015545664
8,0.8643011101\C,0,-5.5897423104,1.9484597325,-0.3821262018\O,0,2.4764
779279,1.1367725486,-0.2559548165\C,0,0.4611514967,-1.9303075337,1.487
7220429\C,0,1.5717975257,-1.1152017455,2.1195494794\C,0,4.3185407707,2
.4213051306,-1.142879378\O,0,-0.7083977872,-1.7113054236,1.7333620359\
O,0,0.7372042998,-2.9776055146,0.6738010071\C,0,1.9718310243,-3.304065
0509,-0.0555814536\C,0,2.219872099,-2.248373617,-1.1377224442\C,0,3.18
42441899,-3.4935261426,0.8661368983\C,0,1.6012676834,-4.6483895874,-0.
6959361646\H,0,-3.7494809531,3.3712872124,-1.4118401257\H,0,-2.0843146
34,-0.0160895674,0.7511731629\H,0,0.1268852656,0.8239900764,0.12299857
11\H,0,-1.4448924862,4.0313995304,-1.9220608746\H,0,-6.5007057286,1.44
08676309,-0.0612531496\H,0,-5.6885991655,-0.2152465107,0.9675956412\H,
0,-4.1955889985,0.1195642436,1.8680233988\H,0,-4.1501556734,-0.8984260
078,0.4152614714\H,0,-5.6320039168,2.057266739,-1.4740966788\H,0,-5.58
62991222,2.9549187329,0.0609099794\H,0,4.9500050961,1.707007258,-0.612
0255776\H,0,4.5159536568,2.35692813,-2.2190646909\H,0,4.5585293189,3.4
426517276,-0.830060686\H,0,1.0999603099,-0.3607816894,2.7507881445\H,0
,2.2099962424,-1.7497783378,2.7413775604\H,0,2.1953659694,-0.608133070
9,1.3783360628\H,0,1.0722498196,2.8110688024,-1.2128630165\H,0,3.60063

98019,-2.5484546662,1.2204094333\H,0,2.9187727807,-4.1133975848,1.7294
098663\H,0,3.9748138713,-4.0113260879,0.3116583531\H,0,0.7010856177,-4
.541327442,-1.3083633626\H,0,2.4181635442,-5.006380184,-1.3317703074\H
,0,1.4032834701,-5.4003418947,0.0749412186\H,0,1.3362521677,-2.1522302
232,-1.7770956163\H,0,2.4543194654,-1.2629997774,-0.7262237499\H,0,3.0
631094643,-2.558483897,-1.7663003991\\Version=x86-Linux-G98RevA.7\HF=-
997.9914622\RMSD=3.264e-09\Dipole=-0.5478256,-0.0806414,-0.2288619\PG=
C01 [X(C15H26N2O4)]\\@

6d

1\1\GINC-NODE-25\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIP03\12-Aug-2004\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\opt of end reverse
irc after 80Pt of nuc271ots freq\\0,1\C,0,-2.15524,1.670357,0.481738\
N,0,-1.113849,0.855585,0.254218\C,0,-1.412314,-0.422106,-0.040497\C,0,
-2.704947,-0.919485,-0.121863\C,0,-3.804326,-0.062744,0.120302\C,0,-3.
485485,1.28153,0.428504\C,0,2.079884,-2.664651,-0.458496\O,0,0.968738,
-2.826225,-0.893812\N,0,-5.102604,-0.508596,0.062066\C,0,-6.201253,0.4
28115,0.236012\C,0,-5.381429,-1.874948,-0.353321\O,0,2.207106,-1.86568
6,0.674383\C,0,3.334977,-1.116889,0.980662\C,0,3.187753,-0.499175,2.33
9127\C,0,3.314316,-3.33518,-1.002254\O,0,4.256537,-0.96292,0.218248\O,
0,1.643456,1.629671,0.575625\C,0,2.109643,2.425744,-0.519036\C,0,3.561
7,2.781577,-0.183479\C,0,2.044052,1.610911,-1.82261\C,0,1.25409,3.6995
07,-0.633089\H,0,-2.844631,-1.963675,-0.372452\H,0,-4.256442,2.016972,
0.62258\H,0,-1.907804,2.703311,0.720532\H,0,-0.571361,-1.08692,-0.2224
75\H,0,-6.458828,-2.044656,-0.323672\H,0,-7.145955,-0.11598,0.190268\H
,0,-6.214569,1.203942,-0.543534\H,0,-6.148718,0.92692,1.212089\H,0,-4.
907691,-2.60102,0.319343\H,0,-5.029802,-2.077143,-1.375228\H,0,3.92928
5,-2.603592,-1.531438\H,0,3.929627,-3.746893,-0.197051\H,0,2.996794,-4
.126231,-1.683368\H,0,2.676567,-1.17159,3.032118\H,0,4.173236,-0.22158
4,2.717335\H,0,2.583281,0.406358,2.202422\H,0,0.696961,1.38909,0.42091
1\H,0,2.657565,0.70807,-1.732024\H,0,1.012322,1.306904,-2.034847\H,0,2
.41023,2.191171,-2.678659\H,0,1.272814,4.25073,0.313634\H,0,1.620434,4
.361582,-1.427209\H,0,0.21215,3.44512,-0.862171\H,0,3.606816,3.341102,
0.757712\H,0,4.157844,1.869767,-0.071191\H,0,4.009822,3.395234,-0.9733
73\\Version=x86-Linux-G98RevA.7\HF=-997.9772633\RMSD=3.434e-09\Dipole=
-2.0044421,-0.6307988,0.1544214\PG=C01 [X(C15H26N2O4)]\\@

6c

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\08-Jul-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT GEOM=CHECKPOINT GUESS=READ INT=FI
NEGRID\\singlepoint\\0,1\C,2.0933661037,-2.2754423978,0.4390836336\N,0
.9444355254,-1.5829075481,0.4370884861\C,1.0581805899,-0.2529553725,0.
2757037885\C,2.257484923,0.421422806,0.1137828652\C,3.4694288601,-0.30
81809211,0.11946588\C,3.3509611637,-1.7095629526,0.2877044174\C,-1.121
0105034,3.0593402261,-0.3218828665\O,0.0631733588,3.0583713832,-0.5358
557092\N,4.6881915673,0.3074673612,-0.0278421959\C,5.9024894441,-0.488
8069831,-0.095210379\C,4.7497086195,1.7420775042,-0.2655928241\O,-1.58
53500548,2.2061521093,0.6796949101\C,-2.8577140927,1.6452760404,0.7143
320428\C,-3.0624386006,0.919428389,2.0097553837\C,-2.1145991324,3.9694
649778,-0.9939316486\O,-3.6297283008,1.6967793011,-0.2103549392\O,-1.8
949743334,-1.7700527936,0.6764420919\C,-2.5157649859,-2.4201135739,-0.
4410661607\C,-4.0247641862,-2.2581160698,-0.2314118423\C,-2.0820042679
,-1.7404920964,-1.7513178866\C,-2.1265044599,-3.9078786493,-0.44541784
19\H,2.2261692797,1.4949906959,-0.0201591649\H,4.2213980739,-2.3540774
322,0.2993251225\H,2.0026840685,-3.3526498062,0.568620818\H,0.12868405
03,0.3080029843,0.2783326043\H,5.7948831814,2.0501089381,-0.3240473675
\H,6.7615935072,0.1759671301,-0.1974144554\H,5.8996609381,-1.177569011
4,-0.9525955533\H,6.0439960092,-1.0824292037,0.8174293098\H,4.27768483
88,2.3015328192,0.5516030849\H,4.2529639092,2.027486266,-1.2035809851\
H,-2.7319236353,3.3943415741,-1.6881548516\H,-2.7920656694,4.423737005
1,-0.2649380159\H,-1.5589413733,4.7402205464,-1.5301065408\H,-2.543294

5788,1.4131939444,2.8341106629\H,-4.1324152427,0.8404817957,2.21167297
7\H,-2.6521896705,-0.091966256,1.8755629189\H,-0.9165763233,-1.8923541
183,0.612966303\H,-2.3620149772,-0.6813392686,-1.7363704426\H,-0.99577
99029,-1.8085552105,-1.8802213763\H,-2.558387029,-2.2088388687,-2.6214
385136\H,-2.4127984484,-4.3751453123,0.5031248803\H,-2.6174037855,-4.4
501645094,-1.2626417018\H,-1.0425309897,-4.0214804344,-0.5688233542\H,
-4.3239145089,-2.7023218531,0.7244407773\H,-4.2962024474,-1.1968757467
,-0.2212501885\H,-4.5875511316,-2.7489809223,-1.0335611753\\Version=x8
6-Linux-G98RevA.7\HF=-997.9767684\RMSD=2.525e-09\Dipole=1.6651613,0.74
37969,-0.0546106\PG=C01 [X(C15H26N2O4)]\\@

6b

1\1\GINC-NODE-26\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIP03\24-Sep-2004\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=(TIGHT,DIRECT) INT=FINEGRID GUESS=READ
GEOM=CHECK\\sp after freq\\0,1\C,-2.6668739607,0.3048254252,-2.484624
7359\C,-2.662675027,0.2818854146,-1.0699885609\C,-1.4589285451,0.32609
23478,-0.3821655902\N,-0.2525878682,0.3964383942,-0.974937679\C,-0.256
3491565,0.4197866455,-2.3169335273\C,-1.3967122923,0.3798645646,-3.104
9519917\N,-3.8305081485,0.25359686,-3.2110833685\C,-5.1143560514,0.235
0562988,-2.5263891532\C,-3.7860292546,0.3412246488,-4.662054911\O,2.10
98022932,0.3238043644,0.719178488\C,3.0432337707,1.3617250442,0.395162
25\C,4.2168543228,1.1817341761,1.3630221829\C,3.5242607344,1.197498175
4,-1.0569519404\C,2.3798260197,2.7346672977,0.5944992984\O,0.167528924
8,-1.512090257,2.1542940076\C,1.2226202517,-2.4104068812,2.1435982184\
C,1.4490838402,-2.902332184,0.7422442018\C,-0.0504702417,-0.534297847,
3.119621278\C,1.0642094451,-0.1926313527,4.0689837414\O,-1.1181496046,
0.023676701,3.0831832455\O,1.8355727479,-2.7416995568,3.1258906642\H,-
1.2925440041,0.4071953523,-4.1826945784\H,-3.5835436528,0.2284679652,-
0.5026964969\H,-1.4621681065,0.2953429906,0.7043155131\H,0.7198588629,
0.4733429599,-2.7960146917\H,-4.8003019818,0.2664178973,-5.0568571765\
H,-5.9135325208,0.175228582,-3.2666573712\H,-5.2733272738,1.1402101852
,-1.9234371202\H,-5.2022411809,-0.6355341076,-1.8638562185\H,-3.195098
1966,-0.4762398122,-5.0954731298\H,-3.3551515341,1.2928038213,-5.00506
07353\H,1.9653411344,0.0409409441,3.4946519037\H,0.7497534208,0.673184
8668,4.653483722\H,1.2966777216,-1.0369122788,4.7201482084\H,2.1150381
971,-3.7661643652,0.7592338299\H,0.5007302532,-3.1518137629,0.25845134
34\H,1.9075828596,-2.0790874884,0.1830169472\H,1.3186512737,0.40840923
57,0.13085075\H,3.8812761207,1.3001904485,2.3992819344\H,4.6465405962,
0.1798048283,1.2564693066\H,5.0036087234,1.9199688914,1.171203287\H,2.
6895106609,1.3160968125,-1.7578401597\H,4.2852287105,1.9438079186,-1.3
153675058\H,3.9548237686,0.2004827928,-1.2016533966\H,1.5171647319,2.8
458834614,-0.0727456527\H,2.0244810835,2.8362616876,1.6256858077\H,3.0
791144258,3.553782738,0.3869132084\\Version=x86-Linux-G98RevA.11.3\HF=
-997.9773103\RMSD=1.927e-09\Dipole=-1.2597828,0.3275297,-2.3316922\PG=
C01 [X(C15H26N2O4)]\\@

6a

1\1\GINC-CICUM82\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\13-Oct-2003\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK
GUESS=READ\\cpy7ix2sp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp min\\0,1
\C,0.988983935,1.6899106459,-1.8513726347\N,0.6220643476,0.7970180606,
-0.9193362942\C,1.371230801,-0.3177030131,-0.8401424512\C,2.4678639979
,-0.5778995912,-1.6486509545\C,2.8570952878,0.3643553039,-2.6302641148
\C,2.0652017748,1.535105436,-2.7118074784\C,-2.6702777603,-2.632869732
,2.3319784021\O,-3.4681112381,-3.2772288495,2.9540114204\N,3.936034985
1,0.1571670679,-3.4521865145\C,4.2825822496,1.1455626891,-4.4614752622
\C,4.7016709694,-1.0761555373,-3.3514200868\O,-1.670261145,-1.97207584
81,3.0702880384\C,-0.4173966486,-1.7114291859,2.5798386417\C,0.2475626
418,-0.624522602,3.3766502225\C,-2.699452569,-2.3778958993,0.849610433
\O,0.0665521498,-2.2962367925,1.6375660641\O,-1.5175222582,0.869262239
4,1.0094322492\C,-2.3314688008,2.0468845903,0.9232686025\C,-3.38936280

93,1.9040590161,2.0214836199\C,-1.4642250754,3.2932751481,1.1699395987
\C,-2.9973731751,2.1159725001,-0.4615660715\H,3.0084059148,-1.50614697
47,-1.5109071441\H,2.2788694148,2.3150656744,-3.4321348144\H,0.3809562
731,2.5909739519,-1.9155326623\H,1.0746789921,-1.0411371966,-0.0838445
625\H,5.5172649341,-1.0511918054,-4.0754495371\H,5.1681594434,0.809688
4064,-5.0026033\H,4.5118369761,2.1201988076,-4.0103110358\H,3.47253152
99,1.288561348,-5.1902414199\H,4.0837420704,-1.9593441639,-3.564221100
9\H,5.1397233248,-1.1989262279,-2.3520416339\H,-1.9289148165,-2.977545
5327,0.3581199362\H,-3.6844243712,-2.6661233812,0.4777898313\H,-2.4867
306295,-1.3246908678,0.6371530674\H,-0.027895996,-0.6800271164,4.43236
64015\H,1.3301709259,-0.6859615123,3.2532632673\H,-0.1142992961,0.3262
14537,2.9668936369\H,-0.8175841948,0.9133800145,0.3098607532\H,-0.9860
635638,3.23509188,2.1538773135\H,-0.673012189,3.3719641614,0.414689895
6\H,-2.0617532917,4.2119723794,1.1308533678\H,-3.6010205133,1.21905191
37,-0.6373667922\H,-3.6487073124,2.9936775601,-0.5504679548\H,-2.24129
79849,2.1740707943,-1.253801746\H,-3.9936970381,1.0057238127,1.8560972
021\H,-2.91086682,1.8144656741,3.0025989462\H,-4.0578360922,2.77203335
66,2.0392147724\\Version=x86-Linux-G98RevA.7\HF=-997.9784356\RMSD=3.04
5e-09\Dipole=2.4831969,1.3872528,-2.3707767\PG=C01 [X(C15H26N2O4)]\\@

7d

1\1\GINC-CICUM90\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\20-Sep-2003\0
\\#BECKE3LYP/6-311+G(D,P) INT=FINEGRID SCF=(DIRECT,TIGHT)\\cpy7cxsp1 b
3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\N,0,-1.2991057209,1.37426887
85,0.9916479433\C,0,-1.3227540396,1.1688731474,2.3227044062\C,0,-0.173
0108627,1.0728342018,3.0705718817\C,0,1.096208365,1.2066467806,2.44429
35653\C,0,1.0811146448,1.4288142217,1.0419902466\C,0,-0.1132128417,1.4
95404624,0.3596041295\N,0,2.2591103998,1.1264659816,3.1456344751\C,0,2
.2345699517,0.8659736427,4.5812959984\C,0,-2.7600766021,1.4866687844,0
.2899016102\O,0,-2.8180299508,-0.2305597539,-0.3784545308\C,0,-2.04738
35569,-0.7496239468,-1.2727448833\O,0,-1.0080823096,-0.227424721,-1.73
2004111\C,0,3.5400799902,1.2508809957,2.4560180412\C,0,-2.7068140566,2
.3125903447,-0.9775387277\O,0,-3.6525890849,1.5586006663,1.1065483442\
C,0,-2.5083252393,-2.1156421723,-1.7682276566\H,0,-0.2631700198,0.9010
4017,4.1348052571\H,0,1.996291594,1.5301116852,0.474626974\H,0,-0.1482
93863,1.595252535,-0.7141618241\H,0,-2.3229208013,1.0950043259,2.73616
63465\H,0,3.2580459783,0.8388456183,4.9555982129\H,0,4.3465196039,1.16
9134286,3.1849335757\H,0,3.6304389447,2.2229189229,1.9557832934\H,0,3.
672660485,0.4602465173,1.7067962514\H,0,1.7620319748,-0.0982320531,4.8
078404368\H,0,1.6956052791,1.6538394187,5.1220083151\H,0,-3.7075185317
,2.2741532532,-1.4133061572\H,0,-2.4870140751,3.3546191028,-0.71496442
99\H,0,-1.9872686797,1.9448858456,-1.7077443744\H,0,-3.5159485826,-2.0
296544238,-2.1883835762\H,0,-1.8218680162,-2.5016392032,-2.5241403393\
H,0,-2.5702296602,-2.8150189721,-0.9275591595\H,0,0.0684806994,-1.1841
647475,-2.8696554869\O,0,0.6256995728,-1.714489767,-3.483726991\C,0,1.
733563295,-2.2435188288,-2.7591937647\C,0,2.655257052,-2.8631271089,-3
.8152713344\H,0,2.1154404598,-3.6305143083,-4.3803231778\H,0,2.9883443
789,-2.0954277904,-4.5220460653\H,0,3.5375001832,-3.3237945813,-3.3555
731431\C,0,2.4623919941,-1.1143667036,-2.0068625048\H,0,1.7922414245,-
0.6608643425,-1.2668249043\H,0,3.3516743585,-1.4878556991,-1.482740147
\H,0,2.7753230129,-0.3349749399,-2.710687729\C,0,1.2545767824,-3.31960
56719,-1.7669466217\H,0,0.5697325861,-2.8824583993,-1.0308273832\H,0,0
.7181928281,-4.1104234441,-2.3025296938\H,0,2.0925806079,-3.7759980554
,-1.2245360051\\Version=x86-Linux-G98RevA.7\HF=-997.9514341\RMSD=2.845
e-09\Dipole=3.0185245,1.0592283,3.0960219\PG=C01 [X(C15H26N2O4)]\\@

7c

1\1\GINC-PIRX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\12-Aug-2003\0\\#
P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECK GUESS=READ INT=
FINEGRID\\cpy7bxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\N,1.040

8333898,-0.0078383071,0.9327543292\C,1.4233517929,-1.2769731037,0.6934
625604\C,2.6291063462,-1.5766565123,0.10356103\C,3.5167259037,-0.53198
88111,-0.2721366736\C,3.0664077128,0.7924805441,-0.0219311094\C,1.8431
003962,1.0163677117,0.5673154972\N,4.7241167288,-0.7844638344,-0.84580
75503\C,5.1314311206,-2.1581798153,-1.1239195064\C,-0.3777949698,0.169
3914172,1.6663753967\O,-1.2117084317,1.0761684473,0.2965671097\C,-1.09
66904794,2.3374389514,-0.0417621709\O,-0.2125570684,3.1115325562,0.345
3067079\C,5.5950051061,0.3192323417,-1.2395752972\C,-0.2993056029,1.20
65630988,2.7679756927\O,-0.9750747124,-0.883635062,1.7852293025\C,-2.1
985285063,2.8242552926,-0.9743400146\H,2.8752732443,-2.6165311408,-0.0
647404113\H,3.6582426957,1.6528756764,-0.304443343\H,1.4251400188,2.01
17617079,0.7011030846\H,0.6976737003,-2.022834222,0.9982598226\H,6.127
9033249,-2.1517872019,-1.565962336\H,6.5191901096,-0.0860699081,-1.651
9040001\H,5.8537400952,0.9481339529,-0.3791607513\H,5.126295725,0.9510
753877,-2.0047234734\H,4.4470651521,-2.6475686802,-1.8286083269\H,5.17
13957705,-2.7557225802,-0.2049527704\H,-1.3108038712,1.3241617295,3.16
35899878\H,0.3387140533,0.811486806,3.5677805088\H,0.0656612407,2.1748
998802,2.4303427598\H,-3.0141119098,3.2329224799,-0.3643939676\H,-1.81
52728726,3.6296818884,-1.6057592814\H,-2.6054475598,2.0084175003,-1.57
55824352\H,-2.3265988216,-0.1111192855,-0.7695303155\O,-2.938543862,-0
.4597928599,-1.4498046364\C,-4.0379578774,-1.0905770354,-0.7801219001\
C,-5.0766951519,-1.362585469,-1.8724103781\H,-5.396119245,-0.422660435
6,-2.3358839305\H,-4.6450249018,-1.9970275979,-2.6545033874\H,-5.95860
2949,-1.8678236371,-1.4619881637\C,-3.5613008828,-2.4070186175,-0.1415
581086\H,-2.7838182328,-2.2059858749,0.6028758681\H,-4.386253901,-2.93
5687953,0.3530093106\H,-3.1427894322,-3.0650239179,-0.9118965855\C,-4.
6103065437,-0.1505466218,0.2940205734\H,-3.8451286875,0.0795152564,1.0
43676912\H,-4.9407593582,0.7900462909,-0.1614296015\H,-5.4664318075,-0
.6044260104,0.8080759553\\Version=x86-Linux-G98RevA.7\HF=-997.9520626\
RMSD=6.548e-09\Dipole=4.4326365,-0.9813681,-0.2097726\PG=C01 [X(C15H26
N2O4)]\\@

7b

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\29-Jul-2003\0\\#P
 BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECK GUESS=READ INT=F
INEGRID\\cpy7axsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp ts\\0,1\N,0.4
374345612,1.3369715386,-0.0258812664\C,0.2469655702,1.4475903619,1.302
5033094\C,1.2927951003,1.4133724322,2.1951669318\C,2.624256628,1.25493
12518,1.724892882\C,2.7810602453,1.1282250327,0.317985167\C,1.68576914
93,1.1687081515,-0.514512602\N,3.6871576795,1.217364776,2.5732612006\C
,3.4780980587,1.2995613573,4.0154320271\C,-0.8919786125,1.4151261887,-
0.9353420152\O,-0.7331369986,-0.2411975045,-1.6814782272\C,0.019109376
6,-0.6265495567,-2.6869473985\O,0.983823333,-0.0055854757,-3.146191791
4\C,5.0358914446,1.0180564181,2.0513418043\C,-0.6895649719,2.354390110
3,-2.1074897079\O,-1.9107758928,1.3941948116,-0.2692318829\C,-0.421226
3741,-1.9531215734,-3.2905234809\H,1.0716756949,1.5032896056,3.2502809
838\H,3.7537762879,0.9756981316,-0.130335756\H,1.7522222258,1.00234154
57,-1.5879771195\H,-0.7916228014,1.5534901922,1.5950318042\H,4.4446836
508,1.2620558697,4.5180241721\H,5.7447841176,1.0399269547,2.8791920297
\H,5.311211753,1.8124975392,1.3472968993\H,5.1335842616,0.0510822582,1
.5415726009\H,2.867866121,0.464802761,4.3832840268\H,2.9868509966,2.23
98767958,4.2940604897\H,-1.5881323983,2.2893720715,-2.7256149762\H,-0.
6135022114,3.3768415014,-1.7185566446\H,0.1793951876,2.111567479,-2.71
65592224\H,-1.2322140742,-1.7613854408,-4.0042917468\H,0.4118981331,-2
.4099428446,-3.829341045\H,-0.8101164738,-2.6246931153,-2.5210120942\H
,-1.5374018304,-1.6157033225,-0.5994079869\O,-1.8178386321,-2.47690420
73,-0.2269915501\C,-3.2002923868,-2.3775703301,0.1385103674\C,-3.64094
67289,-3.8108730451,0.4502083725\H,-3.5238293142,-4.4449322366,-0.4354
574355\H,-3.0224802563,-4.2304719538,1.251488189\H,-4.6896955773,-3.84
29909845,0.7673563244\C,-3.3347407703,-1.482791285,1.3834639366\H,-2.9
860388131,-0.469496559,1.1565677884\H,-4.3758327975,-1.4195988842,1.72

4869298\H,-2.7269548114,-1.8879667391,2.2010521257\C,-4.0130417236,-1.
7950663775,-1.0293976712\H,-3.6594011467,-0.7867776352,-1.2721236219\H
,-3.9025099238,-2.4245997259,-1.9197836638\H,-5.0798601897,-1.73263328
18,-0.7818788802\\Version=x86-Linux-G98RevA.11.3\HF=-997.9523487\RMSD=
3.599e-09\Dipole=3.1081258,1.590995,2.6066703\PG=C01 [X(C15H26N2O4)]\\
@

7a

1\1\GINC-ERIC\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\24-Sep-2003\0\\#
P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GU
ESS=READ\\cpy7gxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\N,-0.89
77575217,0.9157523455,1.4106720011\C,-0.6103646062,0.8461530311,2.7204
538167\C,0.6672120583,0.6185914563,3.1839065759\C,1.7342608364,0.44126
4701,2.2625176631\C,1.3954204743,0.5187922264,0.8874045821\C,0.0921265
577,0.7600969409,0.5103909204\N,3.0124646249,0.2048483821,2.6746335477
\C,3.3159784645,0.0973108145,4.096042074\C,-2.5655541347,1.1621024688,
1.0760688484\O,-2.9223691073,-0.4389725641,0.5780338921\C,-2.524422190
5,-1.0638095211,-0.4927133696\O,-1.7406276371,-0.6329927383,-1.3519906
729\C,4.0681200715,-0.0108191746,1.6905893254\C,-2.682449903,2.0358256
039,-0.1559313844\O,-3.1686461925,1.3719104305,2.1070324974\C,-3.14821
62946,-2.4466944043,-0.6217441331\H,0.8293795941,0.5712995089,4.252841
8382\H,2.1167272751,0.357992717,0.097853727\H,-0.1841927836,0.78489101
14,-0.53248977\H,-1.4721848433,0.9801133175,3.3675611744\H,4.385198593
7,-0.0766349858,4.2205778678\H,5.0138088278,-0.164665462,2.2113807955\
H,4.1798571503,0.8576545371,1.0300007363\H,3.8690698938,-0.8929934396,
1.0688679255\H,2.7769676226,-0.7365718063,4.5651288224\H,3.0581122673,
1.0198544995,4.6313917423\H,-3.7473858888,2.1049245772,-0.3951527148\H
,-2.3227313101,3.0389839661,0.0968177451\H,-2.1509517419,1.6438274653,
-1.0210295409\H,-4.2298854474,-2.3471220833,-0.7638496967\H,-2.7164347
808,-2.9799268365,-1.4708977887\H,-2.9952182327,-3.0170104931,0.299632
1462\H,0.0291259863,-0.8835302154,-1.9201931938\O,0.9674192009,-0.7480
129027,-2.1650644032\C,1.0321135243,-0.6914271952,-3.5982318317\C,2.52
07673833,-0.5740296126,-3.9355827058\H,2.9426310282,0.3303662827,-3.48
26672119\H,3.067938941,-1.4388914583,-3.5446909458\H,2.6777778097,-0.5
232141639,-5.0187238856\C,0.4377015105,-1.9824506756,-4.1838876222\H,-
0.6163815787,-2.0773845075,-3.8966703574\H,0.4935508939,-1.9923783459,
-5.2790308917\H,0.976926827,-2.8556155767,-3.8004145776\C,0.2578430335
,0.5375536039,-4.1031787487\H,-0.7952644657,0.4715225565,-3.8077594192
\H,0.6781195874,1.4526186921,-3.6704564285\H,0.3030582278,0.6214657672
,-5.1958815099\\Version=DEC-AXP-Linux-G98RevA.11.3\HF=-997.9542757\RMS
D=3.741e-09\Dipole=2.9024007,-0.148185,0.8478142\PG=C01 [X(C15H26N2O4)
]\\@

8d

1\1\GINC-ERIC\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\28-Dec-2003\0\\#
P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GU
ESS=READ\\cpy7gxircfsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\N,-
1.0588817695,1.1750457117,1.6273785749\C,-0.564337081,1.2286219055,2.8
912211838\C,0.7433833692,0.9273492994,3.1648873266\C,1.6201206911,0.51
9664485,2.1149399919\C,1.0592372427,0.4570386059,0.8113482294\C,-0.256
743243,0.776499796,0.6034978013\N,2.9129313039,0.1906048561,2.34596949
77\C,3.4603637046,0.2381774089,3.6988983289\C,-2.5122478715,1.48268771
12,1.4317174233\O,-2.7185459038,-0.8698032504,0.4962600892\C,-2.402294
7876,-1.2648948066,-0.6500604021\O,-1.7271136739,-0.5899667549,-1.5102
919127\C,3.7579836259,-0.2653287364,1.2397758643\C,-2.9019195289,2.010
3702777,0.0801670736\O,-3.194624708,1.4980578656,2.4216253359\C,-2.841
3086397,-2.6662559232,-1.0854896851\H,1.0787739958,0.9906219088,4.1914
467102\H,1.6008520564,0.0962857258,-0.0553250268\H,-0.7339060131,0.609
6672823,-0.3627592049\H,-1.2821336668,1.5122654728,3.6502577217\H,4.51
60750338,-0.0304140167,3.6650128404\H,4.7421415897,-0.5241668321,1.630
264891\H,3.8790749688,0.5203844991,0.4851248936\H,3.3317326643,-1.1487

14454,0.752071495\H,2.9481981452,-0.4672132657,4.3653405062\H,3.379771
8693,1.2451805306,4.1255472763\H,-3.9902059709,2.0836264952,0.06743482
82\H,-2.4773682475,3.016953283,-0.0404025732\H,-2.5678204955,1.3703780
764,-0.7389471756\H,-3.4067742461,-2.6026485304,-2.0220067791\H,-1.958
3216441,-3.2848700289,-1.2867160737\H,-3.4524685385,-3.1442199204,-0.3
164759322\H,-0.0231944203,-0.9487228163,-1.8184436862\O,0.9545159642,-
0.9535524309,-1.979769943\C,1.142717075,-0.7341276917,-3.3845911768\C,
2.6519505135,-0.8293645881,-3.6246222341\H,3.1802974279,-0.0666392432,
-3.0399229248\H,3.0239949112,-1.8134699933,-3.3185034271\H,2.895168525
1,-0.679759431,-4.6826864247\C,0.3927399989,-1.8240129556,-4.168270104
7\H,-0.6768724806,-1.777500207,-3.935843426\H,0.518768661,-1.702855821
6,-5.2511615101\H,0.7629350488,-2.8155871684,-3.8843877895\C,0.6136986
13,0.6593719542,-3.7653139879\H,-0.4533273633,0.7308589474,-3.52962819
25\H,1.1445609475,1.4342100836,-3.1991902223\H,0.7477849797,0.86413156
02,-4.8347596517\\Version=DEC-AXP-Linux-G98RevA.11.3\HF=-997.9610496\R
MSD=1.952e-09\Dipole=3.4757299,1.2673175,1.8934473\PG=C01 [X(C15H26N2O
4)]\\@

8c

1\1\GINC-KATHY\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\19-Sep-2003\0\\
#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID\\cpy7kxsp1 b
3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,0,-0.1620732447,1.32063854
94,-1.6961041461\C,0,-0.2637681902,1.334031714,-0.3283474003\N,0,0.851
8873625,1.4048603313,0.4503439355\C,0,2.0849712158,1.4148041965,-0.127
2370424\C,0,2.2432478647,1.404824079,-1.4835606053\C,0,1.1013400652,1.
3604704549,-2.3405242244\C,0,0.7932845821,1.3679864797,1.9333409103\O,
0,1.8434853432,1.3302088796,2.5225784498\N,0,1.2226003771,1.3489518659
,-3.6887869366\C,0,2.5430456571,1.3474687266,-4.315147501\C,0,-0.56566
72936,1.4462394551,2.5481125679\C,0,0.0284302244,1.2638360334,-4.53056
14348\O,0,0.2355326607,-1.3410722415,0.9335337639\C,0,0.5107956928,-2.
6394467151,1.4729313408\C,0,0.122168654,-2.6727896003,2.9612031735\C,0
,-0.2910839808,-3.6910344429,0.6869075287\C,0,2.0170887222,-2.85513231
32,1.2982542918\O,0,-2.3809147051,-0.9309699393,1.418098807\C,0,-3.249
4442897,-0.2293835226,0.8031161424\O,0,-3.0360329235,0.8478169323,0.18
88556703\C,0,-4.687038711,-0.7615389865,0.8473298221\H,0,3.2491690267,
1.4161110045,-1.8809474164\H,0,-1.0904178457,1.2453272173,-2.246201608
9\H,0,-1.2669585968,1.2397724883,0.1266349728\H,0,2.9123629302,1.42809
76623,0.5700032381\H,0,2.4224032862,1.3602642755,-5.3981494413\H,0,0.3
290884305,1.2984626685,-5.5775567426\H,0,-0.6475847247,2.1045635681,-4
.3393005671\H,0,-0.517376353,0.3289644479,-4.3566849026\H,0,3.11578519
51,0.4519060637,-4.0443278856\H,0,3.1195111877,2.2344098208,-4.0271784
24\H,0,-0.4304120554,1.5154199602,3.6282649447\H,0,-1.1175890623,2.320
1178221,2.1856397012\H,0,-1.1679938619,0.5577582182,2.2965327075\H,0,-
5.0172668305,-0.8430335661,1.8893760988\H,0,-5.3692272194,-0.108657767
4,0.2974026319\H,0,-4.7212744375,-1.7722092448,0.4242922766\H,0,-0.745
3326025,-1.1900007608,1.0253241902\H,0,2.2880934259,-2.8009192382,0.23
73199945\H,0,2.5750842999,-2.0786808164,1.8341105698\H,0,2.3260306796,
-3.8330638774,1.6850761041\H,0,-0.9453187305,-2.4550440492,3.072024967
1\H,0,0.3279055201,-3.652701536,3.4100360251\H,0,0.6883537966,-1.91486
20765,3.515048258\H,0,-1.3623897883,-3.4796862915,0.7744788954\H,0,-0.
0202309291,-3.6569950399,-0.3749259464\H,0,-0.1041737295,-4.7057200308
,1.0599942996\\Version=DEC-AXP-Linux-G98RevA.11.3\HF=-997.9625151\RMSD
=2.917e-09\Dipole=2.5737835,1.4896667,-3.4773098\PG=C01 [X(C15H26N2O4)
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8b

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\06-Aug-2003\0\\#P
 B3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GUESS=R
EAD\\cpy7dsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,-0.55291801
99,1.5631656965,-0.75801881\N,-0.5139654985,2.3963751475,0.3296028539\
C,0.6690586968,2.5902580363,0.9936313975\C,1.823857801,1.9931181391,0.

5902830925\C,1.8253167524,1.1076397018,-0.5379156776\C,0.5862145283,0.
9504636228,-1.2091208822\C,-1.7139573359,3.055403197,0.8709203905\O,-1
.78808661,-0.7592170489,-0.0691826066\C,-2.6964003701,-0.7416759562,-0
.9637969948\C,-3.2568841598,-2.0959271427,-1.4147949067\N,2.9367942833
,0.455536826,-0.9327733847\C,2.8370821529,-0.6096034602,-1.9418707736\
C,4.2064889999,0.6483020986,-0.2367058492\C,-2.9532353769,2.9776221484
,0.0379323899\O,-1.6060818154,3.6326388698,1.9258365785\O,-3.163363431
8,0.3006174502,-1.4951966958\O,0.4748989794,-2.2396205013,-0.309876962
6\C,0.6385017258,-2.9014378226,0.9488278124\C,-0.5763605397,-3.8079235
136,1.2117161526\C,1.9183384454,-3.7344832495,0.8307956266\C,0.7702399
712,-1.8524913317,2.0677867259\H,2.7203586072,2.1735485701,1.167971600
8\H,0.4844443745,0.2775980789,-2.0479978683\H,-1.5221596405,1.37274585
41,-1.2215534469\H,0.6014935367,3.2388293904,1.8568943602\H,5.00158068
17,0.185351149,-0.8214705008\H,3.8031671138,-1.1096768821,-2.015383165
1\H,2.5924295221,-0.191963709,-2.925859308\H,2.0765985846,-1.338467397
,-1.6372806649\H,4.1986199267,0.1916302792,0.7619939501\H,4.4408364762
,1.7129846075,-0.1381034868\H,-3.7585874881,3.4523990044,0.5993580876\
H,-2.8020814763,3.5190024818,-0.9048574319\H,-3.2140204434,1.943718613
8,-0.2436612894\H,-3.8456296983,-2.5354752009,-0.6004104779\H,-3.89528
4808,-1.9852794593,-2.2945367225\H,-2.4374658655,-2.7908777874,-1.6293
332804\H,-0.3834252849,-1.7370390699,-0.2631571919\H,1.8328692619,-4.4
435507961,0.0001056317\H,2.7830324371,-3.0873819603,0.6387318615\H,2.1
103823666,-4.2978526317,1.7511041547\H,-0.1254543033,-1.2231214455,2.0
962739459\H,0.8987693938,-2.3211137926,3.0514871649\H,1.6371845033,-1.
2067545883,1.8799562202\H,-1.4895709682,-3.2043303382,1.2304278711\H,-
0.6720897848,-4.5512412242,0.4122238688\H,-0.4867951255,-4.3369967034,
2.1686091613\\Version=x86-Linux-G98RevA.11.3\HF=-997.9622322\RMSD=5.70
2e-09\Dipole=3.4667997,1.1848048,-0.1435504\PG=C01 [X(C15H26N2O4)]\\@

8a

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\11-Aug-2003\0\\#P
BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GUE
SS=READ\\cpy7fxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,-0.793
7381338,0.7735609769,-0.4673433385\N,-1.4711665931,1.5223652335,0.4508
201937\C,-0.9839058713,2.7406789237,0.8322502816\C,0.1871457397,3.2281
311624,0.3297027577\C,0.9459945294,2.457642999,-0.609484908\C,0.390479
8099,1.2126756624,-0.9979607621\C,-2.6953389887,1.0226348781,1.1203800
387\O,0.2937800578,-1.962042532,-1.5182352461\C,-0.8198796952,-2.16250
07875,-2.1071936625\C,-0.8313108748,-3.2516757914,-3.1858685862\N,2.12
90032631,2.8952342811,-1.0964359169\C,2.8937383739,2.0519419091,-2.019
19046\C,2.6773180476,4.1831105205,-0.676927201\C,-2.994917263,-0.42907
48918,0.9360415884\O,-3.3117205483,1.8081443344,1.7968133582\O,-1.8963
630007,-1.5533997626,-1.871857548\O,0.0941291708,-1.4968679395,1.14288
77866\C,0.9852565691,-2.4148518512,1.7837311996\C,2.4194935701,-2.1529
038985,1.2887152051\C,0.8705979138,-2.1420353025,3.2863281207\C,0.5632
579762,-3.8565945504,1.4536576217\H,0.5291846502,4.194240535,0.6760685
515\H,0.8775225631,0.5303451966,-1.682419209\H,-1.2413900741,-0.166091
025,-0.8246600839\H,-1.5896776686,3.2674224126,1.5581959919\H,3.618240
7709,4.3552141535,-1.1989416083\H,3.8232642515,2.5600847578,-2.2751212
793\H,2.3326371856,1.8681805852,-2.9422574111\H,3.1371222491,1.0870360
911,-1.5613386826\H,2.8757619697,4.2027297851,0.4018043486\H,1.9959739
259,5.0055429844,-0.9248768851\H,-3.9001729239,-0.6551423664,1.5006003
463\H,-3.1141788495,-0.7111063135,-0.117120863\H,-2.1414446431,-1.0217
471294,1.2985822025\H,-0.7938893086,-4.2367751088,-2.7039858655\H,-1.7
353107998,-3.1942394214,-3.797357874\H,0.0592086473,-3.1703623312,-3.8
179643637\H,0.1447618346,-1.6733705864,0.160091535\H,1.1349907106,-1.1
010700449,3.5056390558\H,-0.1574978289,-2.3107385,3.6265213091\H,1.535
9365599,-2.7968699233,3.8608314726\H,0.5957772034,-4.0124033204,0.3699
596478\H,1.2225114068,-4.5918196715,1.9319372017\H,-0.462261167,-4.037
3593791,1.795117486\H,2.4696539372,-2.2968448109,0.2038870201\H,2.7127
374699,-1.1205434471,1.5148772199\H,3.1419255821,-2.8286222799,1.76334

66236\\Version=x86-Linux-G98RevA.11.3\HF=-997.9627699\RMSD=2.788e-09\D
ipole=2.2622576,3.5807615,0.1553799\PG=C01 [X(C15H26N2O4)]\\@

9b

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\07-Jan-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK
GUESS=READ\\cpy7s2sp1 b3lyp/6-311+G(d,p)//B3LYP/6-31G(d) sp\\0,1\C,-3.
1190734491,-1.0979574722,-0.3157959629\C,-3.3718082202,0.2566141282,0.
0317226854\C,-2.2559866099,1.1348719269,-0.0214353866\C,-1.0172576658,
0.6747775447,-0.4062230714\N,-0.8263816699,-0.6191789072,-0.751284277\
C,-1.8543022561,-1.48625935,-0.6916127396\N,-4.6082432697,0.6863181095
,0.4009685255\C,-5.7195689137,-0.2567684802,0.4781032805\C,0.589625895
2,-1.2411325461,-1.2072775709\O,1.4201967204,-0.6213295689,0.353655159
7\C,2.3907044657,-1.4424510543,1.0658132518\C,2.9371557026,-0.57400628
77,2.2102179673\O,0.5691465349,-2.4548113041,-1.2763467208\C,1.2474349
045,-0.3567731218,-2.2463917816\C,1.6492919385,-2.6588757652,1.6370964
158\C,3.5309878363,-1.8569767521,0.1249396505\C,-4.8209364626,2.083023
0885,0.7701299572\O,1.7778201922,1.7693963034,0.0398838492\C,2.9619166
723,2.2715833125,-0.1880765687\O,4.0177988777,1.6363152592,-0.18528717
45\C,2.9515183513,3.7744282591,-0.4662908488\H,-3.9013803451,-1.844756
7833,-0.29041059\H,-2.3440893487,2.177334719,0.2536920782\H,-0.1444968
333,1.3240200879,-0.4070800584\H,-1.5908811351,-2.5055108551,-0.951354
8878\H,-6.6201150619,0.2777561553,0.7805736041\H,-5.875433564,2.233012
0312,1.0021905125\H,-4.5547634401,2.7566176131,-0.0532302562\H,-4.2324
058064,2.3621609807,1.6532643707\H,-5.5275209478,-1.0471626084,1.21483
3706\H,-5.9131327903,-0.7260833649,-0.4943166859\H,2.2723657988,-0.707
2108816,-2.3802727306\H,0.7053191669,-0.4912771259,-3.1902482263\H,1.2
736074983,0.6971067832,-1.9747457786\H,2.4935428028,4.3075848661,0.374
6936722\H,3.9676983981,4.1410481968,-0.624650492\H,2.3427004621,3.9896
512285,-1.3526015605\H,1.7377791282,0.4593742749,0.232215914\H,0.82686
66679,-2.3297399753,2.2832032924\H,1.2396244559,-3.2826168839,0.840405
592\H,2.3349009209,-3.2654645779,2.2408561517\H,4.0160388093,-0.961891
9237,-0.2769936147\H,4.281689583,-2.4406247016,0.6719099235\H,3.153711
4196,-2.474828191,-0.6955158481\H,3.5029894299,0.2738209098,1.81495624
29\H,2.1163075369,-0.2007051846,2.8330913525\H,3.6035400359,-1.1727393
027,2.8429879995\\Version=x86-Linux-G98RevA.11.3\HF=-997.9394289\RMSD=
6.681e-09\Dipole=-5.4786609,0.379955,0.1890111\PG=C01 [X(C15H26N2O4)]\
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9a

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\25-Sep-2003\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK
GUESS=READ\\cpy7osp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp ts\\0,1\C,-
1.6371117702,1.0246164722,-2.5778734059\C,-1.8471058152,0.8912753944,-
1.1795824469\C,-0.7840740057,0.8041560163,-0.3099156809\N,0.4902441187
,0.8533671671,-0.7655160848\C,0.73268622,0.9665689949,-2.0864966892\C,
-0.2825305003,1.0559277841,-3.0088230016\C,1.7505490743,0.7486950901,0
.1772168344\O,1.0708952596,-0.8716402249,0.9824643895\C,1.7984156183,-
2.1120516851,0.8462784223\C,1.9695247549,-2.4304702874,-0.6470798334\N
,-2.6724074959,1.1143274419,-3.4557001865\C,-4.0496799775,1.0635146078
,-2.9726328605\O,2.7972891973,0.5791892816,-0.4210367641\C,1.617952809
4,1.6543167326,1.3834937071\C,-2.4140119969,1.2341160664,-4.8867977263
\C,3.1612262022,-2.0034490038,1.5519363662\C,0.94095591,-3.2085765663,
1.5049780038\O,0.3834371625,-0.6566172745,3.3049164264\C,-0.7182048553
,-0.0139187702,3.5248636457\C,-1.2099309111,-0.0905430149,4.9653117539
\O,-1.3608115028,0.6341704936,2.679809043\H,-0.0218298293,1.1475996252
,-4.0546826765\H,-2.8423295318,0.845756661,-0.7579046878\H,-0.93553582
6,0.6796094388,0.765113643\H,1.7839736023,0.968347795,-2.3498539171\H,
-3.3645186272,1.3051099292,-5.4158072026\H,-4.7278801642,1.1571905825,
-3.8209744039\H,-4.2587058304,1.8839629014,-2.2754636237\H,-4.26305612
06,0.1141537602,-2.4660501056\H,-1.8723633818,0.3613816738,-5.27330304

12\H,-1.8303438273,2.1348957944,-5.1140556922\H,2.3654386898,1.3498004
891,2.1179330586\H,1.8523983006,2.6733530284,1.0507505843\H,0.63263304
66,1.6403891201,1.8484076463\H,-0.4223143784,0.2482085769,5.6469760562
\H,-2.10573182,0.5190006946,5.0995515295\H,-1.4310889134,-1.1320598374
,5.2247857782\H,0.7227821563,-0.7223418202,2.1104671133\H,0.9895086837
,-2.4699279081,-1.137711086\H,2.582514798,-1.6753309907,-1.1428730618\
H,2.4510991871,-3.4077546311,-0.7732860429\H,3.015585953,-1.7600447539
,2.6103190851\H,3.7095057228,-2.9518301353,1.4922614084\H,3.7703865268
,-1.2207560091,1.0918827902\H,0.7850299511,-2.9987914149,2.5667098025\
H,-0.0397676575,-3.2647479278,1.0190197693\H,1.4313074553,-4.184922098
,1.407813885\\Version=x86-Linux-G98RevA.7\HF=-997.9473244\RMSD=5.186e-
09\Dipole=-2.1546731,0.8753762,-3.548912\PG=C01 [X(C15H26N2O4)]\\@

10g

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\06-Jul-2004\0\
\#P BECKE3LYP/6-311+G(D,P) GEOM=CHECKPOINT GUESS=READ SCF=TIGHT INT=FI
NEGRID\\b3lyp/6-311+G(d,p) nuc26ircr3optsp singlepoint\\0,1\C,0,-0.766
9729536,1.3520313338,-0.1936983763\N,0,-0.5461106565,2.4583286361,-0.9
27177811\C,0,-1.6314049708,3.1359002706,-1.3324729501\C,0,-2.934198846
7,2.7606937445,-1.0436257255\C,0,-3.1701297023,1.5922522201,-0.2765713
577\C,0,-2.0222204636,0.8851999058,0.1546117296\C,0,2.8577555984,2.123
0251257,-0.8755125451\O,0,2.0554161826,3.0407476818,-1.3937921804\N,0,
-4.4363814039,1.1661645896,0.0311590434\C,0,-4.6208484365,-0.015545664
8,0.8643011101\C,0,-5.5897423104,1.9484597325,-0.3821262018\O,0,2.4764
779279,1.1367725486,-0.2559548165\C,0,0.4611514967,-1.9303075337,1.487
7220429\C,0,1.5717975257,-1.1152017455,2.1195494794\C,0,4.3185407707,2
.4213051306,-1.142879378\O,0,-0.7083977872,-1.7113054236,1.7333620359\
O,0,0.7372042998,-2.9776055146,0.6738010071\C,0,1.9718310243,-3.304065
0509,-0.0555814536\C,0,2.219872099,-2.248373617,-1.1377224442\C,0,3.18
42441899,-3.4935261426,0.8661368983\C,0,1.6012676834,-4.6483895874,-0.
6959361646\H,0,-3.7494809531,3.3712872124,-1.4118401257\H,0,-2.0843146
34,-0.0160895674,0.7511731629\H,0,0.1268852656,0.8239900764,0.12299857
11\H,0,-1.4448924862,4.0313995304,-1.9220608746\H,0,-6.5007057286,1.44
08676309,-0.0612531496\H,0,-5.6885991655,-0.2152465107,0.9675956412\H,
0,-4.1955889985,0.1195642436,1.8680233988\H,0,-4.1501556734,-0.8984260
078,0.4152614714\H,0,-5.6320039168,2.057266739,-1.4740966788\H,0,-5.58
62991222,2.9549187329,0.0609099794\H,0,4.9500050961,1.707007258,-0.612
0255776\H,0,4.5159536568,2.35692813,-2.2190646909\H,0,4.5585293189,3.4
426517276,-0.830060686\H,0,1.0999603099,-0.3607816894,2.7507881445\H,0
,2.2099962424,-1.7497783378,2.7413775604\H,0,2.1953659694,-0.608133070
9,1.3783360628\H,0,1.0722498196,2.8110688024,-1.2128630165\H,0,3.60063
98019,-2.5484546662,1.2204094333\H,0,2.9187727807,-4.1133975848,1.7294
098663\H,0,3.9748138713,-4.0113260879,0.3116583531\H,0,0.7010856177,-4
.541327442,-1.3083633626\H,0,2.4181635442,-5.006380184,-1.3317703074\H
,0,1.4032834701,-5.4003418947,0.0749412186\H,0,1.3362521677,-2.1522302
232,-1.7770956163\H,0,2.4543194654,-1.2629997774,-0.7262237499\H,0,3.0
631094643,-2.558483897,-1.7663003991\\Version=x86-Linux-G98RevA.7\HF=-
997.9914622\RMSD=3.264e-09\Dipole=-0.5478256,-0.0806414,-0.2288619\PG=
C01 [X(C15H26N2O4)]\\@

10f

1\1\GINC-CICUM83\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\13-Oct-2003\0
\\#BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECK GUESS=READ\\cp
y7lxsp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp min\\0,1\C,-2.6400055974
,1.8726185995,-1.7629349842\C,-2.7474778726,1.1856280404,-0.5316191242
\C,-1.5978352813,0.7356409073,0.105773387\N,-0.351441173,0.8995715134,
-0.3665626636\C,-0.252938033,1.5357135175,-1.5440883817\C,-1.329195578
8,2.0295317577,-2.2700151537\N,-3.7443517355,2.3599192826,-2.427770151
5\C,-5.0770113046,2.044075384,-1.9396445334\C,-3.5933016513,2.92572396
72,-3.7585580604\O,2.997849669,-0.0185292379,-1.2776821937\C,2.7760536

322,-0.0423973907,-0.0868115327\O,2.4302640381,-1.1586791108,0.6115594
692\C,2.2613462838,-2.47814601,-0.0552456038\C,1.1552366265,-2.3956333
121,-1.1102222608\C,2.8370718143,1.1629474762,0.8205482928\C,3.6058177
923,-2.9207578652,-0.6399258573\C,1.839479864,-3.3930660037,1.09697917
07\O,1.4237614404,-0.6036350959,3.2167677576\C,0.1328311635,-0.8387629
941,3.5066748238\C,-0.2119967743,-0.3897720861,4.9077935199\O,-0.65106
38588,-1.3519420261,2.7307954326\H,-1.1430200029,2.5222723608,-3.21660
98256\H,-3.7099124199,0.9945990812,-0.0724657709\H,-1.6795911209,0.196
8927211,1.0477603325\H,0.756349267,1.6469643987,-1.9373821832\H,-4.563
4382414,3.2848090284,-4.106671664\H,-5.8158201075,2.543864864,-2.56861
60297\H,-5.2160003105,2.4030132252,-0.9126693388\H,-5.2862881205,0.963
6613061,-1.9541788628\H,-3.2153194825,2.1931384101,-4.4878175279\H,-2.
9058450144,3.7803387059,-3.7484300298\H,3.2894889925,0.9222152195,1.78
58609292\H,3.3996343521,1.9538744128,0.3217850338\H,1.8094358916,1.500
7672376,0.9910074464\H,-0.0697751988,0.6926815731,4.9966871929\H,-1.24
77197399,-0.6464206508,5.1320672621\H,0.4583256834,-0.8656749538,5.630
8622462\H,1.6030459414,-0.8723789004,2.2840668527\H,0.249593333,-1.964
7917954,-0.6741503828\H,1.4596250541,-1.7830899649,-1.9597221464\H,0.9
24943787,-3.4063236133,-1.467204227\H,4.378250471,-2.9294847134,0.1371
665123\H,3.5110352582,-3.9386990099,-1.0348086552\H,3.9225071829,-2.26
05779046,-1.4487395004\H,2.5928446806,-3.3901017928,1.8924698084\H,0.8
792704799,-3.0760914802,1.5157402544\H,1.7339889328,-4.4196734969,0.73
05760404\\Version=x86-Linux-G98RevA.7\HF=-997.9910626\RMSD=3.269e-09\D
ipole=-1.3343992,0.5660275,-0.217412\PG=C01 [X(C15H26N2O4)]\\@

10e

1\1\GINC-NODE-31\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIP03\25-Jul-2004\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\opt of end forward
irc after 80Pt of nuc271ots\\0,1\C,0,1.275511,-0.546759,0.294186\N,0,
1.038988,0.745112,0.014723\C,0,2.107034,1.517231,-0.248987\C,0,3.41241
6,1.05177,-0.249343\C,0,3.672236,-0.309349,0.042104\C,0,2.540203,-1.11
3059,0.32271\C,0,-1.243406,3.28255,-0.206623\O,0,-0.176004,3.820148,-0
.448107\N,0,4.945101,-0.820423,0.051658\C,0,5.165175,-2.221475,0.37580
4\C,0,6.079072,0.042754,-0.242432\O,0,-1.387038,1.975269,0.036921\C,0,
-3.020336,-0.901086,1.386128\C,0,-2.151779,-0.412197,2.523843\C,0,-2.5
64412,4.019299,-0.148583\O,0,-4.232839,-0.867506,1.388458\O,0,-2.25389
1,-1.353949,0.367699\C,0,-2.850443,-1.753518,-0.923282\C,0,-3.739947,-
2.985946,-0.727274\C,0,-3.609334,-0.570963,-1.535878\C,0,-1.623601,-2.
100413,-1.770381\H,0,4.214663,1.743996,-0.472607\H,0,2.638581,-2.16554
6,0.55794\H,0,0.397731,-1.154178,0.500391\H,0,1.879927,2.558362,-0.464
439\H,0,6.996721,-0.545784,-0.202355\H,0,6.234449,-2.434037,0.338609\H
,0,4.661716,-2.887401,-0.338149\H,0,4.805012,-2.46704,1.384147\H,0,6.1
68083,0.861767,0.484394\H,0,6.002085,0.483283,-1.245389\H,0,-3.260861,
3.598143,-0.881395\H,0,-3.020977,3.892942,0.838879\H,0,-2.406692,5.079
118,-0.352199\H,0,-2.766305,-0.277567,3.415261\H,0,-1.334937,-1.11046,
2.727631\H,0,-1.711257,0.548459,2.235154\H,0,-0.477482,1.516034,-0.000
773\H,0,-4.517654,-0.348969,-0.973686\H,0,-2.972384,0.319359,-1.539996
\H,0,-3.884294,-0.809934,-2.56976\H,0,-1.049219,-2.909903,-1.307079\H,
0,-1.937041,-2.428262,-2.767329\H,0,-0.970509,-1.229128,-1.880451\H,0,
-3.172337,-3.795406,-0.254369\H,0,-4.60625,-2.752201,-0.106708\H,0,-4.
091542,-3.343209,-1.702107\\Version=x86-Linux-G98RevA.7\HF=-998.001382
6\RMSD=2.217e-09\Dipole=2.6144309,-1.4755253,-0.2066134\PG=C01 [X(C15H
26N2O4)]\\@

10d

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\15-Aug-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\b3lyp/6-31G(d) sing
lepoint\\0,1\C,0,1.719893,0.067881,1.426626\N,0,1.129576,0.934293,0.58
8752\C,0,1.855058,1.346168,-0.465955\C,0,3.151955,0.928443,-0.720116\C
,0,3.780589,0.01314,0.158433\C,0,3.008905,-0.415298,1.266577\C,0,-1.68
4352,2.697498,-0.31167\O,0,-0.89334,2.879238,-1.222084\N,0,5.059957,-0

.433859,-0.050907\C,0,5.668822,-1.366586,0.885097\C,0,5.820869,0.04597
4,-1.194978\O,0,-1.400478,1.987059,0.788385\C,0,-3.580993,-0.560266,0.
765425\C,0,-3.656653,-0.095913,2.202515\C,0,-3.100312,3.225599,-0.2971
35\O,0,-4.285695,-0.130041,-0.127713\O,0,-2.61318,-1.485456,0.617777\C
,0,-2.278233,-2.06232,-0.698376\C,0,-3.472449,-2.864241,-1.226927\C,0,
-1.837268,-0.963953,-1.67141\C,0,-1.104498,-2.986621,-0.362946\H,0,3.6
62716,1.312121,-1.594475\H,0,3.402772,-1.112611,1.995511\H,0,1.123315,
-0.257092,2.276625\H,0,1.346815,2.042552,-1.128243\H,0,6.807117,-0.420
082,-1.189561\H,0,6.676201,-1.609543,0.544394\H,0,5.099138,-2.303181,0
.951805\H,0,5.745188,-0.940302,1.89485\H,0,5.959079,1.135237,-1.163918
\H,0,5.330034,-0.209405,-2.143564\H,0,-3.799694,2.382284,-0.324617\H,0
,-3.288064,3.780829,0.627879\H,0,-3.262287,3.871733,-1.160908\H,0,-4.6
57867,0.289164,2.405871\H,0,-3.406026,-0.900668,2.897824\H,0,-2.932416
,0.716294,2.328806\H,0,-0.461125,1.613464,0.716873\H,0,-2.670793,-0.31
646,-1.946309\H,0,-1.047743,-0.351601,-1.225144\H,0,-1.43801,-1.425797
,-2.581938\H,0,-1.402065,-3.737399,0.376638\H,0,-0.762692,-3.504232,-1
.265687\H,0,-0.267245,-2.410915,0.045024\H,0,-3.778508,-3.621774,-0.49
6669\H,0,-4.320974,-2.210328,-1.435247\H,0,-3.190057,-3.378755,-2.1526
09\\Version=x86-Linux-G98RevA.7\HF=-998.0017487\RMSD=5.412e-09\Dipole=
2.8484715,-1.438008,0.5019869\PG=C01 [X(C15H26N2O4)]\\@

10c

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\06-Feb-2005\0\
\#BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\new29b b3lyp/6-311+G(
d,p)//b3lyp/6-31G(d) sp reopt ircnucback291last\\0,1\C\C,1,1.38582974\
N,2,1.34364273,1,123.76491834\C,3,1.34414736,2,117.14366318,1,0.003870
26,0\C,4,1.38640276,3,123.60746249,2,0.04555797,0\C,5,1.41579445,4,119
.74474441,3,-0.07888721,0\N,6,1.37271059,5,121.93592483,4,-179.9066618
,0\C,7,1.45444116,6,120.02955607,5,0.41717008,0\C,7,1.4546026,6,120.03
438235,5,179.28616664,0\O,3,2.70051417,2,117.02433906,1,179.76124795,0
\C,10,3.44190479,3,88.04638415,2,-178.98799303,0\C,11,1.51133039,10,77
.43654346,3,103.2645005,0\O,11,1.21765991,10,98.74369793,3,-20.0362606
1,0\O,11,1.3441013,10,91.16619441,3,-145.9555329,0\C,14,1.47566912,11,
121.89476923,10,96.15071572,0\C,15,1.53212039,14,109.79666029,11,66.19
582691,0\C,15,1.53094173,14,102.38643715,11,-175.98887835,0\C,15,1.532
7445,14,110.09114787,11,-58.18821897,0\C,10,1.33583293,3,110.55798283,
2,-0.46478559,0\O,19,1.21934152,10,124.29285107,3,0.9894702,0\C,19,1.5
1501122,10,112.10866361,3,-178.94930596,0\H,5,1.08291675,4,118.7882463
3,3,-179.92014766,0\H,1,1.0829457,2,118.91868444,3,179.92453152,0\H,2,
1.08720126,1,121.17112053,6,179.99632408,0\H,4,1.08767657,3,116.067619
03,2,-179.79086828,0\H,8,1.0910176,7,109.18149589,6,-179.74351487,0\H,
9,1.09100916,7,109.17445973,6,-179.94047814,0\H,9,1.09842382,7,111.679
59468,6,60.71114396,0\H,9,1.09867786,7,111.75851408,6,-60.48384142,0\H
,8,1.0987224,7,111.79440823,6,60.77532081,0\H,8,1.09837774,7,111.66993
181,6,-60.43514298,0\H,12,1.09289581,11,111.31830708,10,123.62792751,0
\H,12,1.09144402,11,109.60659188,10,-113.65711534,0\H,12,1.09583813,11
,107.70185843,10,5.00314433,0\H,21,1.09545166,19,109.9964861,10,60.498
62518,0\H,21,1.09072131,19,109.8387621,10,-178.59010144,0\H,21,1.09516
391,19,110.11713987,10,-57.3837015,0\H,10,1.02630143,3,0.84419679,2,43
.07919106,0\H,18,1.09473412,15,110.21808019,14,-48.30089311,0\H,18,1.0
9088151,15,111.40375507,14,72.00028065,0\H,18,1.09608931,15,109.459649
74,14,-167.66441893,0\H,16,1.09570618,15,110.42701441,14,55.1866435,0\
H,16,1.09610234,15,109.63427013,14,174.14199183,0\H,16,1.09122444,15,1
10.98575346,14,-65.72964816,0\H,17,1.09494939,15,110.67503563,14,-58.9
3006626,0\H,17,1.09480791,15,110.62311431,14,61.14102768,0\H,17,1.0952
2721,15,110.15914279,14,-178.90386551,0\\Version=x86-Linux-G03RevB.03\
State=1-A\HF=-998.0036404\RMSD=3.982e-09\Dipole=0.6378633,-0.1244888,-
1.5243423\PG=C01 [X(C15H26N2O4)]\\@

10b

1\1\GINC-CICUM82\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIPSE\29-Nov-2003\0

\\#BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK G
UESS=READ\\cpy7rx2sp1 b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) sp\\0,1\C,-2.
5686418213,0.4904956234,1.4812838655\C,-2.5753051027,0.4824945809,2.89
6780403\C,-1.306716149,0.4796133066,3.5251135349\C,-0.157664231,0.4914
785075,2.7501036634\N,-0.1631730794,0.5019167924,1.4065132193\C,-1.362
0322316,0.5003650775,0.7986772214\N,-3.7443080419,0.4783053265,3.61766
34376\C,-5.0228800934,0.4103685661,2.9272890323\C,-3.703326636,0.38437
61625,5.0687430215\O,2.2380098775,0.5269478761,0.1650502763\C,3.224563
4648,0.5597474288,1.065006898\O,3.0540138568,0.5423974141,2.2723349109
\C,4.590749051,0.6269960329,0.41368491\C,0.9785596848,1.9282495222,-2.
7286607403\C,0.446976425,0.5235578399,-2.8939677964\O,1.3311875225,-0.
2423067035,-3.556972742\C,1.1360505123,-1.696274954,-3.7172474497\C,2.
4137118505,-2.1213622473,-4.4456353905\O,-0.6224694822,0.139992544,-2.
456007598\C,1.0461793433,-2.3645967095,-2.3408530553\C,-0.0988407856,-
1.9676520359,-4.582848112\H,-3.4892299686,0.4846463015,0.9110668646\H,
-1.2100753644,0.4668955345,4.6036376464\H,0.8290070199,0.4912839796,3.
2066409114\H,-1.3474660997,0.5024645125,-0.288809459\H,-5.8287353229,0
.4439499004,3.6620789784\H,-4.7222107989,0.4123986944,5.45812641\H,-3.
1519107016,1.2252195203,5.5085192517\H,-3.2318747308,-0.5485747545,5.4
095953064\H,-5.1299789525,-0.5151001732,2.3432880697\H,-5.1538296946,1
.2602678434,2.245476703\H,1.5670075687,2.2366000345,-3.5962204379\H,0.
1477308192,2.6164582814,-2.562442008\H,1.6298849041,1.9355351499,-1.84
69662632\H,4.6816578944,1.5513965227,-0.1673907311\H,5.367020774,0.597
4808998,1.1793865124\H,4.7195483737,-0.2076466716,-0.2832015526\H,1.33
14421367,0.5040379109,0.6445290686\H,1.8749298397,-2.0352300596,-1.705
2191923\H,0.1088425838,-2.1185629196,-1.8399112926\H,1.1086589144,-3.4
526636271,-2.4570435522\H,-0.0173054191,-1.4418552444,-5.540683192\H,-
0.1727002918,-3.0414671691,-4.7902273752\H,-1.0108752473,-1.6445532641
,-4.0786801987\H,2.5077184637,-1.5930406505,-5.4000604094\H,3.29705140
45,-1.8968740454,-3.8392322578\H,2.3938258611,-3.198010594,-4.64555321
05\\Version=x86-Linux-G98RevA.7\HF=-998.0038513\RMSD=3.902e-09\Dipole=
-1.6222957,-0.2008301,0.2514585\PG=C01 [X(C15H26N2O4)]\\@

10a

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\23-Sep-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECK GUESS=READ IN
T=FINEGRID\\sp nucback341otsircf\\0,1\N,-1.647426876,0.0674097279,2.00
1667782\C,-1.6355062096,0.1417646356,3.3414373101\C,-0.4812594779,0.15
91716349,4.1087638625\C,0.7822023449,0.0931916954,3.4700374194\C,0.763
2896549,0.0131286352,2.0576349015\C,-0.450306412,0.0066726581,1.391102
8106\N,1.9562393323,0.1063936444,4.1795990323\C,3.229215186,0.03944030
58,3.4763409079\C,1.9309856888,0.190860701,5.6305901242\O,-3.784379952
1,-0.030585433,0.3237174792\C,-3.3992952912,-0.2229121223,-0.931902603
8\C,-4.5742876201,-0.272308123,-1.8867381938\O,-2.235669093,-0.3436802
673,-1.2928680172\O,1.7247126056,-0.296601334,-1.1758720007\C,1.141157
402,-0.9846631002,-1.9945381536\O,0.8843279462,-0.6298155146,-3.264959
494\C,1.1505642919,0.7313698944,-3.7663777536\C,0.5929529628,0.6713460
622,-5.1909828946\C,0.5664384942,-2.3517825984,-1.7051813463\C,0.38075
16995,1.756380634,-2.9260425382\C,2.6594251849,0.9969564565,-3.7815965
904\H,0.7071651941,-3.0280112246,-2.5525133331\H,1.0268075366,-2.76197
4096,-0.8048081155\H,-0.5102936534,-2.2303637376,-1.5395985415\H,-4.22
26332109,-0.4674421302,-2.900661229\H,-5.2769425698,-1.0529103154,-1.5
769805046\H,-5.1157549006,0.6795037899,-1.8583737739\H,-0.6618249829,1
.4424402577,-2.811434798\H,0.8197612225,1.8654856873,-1.9331537836\H,0
.4019882696,2.7304945461,-3.4283805346\H,3.1781993291,0.2270894412,-4.
3637935376\H,2.8569181741,1.9678712998,-4.25057488\H,3.0647503836,1.00
73759618,-2.7685197934\H,1.0955721572,-0.1105372651,-5.7698694374\H,-0
.4795249997,0.4529749873,-5.1749009856\H,0.7461934167,1.6306577641,-5.
6968210856\H,-2.6078676455,0.1901457501,3.8278131027\H,-0.479045066,-0
.0505204791,0.3084629802\H,1.666403988,-0.0484704172,1.4642220619\H,-0
.568648854,0.2219325283,5.1864467636\H,-2.9763325703,0.0047112153,0.94

80292311\H,1.403977838,-0.6624960534,6.0794318012\H,2.9546652943,0.190
3848129,6.0078879818\H,1.4428639138,1.1125324828,5.976489399\H,3.32491
91296,-0.8885142968,2.8971052949\H,3.355535159,0.8839348155,2.78619490
33\H,4.0415608038,0.070837247,4.2040058031\\Version=x86-Linux-G98RevA.
11.3\HF=-998.0041845\RMSD=3.094e-09\Dipole=1.0687201,0.0610496,1.11548
46\PG=C01 [X(C15H26N2O4)]\\@

base catalysis (concerted)

11c

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\19-Sep-2004\0\\#P
BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GUE
SS=READ\\sp after freq\\0,1\C,0.4514584062,-0.684456158,-1.9805028916\
N,0.4074986475,-0.3741573541,-0.6701340764\C,1.5554841857,-0.051328952
5,-0.0366689716\C,2.7728971187,-0.0654105271,-0.6831109884\C,2.8574019
605,-0.4260809156,-2.0521621082\C,1.6257224654,-0.7185402783,-2.698775
2379\C,0.0198079525,2.0353016978,2.3469276844\O,1.1941871045,2.2927032
414,2.1269588994\N,4.0478417619,-0.4847770509,-2.7107808766\C,4.090808
9373,-0.8582527306,-4.1199468167\C,5.2885038938,-0.1725490046,-2.00793
5913\O,-0.4572132335,0.8555066737,1.9198895802\C,-1.8973295367,0.37925
44647,2.1217125352\C,-1.8138365552,-0.6679335636,3.222120319\C,-0.8864
251864,2.9925648591,3.0914030592\O,-2.792493653,1.2042660819,2.0283556
026\O,-1.7761778433,-0.7059073451,0.6749189306\C,-2.9841762237,-0.9696
596303,-0.051373315\C,-4.1548345639,-1.2962733619,0.8984402\C,-3.35045
74204,0.237971123,-0.9362068098\C,-2.7328676499,-2.2222353825,-0.91401
15978\H,3.650110243,0.2154692915,-0.1160135838\H,1.5831379945,-0.97283
44279,-3.7495089746\H,-0.4988939786,-0.9067354635,-2.4502306897\H,1.45
5681322,0.2647650015,0.9935019406\H,6.127262307,-0.2995399375,-2.69272
26817\H,5.1294918769,-0.8852308619,-4.4500200342\H,3.5524881925,-0.136
0912386,-4.747328719\H,3.6569122575,-1.8527338742,-4.2838196869\H,5.44
1932481,-0.8421389189,-1.1524966298\H,5.2970086939,0.8625737313,-1.644
3959654\H,-1.722202458,3.2946237775,2.4576280849\H,-1.3266335781,2.513
3030827,3.9714616817\H,-0.2901731833,3.8545974315,3.3947218438\H,-1.62
43475239,-0.1560477911,4.1743926842\H,-2.7644961401,-1.1978173008,3.30
17166263\H,-1.0108565768,-1.3819279565,3.0350641988\H,-0.579756013,-0.
4448999504,-0.0900126107\H,-3.5029772103,1.1182001719,-0.3079304619\H,
-2.5411317666,0.4603198134,-1.6447641324\H,-4.2617477511,0.0495925098,
-1.5183818141\H,-2.4088066075,-3.0557846811,-0.2816770705\H,-3.6457474
544,-2.5213306072,-1.4434084859\H,-1.9586202799,-2.0564526523,-1.67094
66112\H,-3.9115251737,-2.1683280133,1.5163619763\H,-4.3811060944,-0.45
02928373,1.5489021731\H,-5.0517521434,-1.5394965169,0.3158726247\\Vers
ion=x86-Linux-G98RevA.7\HF=-997.9294911\RMSD=2.948e-09\Dipole=3.087215
7,-1.3927641,-2.9632015\PG=C01 [X(C15H26N2O4)]\\@

11b

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\05-Jul-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT GEOM=CHECKPOINT GUESS=READ INT=FI
NEGRID\\singlepoint 1st order saddlepoint nuc26 b3lyp/6-31G(d)\\0,1\C,
-1.7876888929,-1.5675866049,0.1476747629\N,-0.9110327289,-0.5568381175
,0.0338008024\C,-1.3397752535,0.7136921814,-0.1026628572\C,-2.68694060
57,1.002731054,-0.14690772\C,-3.6499572225,-0.0337546347,-0.0307835591
\C,-3.1480781617,-1.3560774867,0.1215401723\C,2.3822280263,2.151705156
8,-0.4620750985\O,1.2602285496,2.0949957329,-0.9423798675\N,-4.9887217
097,0.2225692984,-0.0615467111\C,-5.9486436901,-0.8644214452,0.0890986
295\C,-5.4677111596,1.5942903349,-0.1955999208\O,2.8989643664,1.369884
7292,0.4776597787\C,2.0236973948,0.4124834789,1.3239441825\C,3.0267333
131,-0.185750145,2.3008435209\C,3.4075292818,3.1768026003,-0.926722648
1\O,0.9446306396,0.848516816,1.7116050819\O,1.6668182201,-0.8197600079
,0.1952030499\C,2.4815893126,-1.6943583589,-0.5905116395\C,3.736883698
6,-1.0014920815,-1.1504772236\C,2.8809311273,-2.9330246758,0.237157502

3\C,1.6063066597,-2.1411359319,-1.7786738753\H,-2.984403987,2.03620417
51,-0.2624612742\H,-3.8098940024,-2.2054685072,0.2235906403\H,-1.36226
44889,-2.5582006291,0.2678222024\H,-0.547622893,1.4530602615,-0.173301
1455\H,-6.5579717037,1.5916245142,-0.2022661439\H,-6.9588908982,-0.458
7186923,0.0302035598\H,-5.8400007534,-1.3693961713,1.0578953569\H,-5.8
370293024,-1.6121849412,-0.7063964461\H,-5.1223587215,2.0487330864,-1.
132434044\H,-5.131648553,2.2223979393,0.6392044084\H,3.6996389801,3.81
88403044,-0.0885684133\H,4.3138936541,2.6731534343,-1.2794987631\H,2.9
850816527,3.7851963331,-1.7285679623\H,3.2827139328,0.5859329761,3.034
8538848\H,2.5463165763,-1.0171466264,2.8222519801\H,3.9455691193,-0.53
14020693,1.8236153883\H,0.172052969,-0.7204497669,0.1007391934\H,3.541
7900871,-2.6632542183,1.0660077942\H,1.9859686727,-3.4045316808,0.6602
170391\H,3.4004114098,-3.6760612178,-0.3812810764\H,1.2628601796,-1.26
6090791,-2.3407038062\H,2.1636003422,-2.796559193,-2.4589320771\H,0.72
60859633,-2.6966523314,-1.4307178361\H,3.4574666035,-0.159501121,-1.79
08297381\H,4.3822693236,-0.6212628987,-0.3555023884\H,4.3168897329,-1.
7120992457,-1.7524886876\\Version=x86-Linux-G98RevA.7\HF=-997.9328206\
RMSD=3.885e-09\Dipole=-3.6604051,-0.9240785,-0.6695756\PG=C01 [X(C15H2
6N2O4)]\\@

11a

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\19-Sep-2004\0\\#P
BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID GEOM=CHECK GUE
SS=READ\\sp after freq\\0,1\C,0.3687431323,-0.1493721464,-2.1218139509
\N,0.3597936975,-0.1117567084,-0.77608778\C,1.5298894281,-0.1078218677
,-0.1026964164\C,2.7400121917,-0.117268535,-0.7664880346\C,2.786115961
2,-0.1294190579,-2.1851899975\C,1.5330723601,-0.15849826,-2.8555038684
\C,0.0291489556,-0.6927630421,3.0907618362\O,1.2356856549,-0.482173008
8,3.0636610632\N,3.9630328756,-0.1164699707,-2.8711718941\C,3.96086034
96,-0.0780695867,-4.3291821345\C,5.2320375183,-0.1143538947,-2.1506333
243\O,-0.6195982905,-0.8203721638,1.9276289957\C,-2.1528917239,-0.7369
522851,1.778708675\C,-2.6077700288,-2.1116258173,1.3196595364\C,-0.720
6788406,-0.8455276845,4.3965032598\O,-2.7588229722,-0.0678772316,2.601
7492395\O,-2.0139846887,0.0339802504,0.1685979431\C,-2.7003376521,1.27
79873956,-0.0440278342\C,-4.2056552506,1.1035831919,0.2313215742\C,-2.
0985763186,2.3920981772,0.8329651231\C,-2.5261731361,1.6419497011,-1.5
315415867\H,3.6445496086,-0.1118456508,-0.1727813799\H,1.4670128431,-0
.1880713873,-3.9347707667\H,-0.6050477919,-0.1656725704,-2.5970248255\
H,1.4679978499,-0.1201129755,0.9846521453\H,6.0500618182,-0.136754941,
-2.8710707617\H,4.9895981197,-0.028532076,-4.6864736533\H,3.4276866752
,0.8041759618,-4.705845968\H,3.4943497244,-0.9745979253,-4.7575096771\
H,5.3245764779,-0.9948582595,-1.5032380898\H,5.3444190556,0.7849945319
,-1.5317289474\H,-1.3917422443,0.0040439471,4.5387634736\H,-1.34912227
45,-1.7411727462,4.392491231\H,0.0102017895,-0.8991362731,5.2051665748
\H,-2.5773204007,-2.7958555077,2.1766707851\H,-3.6396383611,-2.0431881
017,0.966848186\H,-1.9761523586,-2.508294068,0.5230117945\H,-0.6614594
119,-0.0352546077,-0.2570972088\H,-2.2242925158,2.1483247064,1.8890291
881\H,-1.0260059439,2.4980348864,0.6262084244\H,-2.5779044854,3.358092
5809,0.6288504565\H,-2.8639342202,0.8140615292,-2.1671406178\H,-3.1212
365814,2.5275389548,-1.7841715618\H,-1.4820640563,1.8712241735,-1.7733
655533\H,-4.6117315204,0.3123491171,-0.4106138158\H,-4.3802514523,0.83
33736451,1.2730023565\H,-4.7453556606,2.0325793092,0.0088008536\\Versi
on=x86-Linux-G98RevA.7\HF=-997.9336092\RMSD=2.581e-09\Dipole=2.9991534
,-0.1769955,-3.6376531\PG=C01 [X(C15H26N2O4)]\\@

base catalysis (stepwise)

16

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\12-Sep-2004\0\\#P
BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID GEOM=CHECKPOINT GUESS=R
EAD\\singlepoint guess input nucback352ots becke3lyp/6-311+G(d,p)\\0,1

\C,-2.2798947366,0.2711182294,-2.6928824749\C,-2.2884298164,0.2685943001,-1.3195451907\N,-1.1337755779,0.2677555189,-0.626296829\C,0.0784774837,0.257910537,-1.2255861961\C,0.1453446998,0.256089868,-2.6028604749\C,-1.0362216454,0.267769706,-3.3923451809\N,-0.9911409808,0.2709568715,-4.7528289258\C,0.2964882831,0.2643647258,-5.4416978692\C,-2.2239731401,0.280437491,-5.5334360629\O,1.3164261123,0.3114499619,1.1972744993\C,2.1784948454,1.3352022488,1.5523559581\C,3.3686942439,1.4308174663,0.5597692962\C,1.4278351935,2.6934721764,1.557231482\C,2.7591053956,1.0908228468,2.9694469376\O,-2.0892497973,0.122702724,2.0299982541\C,-1.3316661542,-0.543997044,2.712626161\C,-1.0215210959,-0.227774912,4.1475156922\O,-0.7662788403,-1.6283236397,2.1102070175\C,0.3278027769,-2.3531132461,2.6407065547\O,0.406469285,-2.6349334982,3.8057585226\C,1.2914527544,-2.6432779112,1.5443750592\H,1.1244078643,0.2461692623,-3.063863712\H,-3.22515601,0.2753065068,-3.217997666\H,-3.1977329328,0.2651664007,-0.7297950141\H,0.8993777004,0.2660595839,-0.4496875804\H,0.1245128473,0.2726543033,-6.5181097784\H,-1.9736836976,0.2811740963,-6.5943709927\H,-2.8251115839,1.1746220308,-5.3255134496\H,-2.8367284855,-0.6068652234,-5.3295506642\H,0.8781337252,-0.6322535212,-5.1945517136\H,0.8932113045,1.1477266398,-5.1834428336\H,0.0451022563,-0.0062466135,4.2464093928\H,-1.6090560946,0.6456251528,4.432882402\H,-1.2378762372,-1.0792848551,4.7949213134\H,2.072908563,-3.3181286107,1.8968030985\H,0.7769973024,-3.0614469447,0.6731646095\H,1.6840691706,-1.6393272646,1.2635378641\H,-1.1662611921,0.2699528542,0.4034823142\H,1.9500839416,1.0662872404,3.7107414427\H,3.2703933034,0.1209330554,3.0000162697\H,3.4740798465,1.8656325997,3.2809689441\H,3.0010069731,1.6434221761,-0.4536631666\H,4.0913277468,2.216113096,0.8238910801\H,3.9002046215,0.4716171059,0.5285695932\H,1.0514043471,2.9202311953,0.5505939081\H,0.5620757362,2.6300460489,2.2279758857\H,2.0558562913,3.5360436723,1.8805202395\\Version=x86-Linux-G98RevA.11.3\HF=-997.9169912\RMSD=1.308e-09\Dipole=-1.9927109,-0.1609986,-4.6091906\PG=C01 [X(C15H26N2O4)]\\@

15

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\29-Aug-2004\0\\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) GEOM=CHECKPOINT GUESS=READ\\sp b3lyp/6-311+G(d,p)\\0,1\N,0.9676104549,-1.4418369878,-0.7323932839\C,0.9466006405,-0.1673495626,-0.265730245\C,2.1379485475,0.4254728675,0.10036249\C,3.3738942543,-0.2637930099,-0.0016806849\C,3.3229465514,-1.5990524882,-0.5025318161\C,2.1142040213,-2.14574401,-0.8518745688\N,4.5518413124,0.3127940585,0.358836486\C,4.5693634133,1.6833902424,0.8654875398\C,5.8043103585,-0.4259818806,0.2382066043\O,-1.5467376946,-2.3216261706,-1.5289978088\C,-3.6361725339,-1.1921489746,-1.1818783389\O,-2.0150640495,-1.8526035583,0.5630782825\C,-2.8067139251,-1.2926440129,1.6006647154\O,-3.985049462,-1.5043959099,1.6794405828\C,-1.942075348,-0.4672803275,2.4869345773\O,-1.5568191355,1.0548347857,-0.0420122181\C,-1.7154469333,2.3761611346,-0.4251640837\C,-3.072634665,2.9214836618,0.0876860218\C,-0.5879386523,3.2697849778,0.1629411727\C,-1.6821244569,2.5038951446,-1.9714006788\H,2.0894408215,1.4418275656,0.4693235361\H,4.2160600412,-2.1982932556,-0.6158078989\H,2.0221368179,-3.1558902908,-1.2353237744\H,-0.0655442158,0.3674191823,-0.2120607277\H,5.5974404665,1.9642120682,1.0945041943\H,6.6245605305,0.2052485933,0.5801028568\H,6.0058447612,-0.7107105897,-0.8023561829\H,5.7962751356,-1.3348373724,0.8531937227\H,3.9749266098,1.7780823005,1.782178524\H,4.1771703461,2.3890732262,0.1234171299\H,-3.4871963698,-0.1264464017,-0.9570993282\H,-3.7588020716,-1.3403903962,-2.2551277954\H,-4.4979848649,-1.5583166882,-0.6243976289\H,-2.4948982254,-0.1632787923,3.3769922876\H,-1.029783238,-1.0082815695,2.7577855603\H,-1.661495671,0.3976571692,1.8456052036\H,0.0663878261,-1.8828256848,-0.9983958517\H,-3.8954870598,2.3184734341,-0.3160553065\H,-3.1141062931,2.8493695862,1.1814927966\H,-3.2486431988,3.9693317912,-0.19432477\H,0.389554773,2.9556487794,-0.2295914302\H,-0.7120175556,4.3352368376,-0.0773013495\H,-0.5661175525,3.1653408496,1.2550908446\H,-0.7261153445,2.1282775174,-2.3593326984\H,-2

.4798254723,1.894831321,-2.4139967575\H,-1.8083539102,3.538515472,-2.3
215044512\C,-2.3628657265,-1.8471349829,-0.7527200097\\Version=x86-Lin
ux-G98RevA.7\HF=-997.9197832\RMSD=3.387e-09\Dipole=4.9839883,-0.900054
5,0.2993628\PG=C01 [X(C15H26N2O4)]\\@

14

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\31-Aug-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\estimated ts von de
m intermediat zum Edukt\\0,1\N,0,-1.185956,-1.058481,-0.643646\C,0,-1.
319101,-0.010775,0.204747\C,0,-2.576793,0.399472,0.590601\C,0,-3.74007
7,-0.258594,0.107367\C,0,-3.533781,-1.353313,-0.783475\C,0,-2.25574,-1
.718924,-1.129557\N,0,-4.990303,0.131992,0.472242\C,0,-5.168643,1.2702
33,1.370753\C,0,-6.163412,-0.562202,-0.050196\O,0,1.402324,-1.671049,-
1.119408\C,0,1.637345,-1.754064,1.281927\O,0,3.419738,-1.230144,-0.361
835\C,0,4.417064,-0.832882,0.528631\O,0,5.541369,-1.155593,0.246616\C,
0,4.039131,0.016575,1.715233\O,0,1.397606,0.819242,0.324551\C,0,1.5526
89,1.919841,-0.524298\C,0,3.046757,2.252598,-0.762752\C,0,0.903083,1.6
66976,-1.911734\C,0,0.88229,3.156474,0.126253\H,0,-2.649677,1.242709,1
.264798\H,0,-4.36299,-1.907336,-1.20172\H,0,-2.049496,-2.5433,-1.80324
9\H,0,-0.33774,0.460768,0.47749\H,0,-6.234131,1.42735,1.53836\H,0,-7.0
61542,-0.107688,0.367822\H,0,-6.158509,-1.623068,0.229316\H,0,-6.22186
6,-0.48893,-1.143597\H,0,-4.749696,2.188637,0.941795\H,0,-4.692295,1.0
90461,2.342145\H,0,1.52427,-0.852851,1.882748\H,0,0.677595,-2.272581,1
.22527\H,0,2.362247,-2.427633,1.752419\H,0,3.885875,-0.625299,2.590907
\H,0,4.888968,0.668333,1.9312\H,0,3.125666,0.588141,1.510004\H,0,-0.20
2426,-1.341219,-0.902466\H,0,3.54354,2.495991,0.183861\H,0,3.560655,1.
396062,-1.212361\H,0,3.172693,3.111671,-1.435408\H,0,-0.181672,1.5237,
-1.817048\H,0,1.06189,2.505982,-2.603012\H,0,1.325574,0.762914,-2.3628
39\H,0,-0.193898,2.982457,0.262723\H,0,1.319269,3.334562,1.116004\H,0,
1.000476,4.069116,-0.474859\C,0,2.077979,-1.403608,-0.126812\\Version=
x86-Linux-G98RevA.11.3\HF=-997.9039091\RMSD=4.086e-09\Dipole=-6.378775
,-0.593096,1.1889745\PG=C01 [X(C15H26N2O4)]\\@

13c

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\24-Aug-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID GEOM=CHECKPOINT GUES
S=READ\\sp b3lyp/6-311+G(d,p) intermediat von TS zum Edukt\\0,1\N,-1.5
807985532,-0.0217549337,-0.1838099708\C,-2.3831045719,0.9311443657,0.3
158517603\C,-3.7670970325,0.8584638323,0.3321424744\C,-4.4129355352,-0
.2813301425,-0.2068724789\C,-3.5631659076,-1.2830530233,-0.7364934185\
C,-2.1899401219,-1.1029145008,-0.6983582943\N,-5.7775832454,-0.4070142
75,-0.2154456353\C,-6.6112051879,0.6572517456,0.3237057641\C,-6.396792
2235,-1.5908905541,-0.7933057591\O,1.1172648593,-0.4186424259,-0.77318
07149\C,1.3783924968,-1.1706564721,1.5021989971\O,3.0731149056,-1.2635
512032,-0.2852047304\C,4.2985585037,-1.5064428845,0.2542883194\O,5.120
7585619,-2.0517973574,-0.4463012467\C,4.5932598617,-1.1477077922,1.699
2182709\O,2.4567548268,0.7794497694,0.7289333389\C,2.7448475569,1.8882
561809,-0.1850143228\C,3.4993757705,1.4592372638,-1.4502852113\C,1.434
2173297,2.6087335293,-0.5403781217\C,3.6248780075,2.8082073993,0.67133
76695\H,-4.3310062632,1.6790609755,0.7576383944\H,-3.9620161371,-2.189
1762112,-1.1748727601\H,-1.52954828,-1.8656582938,-1.1054913391\H,-1.8
846523109,1.8067224382,0.7265927133\H,-7.6598776945,0.3718519275,0.231
5060781\H,-7.4804885451,-1.5096785504,-0.6998454081\H,-6.0799362925,-2
.5060352821,-0.2757608299\H,-6.1542911271,-1.6984390669,-1.8592659798\
H,-6.4671678417,1.6019863931,-0.2181102508\H,-6.4011005121,0.836592578
6,1.3865832535\H,2.0449664772,-1.1646751521,2.3650874574\H,0.457293280
1,-0.6510986903,1.7803587448\H,1.1365399406,-2.2026031722,1.2342683139
\H,4.1843813558,-1.9237758488,2.3569438259\H,5.6776536773,-1.138860404
8,1.8217208408\H,4.1641015784,-0.1880272245,1.9873900613\H,0.215747716
7,-0.1558144072,-0.4476095822\H,4.4520988527,0.9797557061,-1.206242200
8\H,2.9097690513,0.7666294949,-2.0525078062\H,0.8736997602,2.838169351

6,0.3732882319\H,3.7152149848,2.3506044369,-2.0516392141\H,1.650216253
3,3.5532448674,-1.053850763\H,0.8102771017,1.9962983389,-1.1933993954\
H,3.1058941308,3.0864345758,1.5948388258\H,4.5612950114,2.3083372554,0
.9402128637\H,3.8695404685,3.7235908229,0.1214139923\C,1.998531508,-0.
4729193909,0.2888923508\\Version=x86-Linux-G98RevA.7\HF=-997.9527541\R
MSD=5.228e-09\Dipole=-4.3128113,0.9111732,1.0934453\PG=C01 [X(C15H26N2
O4)]\\@

13b

1\1\GINC-MAX\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\25-Jul-2004\0\\#P
BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID\\opt b3lyp/6-31G(d) nuc
back291ircr\\0,1\N,0,1.363978,-0.780262,0.25246\C,0,2.310487,-1.675728
,0.573668\C,0,3.672351,-1.462554,0.428925\C,0,4.130829,-0.227014,-0.08
9437\C,0,3.128913,0.713456,-0.428155\C,0,1.792105,0.395439,-0.243656\N
,0,5.466207,0.041719,-0.25279\C,0,6.459225,-0.962592,0.094429\C,0,5.88
9095,1.321214,-0.80227\O,0,-1.35358,-1.320293,0.335381\C,0,-2.039014,-
0.220743,0.780338\C,0,-1.849411,0.012392,2.279191\O,0,-1.40454,0.90503
8,0.026864\C,0,-1.699613,2.224929,0.066894\O,0,-0.933389,2.992411,-0.4
79427\C,0,-2.953437,2.713147,0.768533\O,0,-3.395211,-0.313738,0.531389
\C,0,-3.956125,-0.94264,-0.672282\C,0,-3.232063,-0.525719,-1.958165\C,
0,-3.956705,-2.467472,-0.493073\C,0,-5.396964,-0.416742,-0.679061\H,0,
4.361025,-2.247756,0.715248\H,0,3.380173,1.68625,-0.832088\H,0,1.01839
,1.115119,-0.499155\H,0,1.954106,-2.624175,0.971345\H,0,7.455724,-0.56
3284,-0.099502\H,0,6.97859,1.346837,-0.851467\H,0,5.557579,2.15995,-0.
175774\H,0,5.498433,1.478047,-1.816881\H,0,6.338688,-1.878656,-0.50026
6\H,0,6.404963,-1.236038,1.156914\H,0,-2.423301,0.867643,2.641736\H,0,
-2.187017,-0.882944,2.807376\H,0,-0.787807,0.170759,2.488276\H,0,-2.69
0742,3.036535,1.782691\H,0,-3.314527,3.592773,0.230805\H,0,-3.728939,1
.950893,0.830832\H,0,-0.369351,-1.115403,0.331177\H,0,-3.2532,0.560354
,-2.091757\H,0,-2.192332,-0.855133,-1.952742\H,0,-3.740551,-0.981698,-
2.815962\H,0,-4.441092,-2.733315,0.452922\H,0,-4.517277,-2.939586,-1.3
08867\H,0,-2.939983,-2.860987,-0.485989\H,0,-5.901107,-0.667057,0.2601
7\H,0,-5.415186,0.671536,-0.801045\H,0,-5.960833,-0.86444,-1.504623\\V
ersion=x86-Linux-G98RevA.7\HF=-997.9607504\RMSD=5.624e-09\Dipole=1.971
7789,-0.4601711,0.3780349\PG=C01 [X(C15H26N2O4)]\\@

13a

1\1\GINC-NODE-24\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIP03\12-Aug-2004\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID GEOM=CHECKPOINT GUE
SS=READ\\reverse irc freq\\0,1\O,-1.3405355744,-0.4151001322,-0.317405
5219\C,-2.1783342584,0.0869019909,0.6348466372\C,-1.5589674873,0.26338
64654,2.0174115415\O,-2.7100331419,1.4380295532,0.1837999671\C,-1.8737
593357,2.4273259644,-0.1445056746\O,-0.6603960946,2.4005489643,-0.0355
182278\C,-2.6391947559,3.6215025823,-0.681018673\O,-3.3176706261,-0.67
12187445,0.7946471765\C,-3.9990322539,-1.3575063433,-0.3021606606\C,-4
.1155679467,-0.5085128107,-1.5748790994\C,-3.2892304655,-2.6906258636,
-0.5830132504\C,-5.3916276233,-1.6139285437,0.2877640373\H,-2.30959818
55,0.6592544981,2.7055679304\H,-1.2281072495,-0.7143997019,2.378485121
3\H,-0.7069508764,0.9422780876,1.9681578138\H,-3.4397511241,3.90407088
21,0.009581647\H,-1.9555953112,4.4590336469,-0.8284393737\H,-3.1089420
969,3.3595788756,-1.6356013992\H,-4.6142524527,0.4414911746,-1.3642422
129\H,-3.1339991595,-0.3012286888,-2.0052834593\H,-4.711164431,-1.0566
8285,-2.314830701\H,-3.1854242486,-3.2621761642,0.345956902\H,-3.87577
41959,-3.2898452362,-1.2900276793\H,-2.2957287144,-2.5217398199,-1.001
0221138\H,-5.3128150288,-2.1859129072,1.2181519145\H,-5.8932373864,-0.
666385587,0.5095739447\H,-6.0091853036,-2.1808550384,-0.4177146346\C,2
.1656591869,0.9573962827,-0.0806154787\C,2.0131310918,-1.3201884778,-0
.0001373986\H,1.6361098662,1.9044569767,-0.1234941274\C,3.3905036933,-
1.4758437031,0.0256297242\H,1.3684376915,-2.1969102899,0.0194564925\C,
4.2192533013,-0.32819484,-0.0015865715\H,3.8067537247,-2.4748405728,0.
0648370131\C,3.5519395058,0.9187968138,-0.0597095568\H,4.10194417,1.85

12896751,-0.0897945883\N,1.3858845793,-0.1358539872,-0.0504201078\H,-0
.3928342219,-0.1210815468,-0.177156352\C,6.4008418671,0.7844410357,-0.
0436302482\C,6.2299278425,-1.725721219,0.0420412795\H,6.1860466195,1.4
639855182,0.7914551448\H,7.4551366033,0.5092373462,0.0103230423\H,6.23
91726994,1.3343756608,-0.9814181385\H,5.934779801,-2.3100952461,0.9236
555349\H,5.9860076297,-2.3137749889,-0.8540371979\H,7.3122691222,-1.59
28812115,0.075086017\N,5.5887627611,-0.4203882445,0.0275582023\\Versio
n=x86-Linux-G98RevA.7\HF=-997.9697288\RMSD=4.987e-09\Dipole=2.3902056,
-0.2244851,-0.1062186\PG=C01 [X(C15H26N2O4)]\\@

12c

1\1\GINC-NODE-29\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\ZIP03\15-Aug-2004\0
\\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT GEOM=CHECKPOINT GUESS=READ INT=F
INEGRID\\b3lyp/6-311+G(d,p) singlepoint\\0,1\C,1.4603961318,-0.4211260
171,-0.2551439321\N,1.1763621251,0.8828949814,-0.0532469321\C,2.155722
1205,1.7686649864,0.2043670679\C,3.4762871225,1.3894109933,0.275390067
9\C,3.8283671295,0.0250859951,0.0722260679\C,2.7617941341,-0.873264010
4,-0.1969769321\N,5.1226801317,-0.3940999982,0.1338100679\C,5.44738013
89,-1.8018349966,-0.0763109321\C,6.1914541268,0.5574230073,0.416996067
9\O,-1.2037258802,1.9101889691,-0.1665399321\C,-2.0066628769,1.2653909
649,-0.8867759321\O,-2.99883487,-0.0735780402,0.0052670679\C,-3.108127
8687,-0.3251780407,1.4086420679\C,-3.7840318616,-1.6976650442,1.576046
0679\C,-3.1672118808,2.014885959,-1.5093659321\O,-1.4886458715,0.21798
09676,-1.6455879321\C,-2.0122078649,-1.0621860351,-1.1467819321\C,-3.1
059348621,-1.6031600407,-2.0529439321\O,-1.1932918609,-1.8298120309,-0
.6312869321\C,-1.7442018687,-0.3223440337,2.1285780679\C,-4.0038188744
,0.7860389546,1.9827740679\H,4.2236451186,2.1426609971,0.4848360679\H,
2.9421451396,-1.9270640095,-0.3616179321\H,0.5956741351,-1.0632590216,
-0.4517229321\H,1.8385651152,2.7956709848,0.3504280679\H,7.1452481295,
0.0297520122,0.4259910679\H,6.5262151396,-1.934430991,0.0070020679\H,5
.1377881407,-2.1402299982,-1.0728639321\H,4.9650251422,-2.4413269991,0
.6734080679\H,6.0576501243,1.0341300066,1.3964500679\H,6.2449111227,1.
3426070076,-0.3479159321\H,-3.9107318773,1.3415729551,-1.9345909321\H,
-3.6375728841,2.6553719565,-0.7598839321\H,-2.7668628841,2.654431961,-
2.3068109321\H,-2.6337528601,-1.9814930383,-2.9680379321\H,-3.60696485
78,-2.4377600433,-1.5558849321\H,-3.842878866,-0.8455290445,-2.3216009
321\H,0.1400661232,1.238863976,-0.1095959321\H,-1.0983058647,-1.100341
0304,1.7157080679\H,-1.2531038737,0.6472899688,2.0117520679\H,-1.88160
08677,-0.5124250344,3.2009910679\H,-4.9727678745,0.7963339496,1.471411
0679\H,-4.1789728737,0.6362679537,3.0558460679\H,-3.5303028795,1.76433
19571,1.8461450679\H,-4.7528168615,-1.7093540492,1.0640060679\H,-3.152
2808576,-2.481093041,1.1468070679\H,-3.9505428604,-1.9256390451,2.6366
640679\\Version=x86-Linux-G98RevA.7\HF=-997.9131438\RMSD=3.268e-09\Dip
ole=4.6044321,0.3790093,0.3810079\PG=C01 [X(C15H26N2O4)]\\@

12b

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\23-Nov-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=(DIRECT,TIGHT) INT=FINEGRID\\sp\\0,1\N,
0,1.163375,-0.56997,0.356072\C,0,2.023315,-1.561492,0.646673\C,0,3.383
552,-1.445965,0.455456\C,0,3.916359,-0.237692,-0.069969\C,0,2.981624,0
.788559,-0.364247\C,0,1.63308,0.591629,-0.143019\N,0,5.254696,-0.07488
3,-0.279134\C,0,6.183964,-1.150196,0.044242\C,0,5.762908,1.183569,-0.8
14153\O,0,-1.229731,-1.18649,0.733712\C,0,-2.068796,-0.227581,0.960806
\C,0,-2.181979,0.272495,2.396477\O,0,-1.280359,1.073771,0.16714\C,0,-1
.59889,2.336951,-0.039578\O,0,-0.770111,3.107784,-0.518904\C,0,-2.9906
81,2.829055,0.332789\O,0,-3.337286,-0.324646,0.431161\C,0,-3.635002,-1
.138932,-0.746231\C,0,-2.698439,-0.827748,-1.920669\C,0,-3.596928,-2.6
26928,-0.367972\C,0,-5.070534,-0.722054,-1.089655\H,0,4.020599,-2.2821
9,0.711416\H,0,3.298703,1.742522,-0.764327\H,0,0.886844,1.355658,-0.35
0099\H,0,1.577986,-2.467744,1.045645\H,0,7.197959,-0.830254,-0.197098\
H,0,6.846838,1.117309,-0.912108\H,0,5.530586,2.026607,-0.151087\H,0,5.

34288,1.397262,-1.80501\H,0,5.967735,-2.057679,-0.534247\H,0,6.152484,
-1.404476,1.111822\H,0,-2.870095,1.114492,2.493082\H,0,-2.554043,-0.55
4052,3.011937\H,0,-1.193204,0.562922,2.759549\H,0,-2.967147,3.233277,1
.352439\H,0,-3.264382,3.647447,-0.337402\H,0,0.010442,-0.768574,0.5444
65\H,0,-2.729652,0.236468,-2.172924\H,0,-1.66937,-1.095354,-1.679765\H
,0,-3.019515,-1.398776,-2.800445\H,0,-4.257243,-2.814036,0.48643\H,0,-
3.734224,2.03171,0.295668\H,0,-3.946267,-3.237641,-1.209571\H,0,-2.584
458,-2.929503,-0.099414\H,0,-5.733472,-0.889673,-0.234256\H,0,-5.11371
6,0.33935,-1.355955\H,0,-5.444185,-1.306482,-1.937879\\Version=x86-Lin
ux-G98RevA.7\HF=-997.9518316\RMSD=1.688e-09\Dipole=3.6110964,-1.246029
7,0.1163652\PG=C01 [X(C15H26N2O4)]\\@

12a

1\1\GINC-GRETEL\SP\RB3LYP\6-311+G(d,p)\C15H26N2O4\IHELD\15-Aug-2004\0\
\#P BECKE3LYP/6-311+G(D,P) SCF=TIGHT INT=FINEGRID GEOM=CHECKPOINT GUES
S=READ\\singlepoint guess input nucback34ots ts becke3lyp/6-311+G(d,p)
\\0,1\O,0,-1.2080135312,-0.5478075276,-0.0879537582\C,0,-2.0688278095,
-0.1252677423,0.7593106237\C,0,-1.6475035186,0.2415984087,2.1705842772
\O,0,-2.6147636125,1.5643946636,0.1860992878\C,0,-1.7363056667,2.47920
48054,-0.0523051113\O,0,-0.5199728368,2.4221781584,0.1959891331\C,0,-2
.3224803213,3.7294690399,-0.712540133\O,0,-3.2964900749,-0.7074668688,
0.7960521409\C,0,-3.8792117768,-1.408438642,-0.3458584465\C,0,-3.82097
09305,-0.5753384597,-1.6319694313\C,0,-3.1919325305,-2.7709708765,-0.5
187589396\C,0,-5.3351359434,-1.6009708817,0.095326874\H,0,-2.487107424
6,0.6742773682,2.7167964561\H,0,-1.3225616296,-0.6718123,2.6858392559\
H,0,-0.8258916338,0.9570872425,2.1311974436\H,0,-3.2347028729,4.043635
2806,-0.1957887294\H,0,-1.5905025727,4.5407612256,-0.7102068818\H,0,-2
.5994340031,3.4993826795,-1.7484416263\H,0,-4.259682744,0.4111350994,-
1.4647793735\H,0,-2.7909237316,-0.438743564,-1.9640484434\H,0,-4.38478
20832,-1.0899297403,-2.4200548301\H,0,-3.215595266,-3.3285417738,0.424
5382093\H,0,-3.7159345235,-3.3632044025,-1.2788493022\H,0,-2.152590419
7,-2.6418773896,-0.824611914\H,0,-5.3804989304,-2.1570170411,1.0379777
317\H,0,-5.8183356757,-0.6305582957,0.2465004636\H,0,-5.8954934152,-2.
1576301477,-0.6641315487\C,0,1.9787870828,0.9918346629,-0.1045315947\C
,0,1.8479386041,-1.3267503282,0.0327330069\H,0,1.4041083748,1.91214336
93,-0.134286383\C,0,3.2191257746,-1.4621594832,0.0043565777\H,0,1.1854
15809,-2.1839348461,0.0995208882\C,0,4.0352608673,-0.302090414,-0.0849
932657\H,0,3.6475478446,-2.4544862756,0.0512833532\C,0,3.3581327236,0.
9443730713,-0.1407382503\H,0,3.9030020391,1.8766214267,-0.2097894613\N
,0,1.2384642987,-0.1300130111,-0.0186853141\H,0,0.0589533557,-0.148360
1105,-0.0065703874\C,0,6.2019979005,0.8282122033,-0.2037370942\C,0,6.0
537600165,-1.6847731924,-0.0581750296\H,0,6.0227327026,1.4933154386,0.
6504345666\H,0,7.2577078203,0.55581678,-0.205063886\H,0,5.9923557698,1
.3848190344,-1.1261263981\H,0,5.8138646092,-2.2183915179,0.8706756942\
H,0,5.7662482754,-2.3196094045,-0.9062623632\H,0,7.1338485033,-1.54079
97706,-0.0953325603\N,0,5.3967307632,-0.3845696745,-0.1147630833\\Vers
ion=x86-Linux-G98RevA.11.3\HF=-997.9595449\RMSD=2.253e-09\Dipole=4.436
6458,-1.2762941,-0.2934427\PG=C01 [X(C15H26N2O4)]\\@