Electronic Supplementary Material (ESI) for Polymer Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION

Which Side-Reactions Compromise Nitroxide Mediated Polymerization?

Ganna Gryn'ova, Ching Yeh Lin and Michelle L. Coote*

Australian Research Council Centre of Excellence for Free Radical Chemistry and Biotechnology, Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

*Correspondence to mcoote@rsc.anu.edu.au

Table of Contents

Details of the Theoretical Procedures

Quantum-Chemical Calculations

Standard *ab initio* molecular orbital theory and density functional theory (DFT) calculations were carried out using Gaussian 09,[1] Molpro 2009.1,[2] ADF 2010.01[3] and Q-Chem 3.2 and 4.0.[4] Calculations on radicals were performed with an unrestricted wave function except in cases designated with an "R" prefix where a restricted open-shell wave function was used. Calculations were performed at a high-level of theory, previously shown to predict accurate values of the

1 Gaussian 09, Revision **B.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

2 MOLPRO 2009.1, H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, P. Celani, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K. R. Shamasundar, T. B. Adler, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Hrenar, G. Jansen, C. Köppl, Y. Liu, A. W. Lloyd, R. A. Mata, A. J. May, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß, D. P. O'Neill, P. Palmieri, D. Peng, K. Pflüger, R. Pitzer, M. Reiher, T. Shiozaki, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson, M. Wang.

3 ADF **2010.01**, E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

4 Q-Chem, Versions **3.2** and **4.0**, Q-Chem, Inc., Pittsburgh, PA (2007); Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, R. A. Distasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M., Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2006, **8**, 3172.

kinetics[5] and thermodynamics[6] of radical reactions, including the specific case of nitroxide mediated polymerization (NMP).[7,8]

Propagating radicals and products of their transformations were modelled as dimers to include the penultimate unit effect.[9] For all species either full systematic conformational searches (at a resolution of 120°) or, for more complex systems, energy-directed tree searches[10] were carried out to ensure global, and not merely local minima were located. These conformational searches were performed in a solution phase using UAKS-CPCM[11]/B3LYP/6-31G(d) method. Toluene was used as a solvent for conformational searches of species participating in model styrene polymerizations, and ethyl acetate – in acrylate and methacrylate polymerizations.[12] Geometries of all species were then refined *via* full optimisation at the B3LYP/6-31G(d) level and frequencies were also calculated at the same level and scaled by recommended scaling factors.[13] All transition state geometries were characterized by a single imaginary frequency. Accurate energies for all species were then calculated using double-layer ONIOM-type method.[5] The core layer was calculated using composite high-level *ab initio* G3(MP2)-RAD method,[14] and the full system was calculated with the R(O)MP2/6-311+G(3df,2p) method, using either Gaussian 09[1] or a resolution of identity rational as implemented in Q-Chem[4] with aug-cc-pVTZ auxiliary basis. For several large species RI-R(O)MP2/6-31+G(2df,p) method with the cc-pVDZ auxiliary basis was used for the outer layer instead. For kinetics of *ß*-H abstraction from SG1-PBA three-layer ONIOM was applied where the B3LYP/6-31G(d) method was used for the outermost ONIOM layer. These approximations are shown in the Appendix S1.

Free energies of each species in bulk monomer solutions at 120 °C were calculated as the sum of the corresponding gas-phase free energies and the obtained free energies of solvation and included a phase change correction term $RTln(\frac{RT}{P})$, where R is the universal gas constant, T is the

5 For a review, see M. L. Coote, *Macromol. Theory Simul.*, 2009, **18**, 388.
6 M. L. Coote, C. Y. Lin, A. L. J. Beckwith and A. A. Zavitsas, *Phys. Chem. Chem. Phys.*, 2010, **12**, 9597.
7 J. L. Hodgson, L. B. Roskop, M. S. Gordon, C. Y. Lin and M. L. Coote, *J. Phys. Chem. A*, 2010, **114**, 10458
8 J. L. Hodgson, C. Y. Lin, M. L. Coote, S. R. A. Marque and K. Matyaszewski, *Macromolecules*, 2010, **43**, 3728.
9 D. Bertin, P.-E. Dufils, I. Durand, D. Gigmes, B. Giovanetti, Y. Guillaneuf, S. R. A. Marque, T. Phan and P. Tordo, *Macromol. Chem. Phys.*, 2008, **209**, 220.
10 E. I. Izgorodina, C. Y. Lin and M. L. Coote, *Phys. Chem. Chem. Phys.*, 2007, **9**, 2507.
11 E. Cances, B. Mennucci and J. Tomasi, *J. Chem. Phys.*, 1997, **107**, 3032.
12 For toluene, sphere's radii were scaled by 1.3; for ethyl acetate, sphere's radii were scaled by 1.2, and the following additional solvent specifications were used: EPS=5.9867, DENSITY=0.00613, RSOLV=2.734 and VMOL=98.5, see M. H. Abraham and J. Liszi, *J. Inorg. Nucl. Chem.*, 1981, **43**, 143.
13 J. P. Merrick, D. Moran and L. Radom, *J. Phys. Chem. A*, 2007, **111**, 11683.
14 D. J. Henry, M. B. Sullivan and L. Radom, *J. Chem. Phys.*, 2003, **118**, 4849.

absolute temperature and *P* is the pressure. The entropies and thermal corrections at 25 and 120 °C (298.15 and 393.15 K) were calculated using standard textbook formulae[15] for the statistical thermodynamics of an ideal gas under the harmonic oscillator approximation in conjunction with the optimised geometries and scaled frequencies. Free energies of solvation in bulk monomer (styrene, butyl acrylate or methyl methacrylate) solutions at 120 °C were obtained using the COSMO-RS (COnductor-like Screening MOdel for Realistic Solvents) method.[16] The ADF package[3] was used to compute COSMO-RS solvation free energies in conjunction with the solution-phase CPCM-UAKS/B3LYP/6-31G(d) geometries (obtained as described above) at the BP/TZVP level of theory, and the remaining parameters (e.g., atomic cavity radii, radius of the probing sphere, and cavity construction) were kept as default values for the corresponding solvents.[17]

Transition-state theory rate coefficients were calculated according to the standard textbook formulae:[18]

$$k(T) = a\,\kappa(T)\frac{k_B T}{h}(c^o)^{1-m}\exp\left(\frac{-\Delta G^{\ddagger}}{RT}\right) \qquad \text{(Eq. 1)}$$

In this formula, *a* is the reaction path degeneracy, $\kappa(T)$ is the tunnelling correction factor,[19,20] k_B is Boltzmann's constant, *h* is Planck's constant, $\Delta G^{\ddagger}$ is the Gibbs free energy of activation, c^o is the standard unit of concentration (equal to P/RT for gas-phase $\Delta G^{\ddagger}$ and to 1 for already corrected solution-phase $\Delta G^{\ddagger}$) and *m* is the molecularity of the reaction.[21]

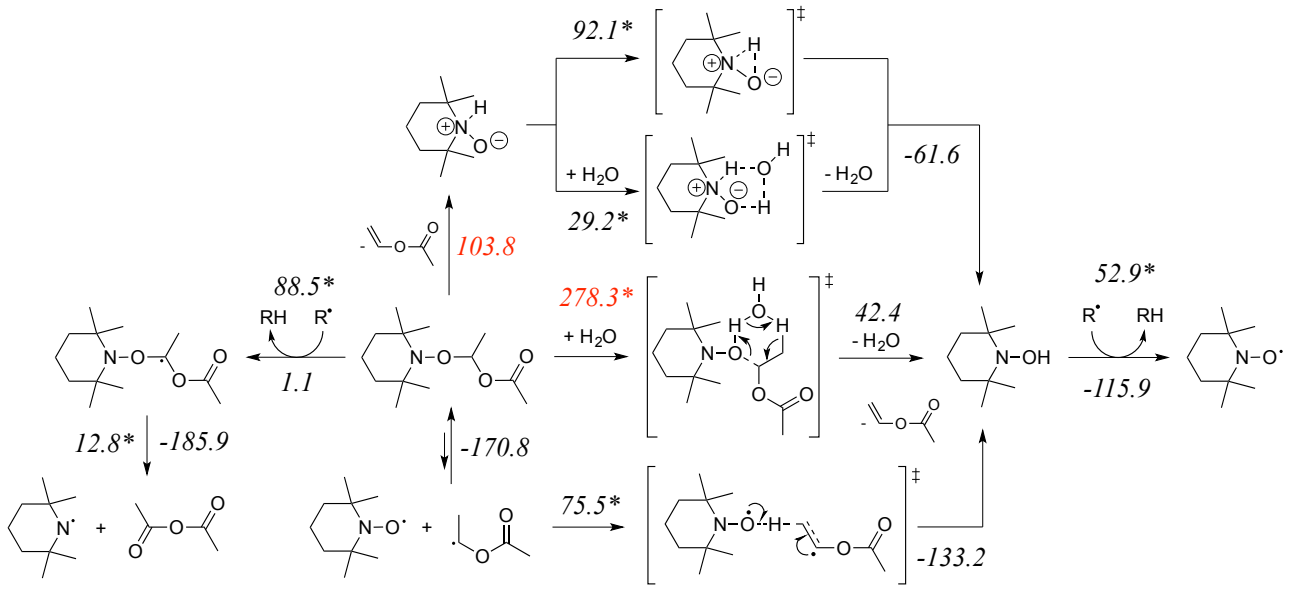
Kinetic Modelling

The PREDICI program[22] was used to model kinetics of NMP in different systems and under various scenarios (different starting concentrations and/or rate constants of different reaction steps) at 120 °C in the bulk solution of relevant monomers. The kinetic model comprised the main alkoxyamine dissociation equilibrium, propagation and bimolecular termination of P• (experimental

15 J. I. Steinfeld, J. S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics*, Prentice Hall, Englewood Cliffs, 1989.
16 a) A. Klamt, *J. Phys. Chem.*, 1995, **99**, 2224; b) A. Klamt, *COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design*, Elsevier, Amsterdam, 2005; c) A. Klamt, V. Jonas, T. Burger and J. C. W. Lohrenz, *J. Phys. Chem. A*, 1998, **102**, 5074.
17 C. C. Pye, T. Ziegler, E. van Lenthe and J. N. Louwen, *Can. J. Chem.*, 2009, **87**, 790.
18 For the summary of the formulas see: M. L. Coote, in *Encyclopedia of Polymer Science and Technology*, ed. J. I. Kroschwitz, John Wiley and Sons, New York, 3rd ed., 2004.
19 C. Eckart, *Phys. Rev.*, 1930, **35**, 1303.
20 M. L. Coote, M. A. Collins and L. Radom, *Mol. Phys.*, 2003, **101**, 1329.
21 For the detailed description of kinetic calculations see: M. L. Coote, *Macromol. Theory Simul.,* 2009, **18**, 388.
22 M. Wulkow, *Macromol. React. Eng.*, 2008, **2**, 461.

values for rate constants are taken from literature and set to be chain-length independent), inter- and intramolecular H-transfer between P• and NO•, β-hydrogen abstraction from alkoxyamine, conversion of *N*-oxide into hydroxylamine and back H-transfer from NOH to propagating radicals (rate constants calculated in this work), decomposition of alkoxyamine radicals and oxidation of formed aminyl radicals into nitroxides (rates of which are close to diffusion-limited, as shown in our previous study[23]). The kinetic model was chain-length-dependent with respect to the concentrations of the growing polymer chains, *i.e.* the simulations were run in the distribution mode of PREDICI. Reactions that were close to thermoneutral ($\Delta G^{393} = \pm 20$ kJ mol^{-1}) were modelled as reversible. Thermal self-initiation of styrene (according to the Mayo mechanism)[24] was also included in the modelling. For methyl methacrylate, H-abstractions from both α-C**H$_2$**~ and α-C**H$_3$** were studied, and the more energetically favoured site was used in kinetic simulations. All the individual reactions are shown in Figures 1 and 2 of the manuscript. The primary aim of this study is to identify the major side-reactions disrupting NMP, thus certain assumptions were introduced in the modelling, however none of them is expected to influence our trends and conclusions. In particular, we did not include disproportionation between propagating radicals, as it is typically supressed in NMP, although would be more important for methacrylate monomers compared with styrenics.[25] We also discarded trapping of transient radicals by oxygen provided low O_2 concentrations under typical NMP conditions (degassing) because it is expected to influence different polymerizing systems in the same manner (forming relatively inactive peroxide radicals with diffusion-limited rates), however we emphasise that for other tasks (experimental optimisation of NMP or accurate experimental measurement of its kinetic parameters) it might be more significant.[26] All systems in this work were modelled under 120 °C to afford direct comparison, however the temperature in typical NMP varies within *ca.* 80-130 °C, which should be taken into account when comparing results reported here with the referenced experimental data. Finally, we did not include effects of changing viscosity, diffusional limitations and chain-length dependency in the propagation and self-termination rates as they are also expected to be similar in the various scenarios considered in the present work.

23 G. Gryn'ova, K. U. Ingold and M. L. Coote, *J. Am. Chem. Soc.*, 2012, **134**, 12979.
24 G. Pan, D. Sudol, V. L. Dimonie and M. S. El-Aasser, *J. Polym. Sci., Part A: Polym. Chem.*, 2004, **42**, 4921.
25 M. Buback, M. Egorov, R. G. Gilbert, V. Kaminsky, O. F. Olaj, G. T. Russell, P. Vana and G. Zifferer, *Macromol. Chem. Phys.*, 2002, **203**, 2570.
26 M. Edeleva, S. R. A. Marque, K. Kabytaev, Y. Guillaneuf, D. Gigmes and E. Bagryanskaya, *J. Polym. Sci., Part A: Polym. Chem.*, 2013, **51**, 1323.



Scheme S1. Nitroxide Cycling in HALS-inhibited Polymer Degradation

Calculated Gibbs free energies (kJ mol^{-1}, gas phase, 25 ^{O}C) of reactions and activation (denoted by an asterisk), relevant to possible NMP side-reactions. Red colour is used to indicate unfeasible energetics.[23]

Data Used in Kinetic Modelling

Table S1. Kinetic scheme used for PREDICI simulations of NMP in this work

Reaction scheme[a]	Reaction description [b]	Rate coefficient
M + M → D	Styrene thermal self-initiation *via* Mayo mechanism[24] [c]	k_{dim}
D + M → P• + D•		k_{i1}
D• → P•		k_{i2}
NOP(s) → P•(s) + NO•	Alkoxyamine decomposition (1)	k_d
P•(s) + NO• → NOP(s)	Combination to alkoxyamine	k_c
P•(s) + M → P•(s+1)	Propagation	k_p
P•(s) + P•(r) → PP(s+r)	Self-termination	k_t
NOP(s) → P(-H)(s) + NOH	Intramolecular H-transfer (3a)	k_{H1a}
NOP(s) → P(-H)(s) + NOx	Intramolecular H-transfer (3b)	k_{H1b}
P(-H)(s) + NOx → NOP(s)	Reverse of above	k_{H1b_r}
NOx → NOH	*N*-oxide to hydroxylamine	k_b
P•(s) + NO• → P(-H)(s) + NOH	Intermolecular H-transfer (2)	k_{H2}
NOP(s) + P•(r) → NOP•(s) + PH(r)	β-Hydrogen abstraction (6)	$k_{\beta H}$
NOH + P•(s) → NO• + PH(s)	Back hydrogen transfer	k_{ox}
NO• + PH(s) → NOH + P•(s)	Reverse of above	k_{ox_r}
NOP•(s) → N• + O=P(s)	Alkoxyamine radical decomposition	k_{ad}
N• + O_2 → NO•	Oxidation of aminyl	k_{o2}

[a] Chain-length dependent concentrations are denoted with (s), (r) and (s+r); [b] Reaction numbers corresponding to Figures 1 and 2 of the main text are given in brackets; [c] $k_{dim} = 3\times10^{-8}$ L mol^{-1} s^{-1}, $k_{i1} = 5\times10^{-8}$ L mol^{-1} s^{-1}, $k_{i2} = 1\times10^{10}$ s^{-1}.

Table S2. Typical starting concentrations of the reactive species in NMP [a]

System	Monomer M	Alkoxyamine R'R"NO-P	Nitroxide R'R"NO•	Ref.
TEMPO-PS $\mathbf{A1_n}$	$1.0*10^{1}$	$1.0*10^{-2}$	$1.0*10^{-4}$	27
SG1-PBA $\mathbf{B2_n}$	$1.0*10^{1}$	$1.0*10^{-2}$	$5.0*10^{-4}$	28
TEMPO-PMMA $\mathbf{A3_n}$	$1.0*10^{1}$	$1.0*10^{-2}$	$1.0*10^{-4}$	29
SG1-PMMA $\mathbf{B3_n}$	$1.0*10^{1}$	$5.0*10^{-2}$	$5.0*10^{-3}$	30
DPAIO-PMMA $\mathbf{D3_n}$	$1.0*10^{1}$	$2.5*10^{-2}$	0.0	31

[a] Concentration of O_2 was set constant and equal to 10^{-3}, and all concentrations are given in mol L^{-1}.

27 T. Fukuda, T. Terauchi, A. Goto, K. Ohno, Y. Tsujii, T. Miyamoto, S. Kobatake and B. Yamada, *Macromolecules*, 1996, **29**, 6393.

28 D. Benoit, S. Grimaldi, S. Robin, J.-P. Finet, P. Tordo and Y. Gnanou, *J. Am. Chem. Soc.*, 2000, **122**, 5929.

29 C. Burguière, M.-A. Dourges, B. Charleux and J.-P. Vairon, *Macromolecules*, 1999, **32**, 3883.

30 Y. Guillaneuf, D. Gigmes, S. R. A. Marque, P. Tordo and D. Bertin, *Macromol. Chem. Phys.*, 2006, **207**, 1278.

31 Y. Guillaneuf, D. Gigmes, S. R. A. Marque, P. Astolfi, L. Greci, P. Tordo and D. Bertin, *Macromolecules*, 2007, **40**, 3108.

Table S3. Literature experimental rate constants of various reactions in NMP at 120 °C

System	k_c, L mol^{-1} s^{-1}	k_d, s^{-1}	K_{eq}	Solv.[a]	Ref	k_p, L mol^{-1} s^{-1}	Ref	k_t, L mol^{-1} s^{-1}	Ref
TEMPO-S **A1**	$2.5*10^{8}$	$5.2*10^{-4}$	$4.8*10^{11}$	*t*BB	32			$5.0*10^{9}$	33
TEMPO-PS **A1$_n$**	$7.6*10^{7}$ [b]	$1.0*10^{-3}$	$7.6*10^{10}$	S	34	$2.0*10^{3}$	35	$1.8*10^{8}$	36
SG1-PS **B1$_n$**	$5.7*10^{5}$	$3.4*10^{-3}$	$1.7*10^{8}$	S	28				
SG1-PBA **B2$_n$**	$4.2*10^{7}$	$7.1*10^{-3}$	$5.9*10^{9}$	BA	28	$9.3*10^{4}$	37	$7.3*10^{7}$	36
TEMPO-MMA **A3$_n$**	$5.9*10^{8}$	$2.2*10^{-2}$	$2.7*10^{10}$	ACN	32				
SG1-MMA **B3**	$1.1*10^{6}$	$5.0*10^{-2}$	$2.2*10^{7}$	ACN	32				
SG1-PMMA **B3$_n$**	$5.0*10^{5}$	$2.4*10^{0}$	$2.1*10^{5}$	MMA	30	$2.9*10^{3}$	35	$3.6*10^{7}$	38
DPAIO-PMMA **D3$_n$**	$1.4*10^{6}$	$2.0*10^{-4}$	$7.0*10^{9}$	MMA	31				

[a] Solvent, '*t*BB' stands for *tert*-butyl benzene, 'ACN' – acetonitrile; [b] Measured at 125 °C.

32 J. Sobek, R. Martschke and H. Fischer, *J. Am. Chem. Soc.*, 2001, **123**, 2849.
33 G. S. Ananchenko and H. Fischer, *J. Polym. Sci., Part A: Polym. Chem.*, 2001, **39**, 3604.
34 A. Goto, T. Terauchi, T. Fukuda and T. Miyamoto, *Macromol. Rapid. Commun.*, 1997, **18**, 673.
35 R. G. Gilbert, *Pure & Appl. Chem.*, 1996, **68**, 1491.
36 F. Chauvin, P.-E. Dufils, D. Gigmes, Y. Guillaneuf, S. R. A. Marque, P. Tordo and D. Bertin, *Macromolecules*, 2006**, 39***,* 5238.
37 J. M. Asua, S. Beuermann, M. Buback, P. Castignolles, B. Charleux, R. G. Gilbert, R. A. Hutchinson, J. R. Leiza, A. N. Nikitin, J.-P. Vairon and A. M. van Herk, *Macromol. Chem. Phys.*, 2004, **205**, 2151.
38 E. Bagryanskaya, D. Bertin, D. Gigmes, I. Kirilyuk, S. R. A. Marque, V. Reznikov, G. Roshchupkina, I. Zhurko and D. Zubenko, *Macromol. Chem. Phys.*, 2008, **209**, 1345.

Table S4. Calculated rate constants of various side-reactions interfering with NMP

(at 120 °C in corresponding bulk monomer solutions)

System	k_{H1a}, s^{-1}	k_{H1b}, [a] s^{-1}	k_b, s^{-1}	k_{H2}, L mol^{-1} s^{-1}	$k_{\beta H}$, L mol^{-1} s^{-1}	k_{ox}, [a] L mol^{-1} s^{-1}
TEMPO-PS **A1**$_n$	$6.0*10^{-15}$	0.0 [b]	0.0 [c]	$5.2*10^{1}$	$3.0*10^{1}$	$1.4*10^{3}$
						$5.5*10^{-9}$
SG1-PBA **B2**$_n$	$1.4*10^{-13}$	0.0 [b]	0.0 [c]	$1.2*10^{2}$	$7.7*10^{-7}$	$3.7*10^{2}$
						$2.0*10^{-14}$
TEMPO-PMMA **A3**$_n$	$1.1*10^{-14}$	$4.8*10^{-4}$	$5.6*10^{-2}$	$8.1*10^{2}$	0.0 [d]	$1.4*10^{-5}$
		$8.3*10^{-2}$				$1.9*10^{-17}$
SG1-PMMA **B3**$_n$	0.0 [e]	$1.1*10^{-2}$	$1.2*10^{-2}$	$1.1*10^{2}$	0.0 [d]	$1.4*10^{1}$
		$3.78*10^{-2}$				$2.9*10^{-13}$
DPAIO-PMMA **D3**$_n$	0.0 [e]	0.0 [b]	0.0 [c]	$1.3*10^{2}$	0.0 [d]	$6.4*10^{3}$
						$3.0*10^{-8}$

[a] Given are forward and reverse rate coefficients; [b] Reaction is highly endoergic and is unlikely to be significant, therefore its barrier was not calculated; [c] Species participating in this reaction are not expected to form in appreciable amount, therefore its barrier was not calculated; [d] Dormant alkoxyamine species do not have an abstractable β-hydrogen; [e] Transition state structure was not located.

Table S5. Unimer *vs.* dimer in TEMPO-styrene

Calculated rate coefficients (in L mol^{-1} s^{-1}) of various side-reactions for TEMPO-PS system modelled as a dimer and as a unimer (in the gas phase and in bulk styrene solution at 120 °C).

Reaction	Gas phase		Styrene solution	
	unimer [a]	dimer	unimer [a]	dimer
Intermolecular H-transfer (2)	$1.93*10^{1}$	$1.62*10^{2}$	4.44	$5.16*10^{1}$
β-H abstraction (6)	$7.35*10^{-1}$	$4.87*10^{2}$	$4.59*10^{-2}$	$3.04*10^{1}$

[a] Calculated using ONIOM core layer of the corresponding dimer reactions, with TEMPO modelled as $(CH_3)_2NO•$.

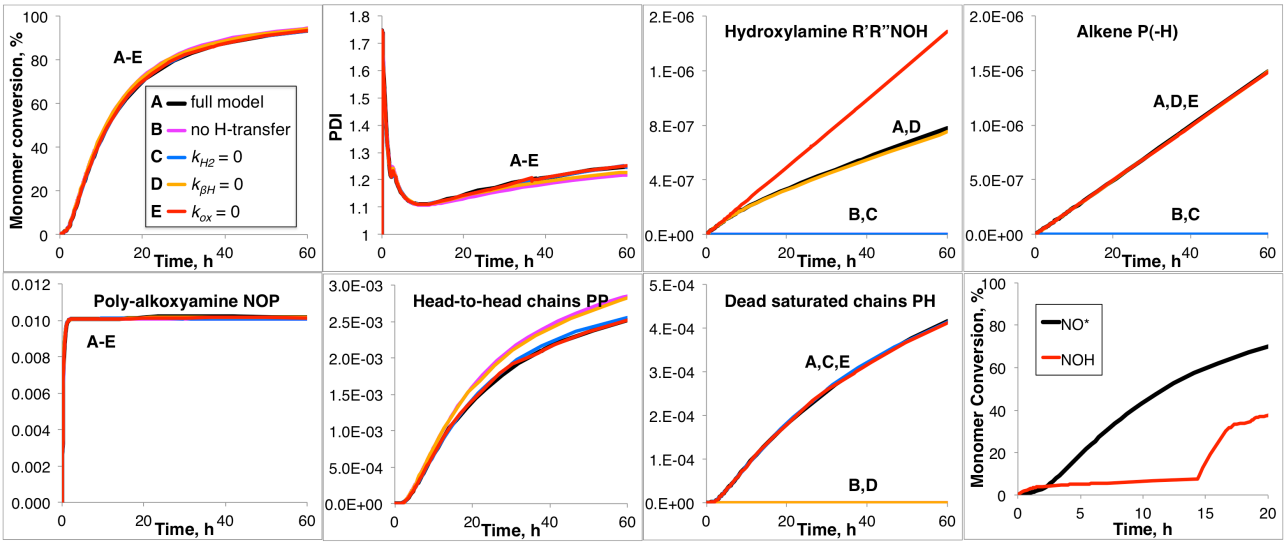


Figure S1. Kinetic simulations of TEMPO-mediated polymerization of styrene

Simulations carried out using kinetic parameters in Tables S2-S4 as given (full model) or setting all (no H-transfer) or some of the side-reactions rate coefficients to zero. Shown are time-profiles of monomer conversion, PDI and concentrations (in mol L^{-1}) of macro-alkoxyamine and various by-products, as well as the simulated monomer conversions in TEMPO-mediated polymerizations of styrene with initially added 0.0001 mol L^{-1} of TEMPO (NO•) or its hydroxylamine (NOH) (bottom right).

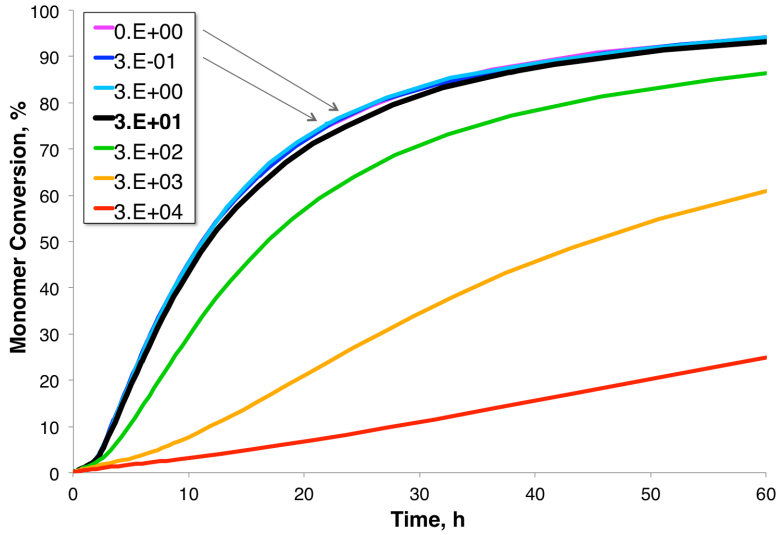


Figure S2. Effect of varying $k_{\beta H}$ on monomer conversion in TEMPO-mediated polymerization of styrene

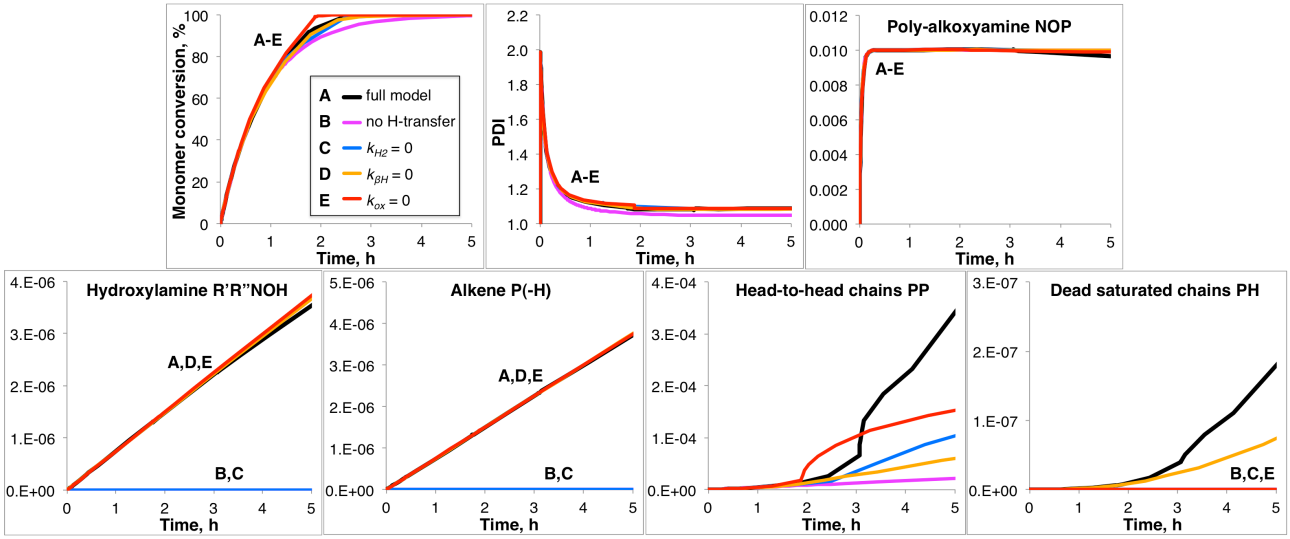


Figure S3. Kinetic simulations of SG1-mediated polymerization of butyl acrylate

Simulations carried out using kinetic parameters in Tables S2-S4 as given (full model) or setting all (no H-transfer) or some of the side-reactions rate coefficients to zero. Shown are time-profiles of monomer conversion, PDI and concentrations (in mol L^{-1}) of macro-alkoxyamine and various by-products.

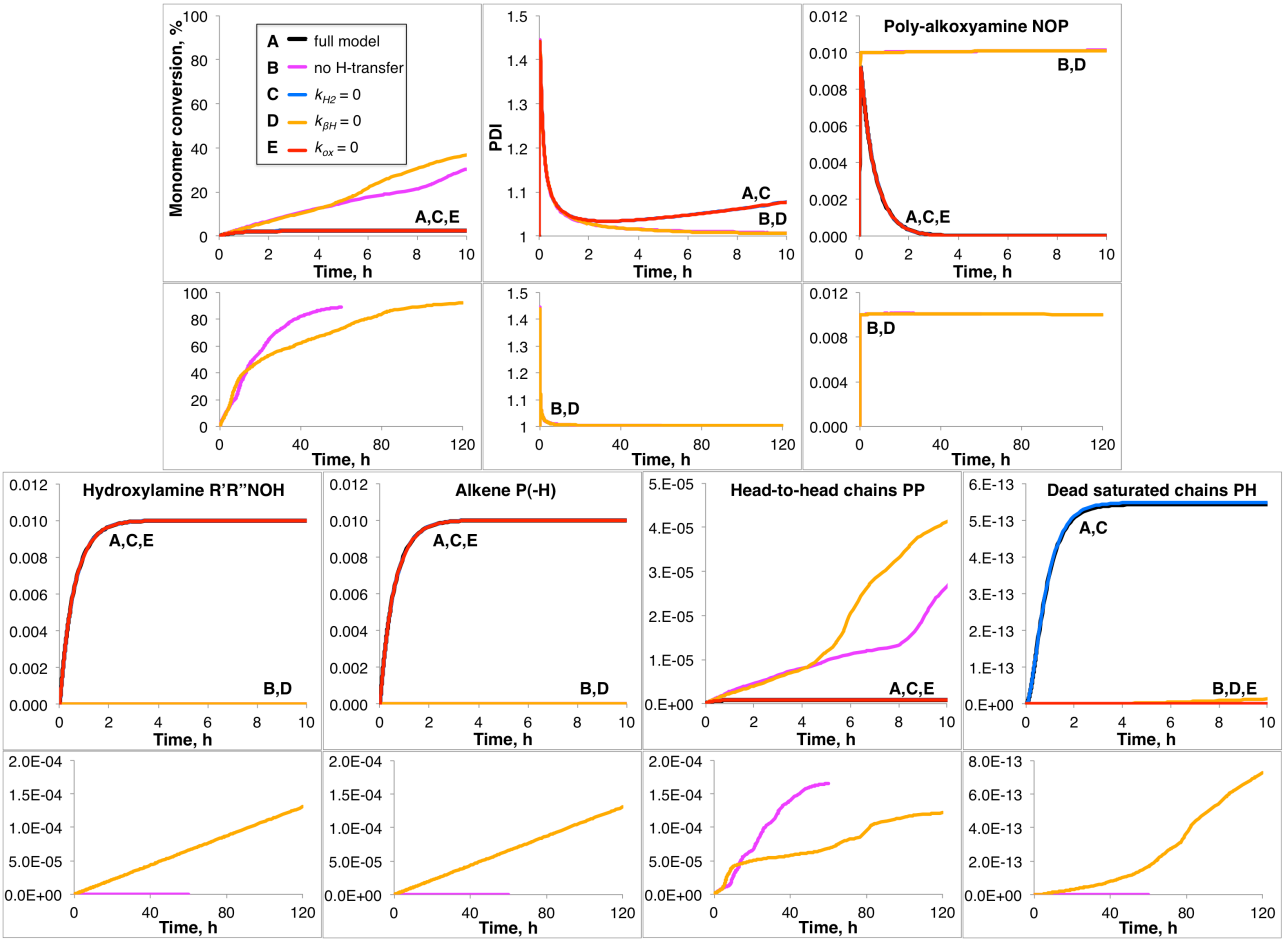
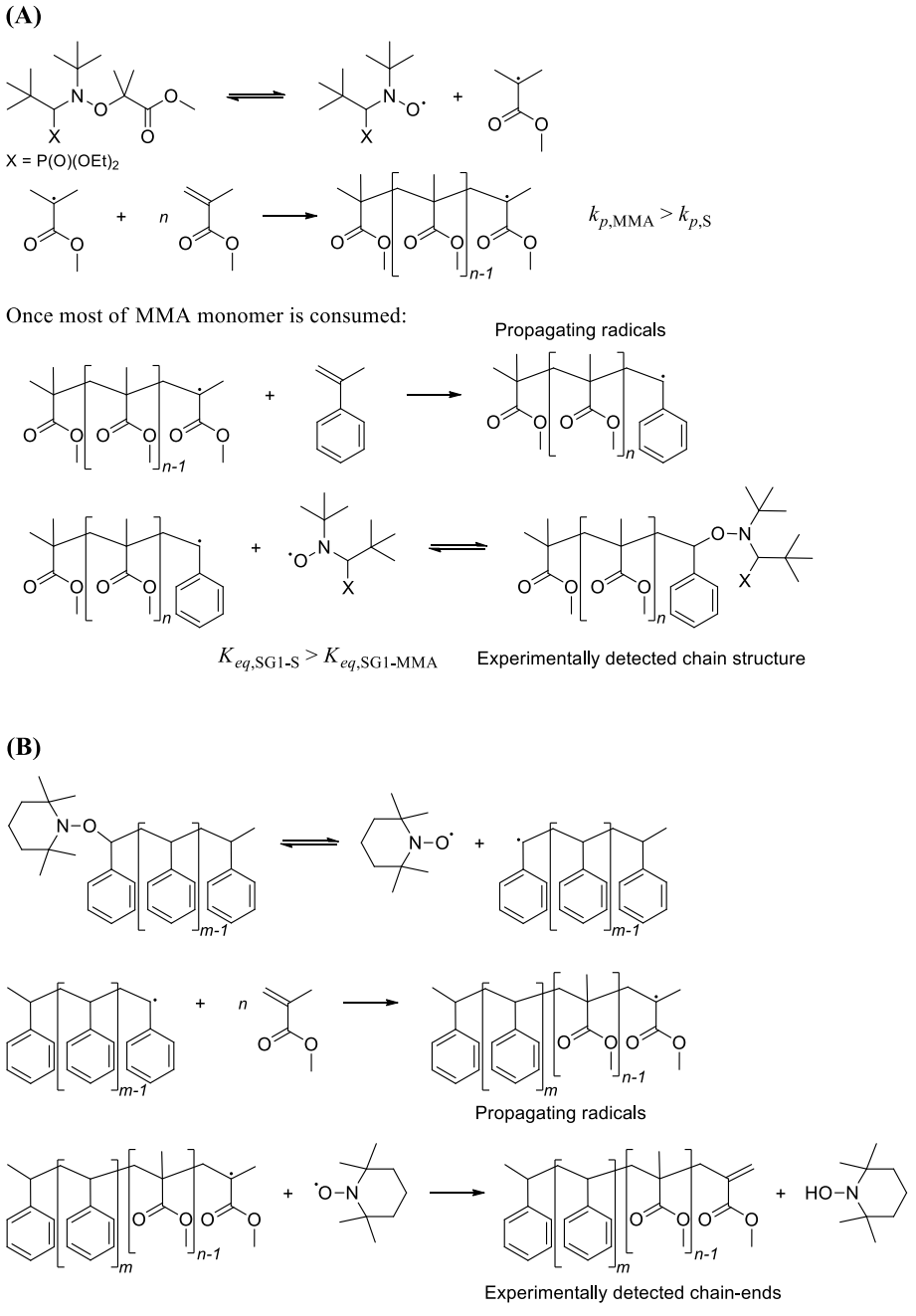


Figure S4. Kinetic simulations of TEMPO-mediated polymerization of methyl methacrylate

Simulations carried out using kinetic parameters in Tables S2-S4 as given (full model) or setting all (no H-transfer) or some of the side-reactions rate coefficients to zero. Shown are time-profiles of monomer conversion, PDI and concentrations (in mol L^{-1}) of macro-alkoxyamine and various by-products in two time scales – 10 hours (top, for all five scenarios) and 120 hours (bottom, for scenarios with either all decomposition or only pathway 3b turned off).



Scheme S2. Different scenarios of styrene and methacrylate copolymerizations[39,40]

39 J. Nicolas, C. Dire, L. Mueller, J. Belleney, B. Charleux, S. R. A. Marque, D. Bertin, S. Magnet and L. Couvreur, *Macromolecules*, 2006, **39**, 8274.

40 I. C. Wienhöfer, H. Luftmann and A. Studer, *Macromolecules*, 2011, **44**, 2510.

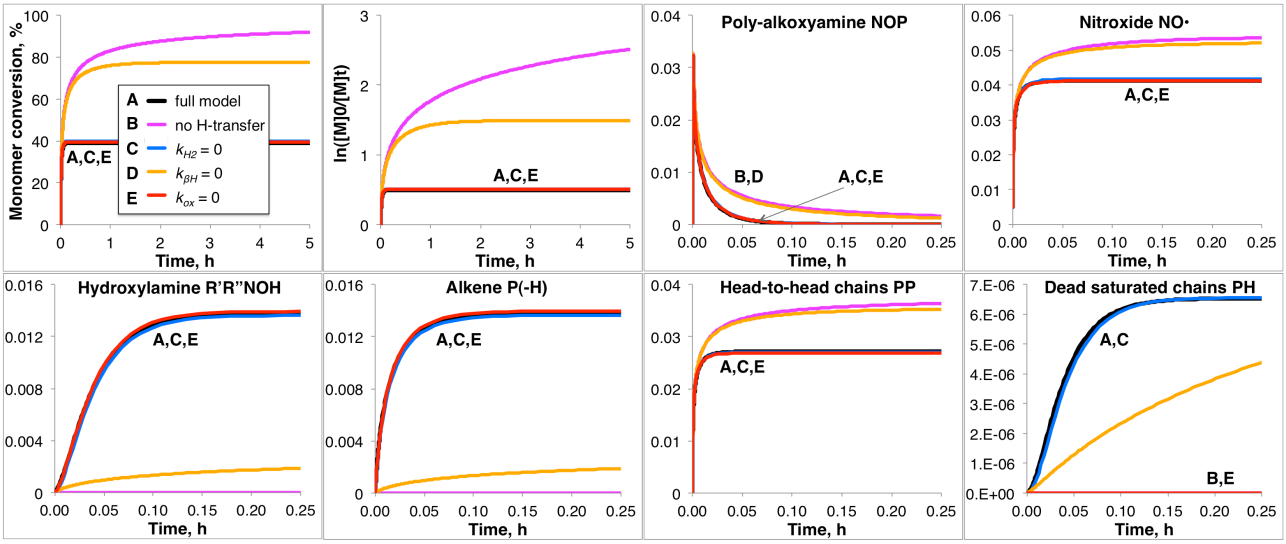


Figure S5. Kinetic simulations of SG1-mediated polymerization of methyl methacrylate

Simulations carried out using kinetic parameters in Tables S2-S4 as given (full model) or setting all (no H-transfer) or some of the side-reactions rate coefficients to zero. Shown are time-profiles of monomer conversion and $\ln([M]_0/[M]_t)$ in 5 hour time scale, and concentrations (in mol L^{-1}) of macro-alkoxyamine, nitroxide and various by-products in 15 min time scale.

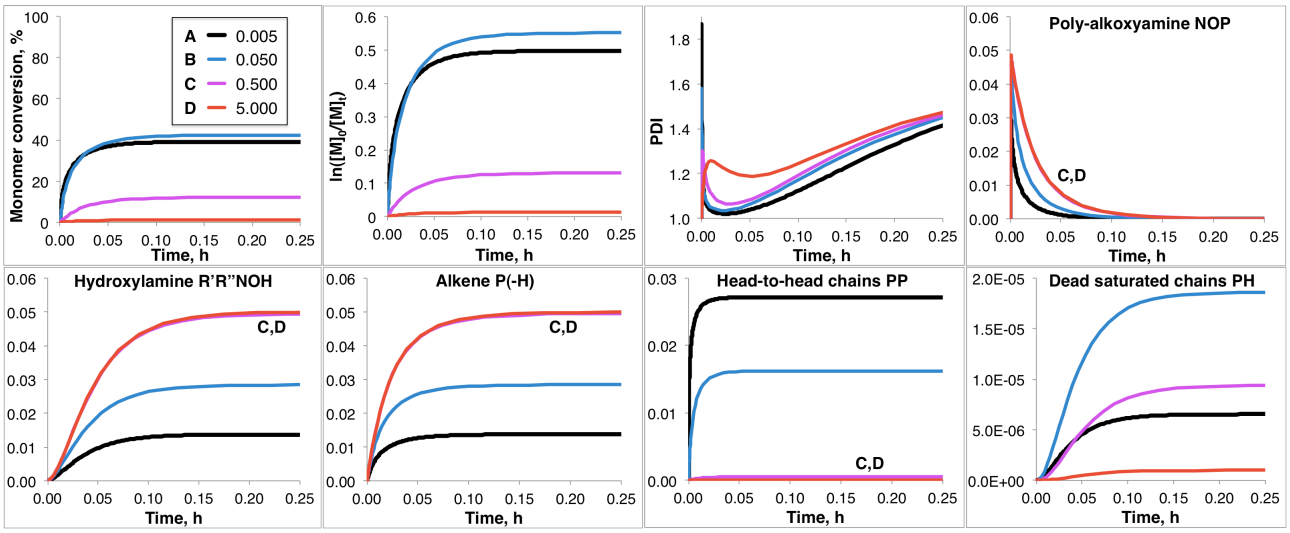


Figure S6. Varying SG1 starting concentration

Kinetic plots of monomer conversion, $\ln([M]_0/[M]_t)$ and concentrations (in mol L^{-1}) of macro-alkoxyamine and various by-products in 15 min time scale for varying starting concentrations of free SG1 in NMP of MMA.

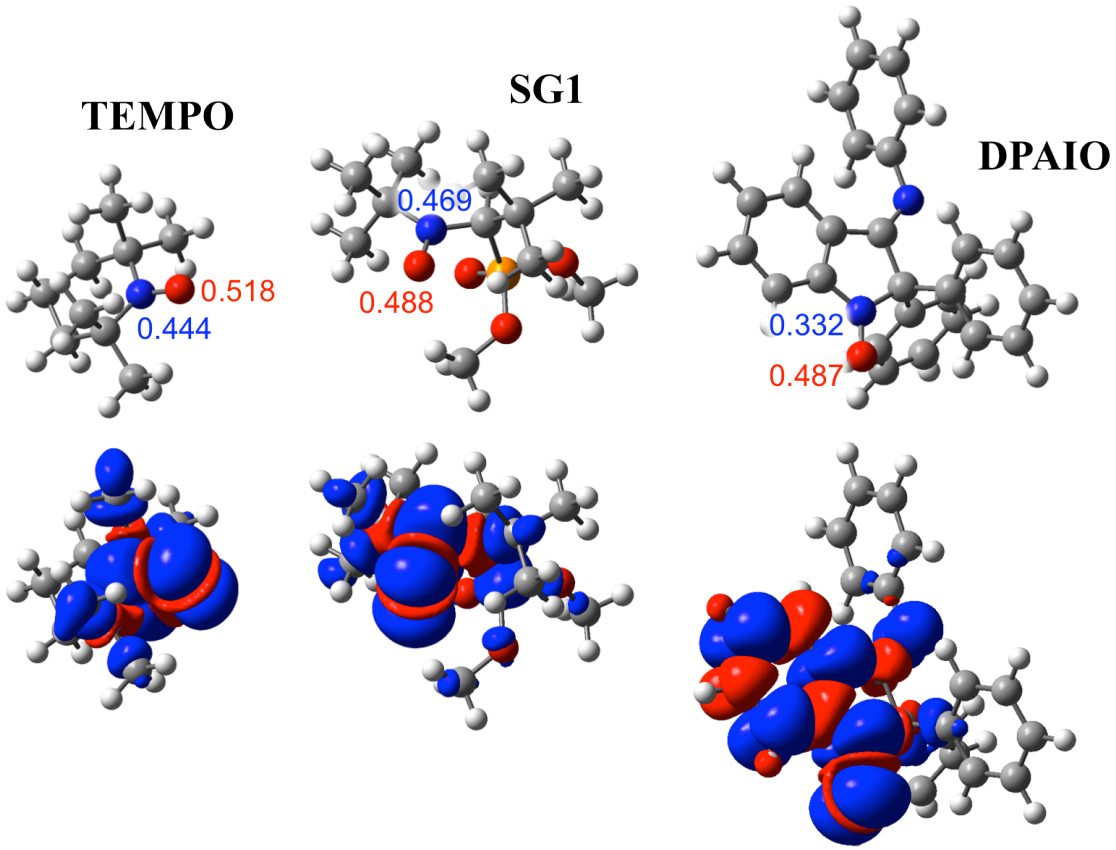


Figure S7. Geometries of TEMPO, SG1 and DPAIO

Geometries optimised in the gas phase using B3LYP/6-31G(d) method, also shown the corresponding Mulliken spin densities on nitrogen (blue) and oxygen (red) atoms of the NO• moiety (top row) and α and β spin density surfaces (bottom row).

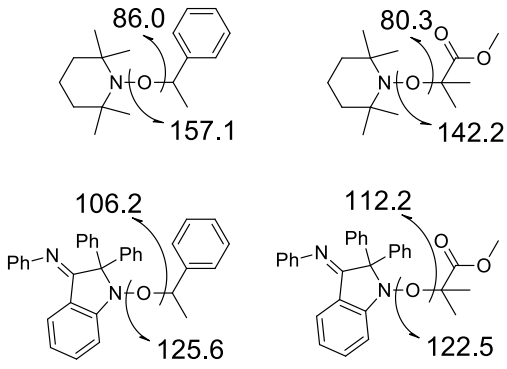


Figure S8. Bond dissociation Gibbs free energies in TEMPO and DPAIO alkoxyamines

NO–C and N–OC BDFEs of typical NMP initiators, calculated in toluene solution at 120 °C.[7]

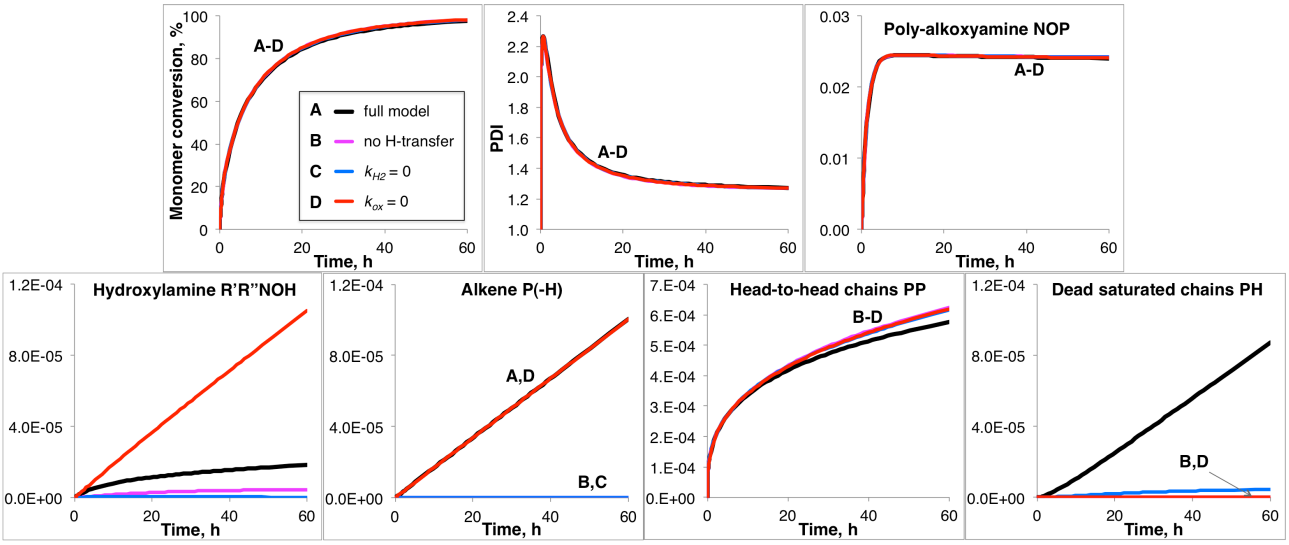


Figure S9. Kinetic simulations of DPAIO-mediated polymerization of methyl methacrylate

Simulations carried out using kinetic parameters in Tables S2-S4 as given (full model) or setting all (no H-transfer) or some of the side-reactions rate coefficients to zero. Shown are time-profiles of monomer conversion, PDI and concentrations (in mol L^{-1}) of macro-alkoxyamine and various by-products.

Table S6. Calculated kinetic and thermodynamic parameters of side-reactions (2)-(6) in five studied systems [a]

Reaction [b]	Imaginary	Thermodynamics				Kinetics					
	frequency in TS‡	ΔS, J mol^{-1} K^{-1}	ΔH, kJ mol^{-1}	ΔG, kJ mol^{-1}	ΔG_{soln}, [c] kJ mol^{-1}	ΔS‡, J mol^{-1} K^{-1}	ΔH‡, kJ mol^{-1}	ΔG‡, kJ mol^{-1}	k, [d] X s^{-1}	ΔG_{soln}‡, [c] kJ mol^{-1}	k_{soln}, [c,d] X s^{-1}
					TEMPO-PS						
					298.15 K						
(2)	-401.820	-14.393	-116.609	-112.318		-188.450	20.488	76.674	1.32E+01		
(3a)	-351.078	210.220	74.521	11.844		-4.123	204.575	205.804	1.24E-23		
(3b)		206.044	134.789	73.357							
(5)	-1885.466	1.325	-75.906	-76.301		-172.917	22.840	74.395	2.86E+02		
(-5)								156.904	1.00E-12		
(6)	-1867.372	-0.042	-11.172	-11.160		-196.424	16.705	75.269	1.39E+02		
					393.15 K						
(2)	-401.820	-14.044	-116.489	-110.967	-108.319	-186.642	21.114	94.492	1.62E+02	86.873	5.16E+01
(3a)	-351.078	209.935	74.412	-8.123	-3.596	-5.644	204.051	206.270	6.92E-15	206.768	5.95E-15
(3b)		204.106	134.113	53.868	45.948						
(5)	-1885.466	-1.113	-76.746	-76.308	-79.534	-171.697	23.263	90.766	1.36E+03	79.423	1.35E+03
(-5)								173.283	1.48E-08	165.166	5.49E-09
(6)	-1867.372	-0.185	-11.223	-11.150	-12.406	-193.586	17.684	93.792	4.87E+02	91.508	3.04E+01
					SG1-PBA						
					298.15 K						
(2)	-351.731	-18.383	-118.224	-112.743		-206.080	9.700	71.143	1.18E+02		
(3a)	-383.100	231.238	68.997	0.053		20.223	205.091	199.062	1.93E-22		
(3b)		225.076	134.873	67.766							
(5)	-1736.913	4.951	-115.362	-116.838		-165.963	24.373	73.855	4.02E+01		
(-5)								190.693	1.36E-19		
(6)	-901.192	13.147	-11.592	-15.512		-194.768	69.899	127.969	5.54E-07		
					393.15 K						
(2)	-351.731	-18.702	-118.330	-110.977	-108.885	-203.976	10.429	90.622	5.16E+02	83.957	1.23E+02
(3a)	-383.100	230.248	68.648	-21.874	-16.795	18.889	204.631	197.204	1.12E-13	196.598	1.35E-13
(3b)		223.138	134.196	46.470	31.315						
(5)	-1736.913	3.670	-115.808	-117.251	-122.410	-163.610	25.182	89.506	5.41E+02	79.422	3.67E+02
(-5)								206.756	1.43E-13	201.832	2.00E-14
(6)	-901.192	13.462	-11.488	-16.780	-25.742	-191.629	70.981	146.320	8.27E-05	150.240	7.73E-07

TEMPO-PMMA										
298.15 K										
(2)	-1144.276	-22.243	-119.266	-112.634		-205.222	1.610	62.797	3.84E+03	
(2) M	-1355.282	-36.562	-120.464	-109.564		-202.202	34.491	94.777	9.46E-02	
(3a)	-362.867	219.111	52.709	-12.619		-9.473	198.615	201.440	7.24E-23	
(3a) M	-470.148	204.793	46.656	-14.403		18.993	215.990	210.327	3.32E-24	
(3b)	-1355.524	214.935	112.977	48.894		14.601	180.778	176.425	2.00E-17	
(3b) M	-1207.846	200.616	106.924	47.110		-3.823	137.721	138.861	4.43E-11	
(-3b) M								91.751	7.94E-03	
(4)	-1623.308	4.177	-60.223	-61.468		0.657	104.627	104.431	4.47E-04	
(5)	-1465.419	-17.593	-96.800	-91.554		-185.396	74.051	129.327	2.59E-07	
(-5)								220.881	2.36E-23	
393.15 K										
(2)	-1144.276	-21.576	-119.035	-110.552	-109.866	-202.925	2.406	82.186	7.19E+03	77.986	8.06E+02
(2) M	-1355.282	-36.511	-120.441	-106.086	-103.505	-200.238	35.175	113.899	1.80E+00	109.841	1.93E-01
(3a)	-362.867	218.061	52.336	-33.394	-34.210	-11.385	197.957	202.433	2.22E-14	201.617	2.85E-14
(3a) M	-470.148	203.125	46.076	-33.783	-32.703	17.160	215.358	208.612	5.37E-15	206.407	1.05E-14
(3b)	-1355.524	212.232	112.036	28.597	15.376	14.325	180.679	175.047	3.11E-10	168.039	2.65E-09
(3b) M	-1207.846	197.297	105.776	28.209	16.883	-4.893	137.353	139.277	1.85E-05	128.658	4.76E-04
(-3b) M								111.068	1.03E-01	111.775	8.33E-02
(4)	-1623.308	5.828	-59.655	-61.947	-49.541	0.890	104.706	104.356	8.45E-01	113.251	5.56E-02
(5)	-1465.419	-19.737	-97.537	-89.777	-89.308	-183.910	74.567	146.871	3.61E-05	138.574	1.42E-05
(-5)								236.648	4.27E-17	227.883	1.93E-17
SG1-PMMA										
298.15 K										
(2)	-812.434	-22.666	-103.200	-96.442		-212.898	-1.587	61.888	4.12E+03	
(2) M	-318.349	-36.985	-109.253	-98.226		-205.766	13.999	75.348	3.18E+01	
(3a)		232.766	44.540	-24.859						
(3a) M		218.448	38.487	-26.644						
(3b)	-1366.852	226.604	110.416	42.854		-13.451	162.132	166.142	1.14E-15	
(3b) M	-1256.479	212.285	104.362	41.069		1.592	125.508	125.034	1.13E-08	
(-3b) M								83.964	1.77E-01	
(4)	-1656.563	6.163	-65.855	-67.693		8.545	109.054	106.506	6.43E-01	
(5)		-17.170	-108.011	-102.892		-179.217	32.226	85.659	5.80E+00	
(-5)	-1523.683							188.551	5.47E-18	
393.15 K										
(2)	-812.434	-22.713	-103.212	-94.282	-91.420	-209.958	-0.572	81.973	6.27E+03	83.784	1.12E+02

(2) M	-318.349	-37.649	-109.472	-94.671	-89.913	-203.967	14.626	94.816	2.12E+02	93.251	1.06E+01
(3a)		230.913	43.892	-46.891	-46.318						
(3a) M		215.977	37.632	-47.280	-44.811						
(3b)	-1366.852	223.802	109.441	21.453	2.479	-14.169	161.882	167.453	3.15E-09	168.252	2.46E-09
(3b) M	-1256.479	208.867	103.181	21.065	3.986	0.523	125.142	124.937	1.50E-03	118.385	1.12E-02
(-3b) M								103.872	9.47E-01	114.399	3.78E-02
(4)	-1656.563	7.110	-65.528	-68.324	-48.776	9.023	109.216	105.669	6.43E-01	118.819	1.15E-02
(5)		-18.600	-108.505	-101.192	-102.899	-176.607	33.124	102.557	2.50E+01	93.168	1.37E+01
(-5)	-1523.683							203.750	8.98E-13	196.068	2.92E-13
					DPAIO-PMMA						
					298.15 K						
(2)	-378.085	-21.524	-112.429	-106.012		-223.458	-2.202	64.422	7.84E+02		
(2) M		-35.843	-118.482	-107.796							
(3a)		226.106	85.533	18.119							
(3a) M		211.788	79.480	16.335							
(3b)		222.879	181.648	115.196							
(3b) M		208.561	175.594	113.412							
(5)	-1701.576	-18.312	-98.782	-93.322		-178.464	3.103	56.312	3.25E+04		
(-5)								151.452	6.99E-13		
					393.15 K						
(2)	-378.085	-20.812	-112.184	-104.002	-110.864	-221.298	-1.454	85.549	1.12E+03	81.139	1.34E+02
(2) M		-35.748	-118.445	-104.391	-109.357						
(3a)		225.132	85.186	-3.325	-4.977						
(3a) M		210.197	78.925	-3.713	-3.471						
(3b)		220.364	180.772	94.136	87.538						
(3b) M		205.428	174.512	93.748	89.045						
(5)	-1701.576	-20.501	-99.532	-91.472	-83.456	-176.648	3.731	73.181	6.53E+04	69.444	6.35E+03
(-5)								166.471	2.63E-08	154.718	2.97E-08

[a] Calculated using G3(MP2)-RAD method or an ONIOM approximation to it; [b] 'M' denotes reactions of H-abstraction from methyl group of PMMA model; [b] Solution of a corresponding monomer, solvation free energies are calculated using COSMO-RS method; [d] 'X' is 1 for unimolecular reactions and L mol^{-1} for bimolecular reactions.

Appendix S1. Contributions to the gas and solution-phase free energies of species

Table S7. Calculated energies

Raw electronic energies, zero-point vibrational, entropic and thermal corrections, gas-phase Gibbs free energies at 25 and 120 °C (298.15 and 393.15 K, respectively), as well as free energies of solvation in bulk monomer solutions at 120 °C.[a]

Species[b]	Raw $E°$, Hartrees[c]		$E°_{ONIOM}$,	S, J mol^{-1} K^{-1}		T_c, Hartrees		$ZPVE$,	G_{gas}, Hartrees		ΔG_{solv},[d]
	low	high	Hartrees	298 K	393 K	298 K	393 K	Hartrees	298 K	393 K	kcal mol^{-1}
TEMPO-PS											
•CH(Et)Ph (c)	-348.73335	-349.06389									
•P	-618.50261		-618.83314	527.1163	604.7612	0.01529	0.02554	0.27666	-618.60105	-618.62150	-11.346
Me_2NO• (c)	-209.31176	-209.47574									
TEMPO•	-482.68701		-482.85099	436.0087	501.4818	0.01291	0.02154	0.25852	-482.62907	-482.64602	-7.822
MeCH=CHPh (c)	-348.16860	-348.48815									
P(-H)	-617.93645		-618.25600	520.1564	595.7729	0.01506	0.02504	0.26682	-618.03318	-618.05335	-11.639
Me_2NOH (c)	-209.93496	-210.10521									
TEMPOH	-483.30210		-483.47234	428.5752	496.4265	0.01307	0.02202	0.27004	-483.23790	-483.25462	-6.896
•CH(Et)Ph (c)	-348.73325	-349.06389									
•P	-618.50240		-618.83303	527.1163	604.7612	0.01529	0.02554	0.27666	-618.60094	-618.62139	-11.346
Me_2NO• (c)	-209.31173	-209.47574									
TEMPO•	-482.68690		-482.85091	436.0087	501.4818	0.01291	0.02154	0.25852	-482.62899	-482.64594	-7.822
MeCH=CHPh (c)	-348.16849	-348.48815									
P(-H)	-617.93627		-618.25592	520.1564	595.7729	0.01506	0.02504	0.26682	-618.03311	-618.05328	-11.639
Me_2NOH (c)	-209.93491	-210.10521									
TEMPOH	-483.30194		-483.47224	428.5752	496.4265	0.01307	0.02202	0.27004	-483.23780	-483.25452	-6.896
TS2 (c)	-558.02536	-558.52678									
TS2	-1101.17288		-1101.67430	774.6754	919.6015	0.02826	0.04738	0.53328	-1101.20072	-1101.23134	-18.275
$Me_2NOCH(Et)Ph$ (c)	-558.13545	-558.62086									
TEMPOP	-1101.27489		-1101.76031	738.5113	882.2649	0.02736	0.04632	0.54139	-1101.27542	-1101.30470	-16.903
TS3a (c)	-558.03983	-558.52400									
TS3a	-1101.19430		-1101.67847	734.3882	876.6206	0.02701	0.04578	0.53781	-1101.19704	-1101.22614	-16.784
$Me_2NH{\rightarrow}O$ (c)	-209.90719	-210.07647									
TEMPH→O	-483.28088		-483.45015	424.3985	490.5982	0.01276	0.02149	0.27122	-483.21437	-483.23091	-9.871
CH_2(Et)Ph (c)	-349.38421	-349.71747									
PH	-619.15390		-619.48716	521.0078	598.5929	0.01532	0.02556	0.29036	-619.24064	-619.26087	-11.191
•CH(Et)Ph (c)	-348.61602	-349.06389									
•P	-618.29943		-618.74730	527.1163	604.7612	0.01529	0.02554	0.27666	-618.51520	-618.53566	-11.346

Me_2NOH (c)	-209.84617	-210.10521									
TEMPOH	-483.11606		-483.37509	428.5752	496.4265	0.01307	0.02202	0.27004	-483.14065	-483.15737	-6.896
Me_2NO• (c)	-209.22637	-209.47574									
TEMPO•	-482.50487		-482.75424	436.0087	501.4818	0.01291	0.02154	0.25852	-482.53232	-482.54927	-7.822
CH_2(Et)Ph	-349.26480	-349.71747									
PH	-618.94881		-619.40148	521.0078	598.5929	0.01532	0.02556	0.29036	-619.15496	-619.17519	-11.191
TS5 (c)	-558.45080	-559.15193									
TS5	-1101.40960		-1102.11073	782.7746	929.4904	0.02851	0.04787	0.54358	-1101.62752	-1101.65846	-18.239
•CH(Me)CH=CH_2 (c1)	-156.14026	-156.36367									
•CH(Me)Ph (c2)	-309.41196		-309.41196	362.2665	402.0602	0.00841	0.01366	0.14049			
•P	-618.29943		-618.56838	527.1163	604.7612	0.01529	0.02554	0.27666	-618.33628	-618.35674	-11.346
Me_2NOCH(Me)CH=CH_2 (c1)	-365.44191	-365.91304									
TEMPOCH(Me)Ph (c2)	-791.99446		-791.99446	583.2595	689.0722	0.02020	0.03416	0.40539			
TEMPOP	-1100.88951		-1101.50351	738.5113	882.2649	0.02736	0.04632	0.54139	-1101.01862	-1101.04790	-16.903
TS6 (c1)	-521.55556	-522.24824									
TS6 (c2)	-1101.38961		-1101.38961	754.5216	902.5753	0.02841	0.04794	0.54358			
TS6	-1719.18150		-1720.06285	1069.203	1293.440	0.04294	0.07252	0.81509	-1719.32624	-1719.36892	-26.081
EtCH=CH_2 (c1)	-156.77618	-157.01126									
CH_3CH_2Ph (c2)	-310.05985		-310.05985	356.2507	395.8788	0.00827	0.01349	0.15443			
PH	-618.94881		-619.22952	521.0078	598.5929	0.01532	0.02556	0.29036	-618.98300	-619.00323	-11.191
Me_2NOC•(Me)CH=CH_2 (c1)	-364.80700	-365.26855									
TEMPOC•(Me)Ph (c2)	-791.35484		-791.35484	599.2759	705.0606	0.02050	0.03445	0.39182			
TEMPOP•	-1100.24306		-1100.84726	744.5779	888.2480	0.02745	0.04641	0.52820	-1100.37616	-1100.40566	-17.358
SG1-PBA											
•CH(Et)COOMe (c)	-345.68371	-345.95005									
•P	-612.40945		-612.67578	520.9942	585.6444	0.01516	0.02367	0.20251	-612.51728	-612.53730	-9.006
Me_2NO• (c)	-209.31176	-209.47574									
SG1•	-1129.25885		-1129.42283	646.0508	753.0813	0.02310	0.03719	0.35903	-1129.11407	-1129.13938	-11.132
MeCH=CHCOOMe (c)	-345.12483	-345.38298									
P(-H)	-611.84697		-612.10512	510.4676	573.1348	0.01485	0.02310	0.19250	-611.95574	-611.97535	-9.458
Me_2NOH (c1)	-209.93115	-210.10132									
SG1H	-1129.86960		-1130.03977	638.1943	746.8886	0.02309	0.03740	0.37061	-1129.71855	-1129.74360	-10.180
•CH(Et)COOMe (c1)	-345.68366	-345.95005									
•P	-612.40938		-612.67576	520.9942	585.6444	0.01516	0.02367	0.20251	-612.51726	-612.53728	-9.006
Me_2NO• (c)	-209.31173	-209.47574									
SG1•	-1129.25873		-1129.42274	646.0508	753.0813	0.02310	0.03719	0.35903	-1129.11397	-1129.13928	-11.132
CH_3CH=CHCOOMe (c)	-345.12478	-345.38298									
P(-H)	-611.84690		-612.10510	510.4676	573.1348	0.01485	0.02310	0.19250	-611.95572	-611.97533	-9.458
Me_2NOH (c1)	-209.93110	-210.10132									

SG1H	-1129.86947		-1130.03969	638.1943	746.8886	0.02309	0.03740	0.37061	-1129.71846	-1129.74352	-10.180
TS2 (c)	-554.99310	-555.41433									
TS2	-1741.67079		-1742.09202	960.9648	1134.750	0.03825	0.06114	0.55876	-1741.60413	-1741.64204	-19.017
$Me_2NOCH(Et)COOMe$ (c)	-555.08752	-555.51250									
SG1P	-1741.74981		-1742.17479	917.4235	1089.776	0.03699	0.05969	0.56777	-1741.67421	-1741.71051	-18.138
TS3a (c)	-554.99037	-555.41362									
TS3	-1741.66998		-1742.09323	937.6468	1108.665	0.03704	0.05956	0.56429	-1741.59839	-1741.63540	-18.283
$Me_2NH{\rightarrow}O$ (c)	-209.90719	-210.07647									
SG1H→O	-1129.84634		-1130.01562	632.0318	739.7782	0.02292	0.03711	0.37180	-1129.69267	-1129.71749	-15.016
$EtCH_2COOMe$ (c)	-346.34115	-346.61328									
PH	-613.06621		-613.33834	518.0892	583.1221	0.01531	0.02387	0.21561	-613.16625	-613.18617	-9.287
TS5 (c)	-555.60343	-556.03991									
TS5	-1742.26696		-1742.70344	993.2251	1168.923	0.03883	0.06197	0.56980	-1742.20759	-1742.24670	-18.882
•CH(Me)COOH (c)	-267.26300	-267.44273									
•P	-612.40938		-612.58911	520.9942	585.6444	0.01516	0.02367	0.20251	-612.43061	-612.45063	-9.006
$Me_2NOCH(Me)COOH$ (c)	-476.66521	-477.00383									
SG1P	-1741.74981		-1742.08843	917.4235	1089.776	0.03699	0.05969	0.56777	-1741.58785	-1741.62415	-18.138
CH_3CH_2COOH (c)	-267.91990	-268.10549									
PH	-613.06621		-613.25180	518.0892	583.1221	0.01531	0.02387	0.21561	-613.07971	-613.09963	-9.287
$Me_2NOC•(Me)COOH$ (c)	-476.01778	-476.35043									
SG1P•	-1741.09759		-1741.43024	933.4753	1105.760	0.03731	0.05999	0.55428	-1740.94465	-1740.98154	-19.999
•CH(Me)COOH (c1)	-267.15804	-267.44273									
•P	-612.17212		-613.24959	520.9942	585.6444	0.01516	0.02367	0.20251	-613.09108	-613.11110	-9.006
$Me_2NOCH(Me)COOH$ (c1)	-476.47435	-477.00383									
SG1P	-1741.16687		-1744.28706	917.4235	1089.776	0.03699	0.05969	0.56777	-1743.78648	-1743.82278	-18.138
CH_3CH_2COOH (c1)	-267.81260	-268.10549									
PH	-612.82637		-613.91201	518.0892	583.1221	0.01531	0.02387	0.21561	-613.73993	-613.75985	-9.287
$Me_2NOC•(Me)COOH$ (c1)	-475.82883	-476.35043									
SG1P•	-1740.51665		-1743.62718	933.4753	1105.760	0.03731	0.05999	0.55428	-1743.14160	-1743.17849	-19.999
TS6 (c1)	-743.61766	-744.42768									
TS6	-2353.21485		-2357.50660	1243.649	1483.791	0.05255	0.08417	0.76646	-2356.82882	-2356.87816	-23.493
TEMPO-PMMA											
•CH(Et)(Me)COOMe (c)	-384.91070	-385.21922									
•P	-690.86104		-691.16956	563.4392	642.6184	0.01801	0.02844	0.25777	-690.95776	-690.97958	-9.389
$Me_2NO•$ (c)	-209.31176	-209.47574									
TEMPO•	-482.68701		-482.85099	436.0087	501.4818	0.01291	0.02154	0.25852	-482.62907	-482.64602	-7.751
MeCH=C(Me)COOMe (c)	-384.34710	-384.64731									
P(-H)	-690.29271		-690.59292	548.6295	626.0979	0.01759	0.02779	0.24761	-690.39002	-690.41127	-9.610

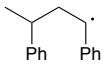
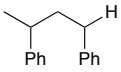
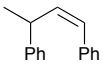
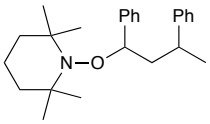
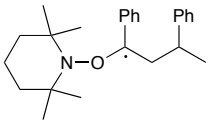
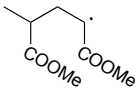
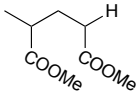
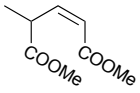
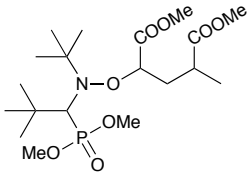
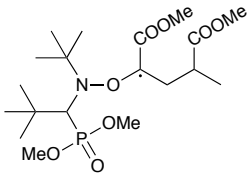
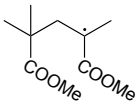
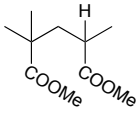
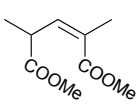
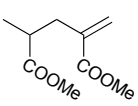
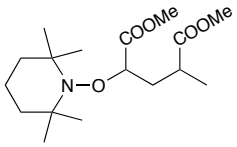
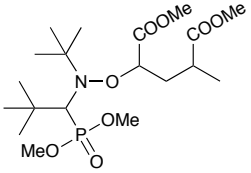
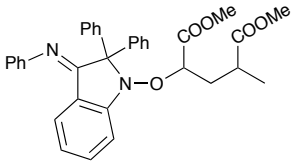
Me_2NOH (c)	-209.93496	-210.10521									
TEMPOH	-483.30210		-483.47234	428.5752	496.4265	0.01307	0.02202	0.27004	-483.23790	-483.25462	-7.366
•CH(Et)(Me)COOMe (c)	-384.91064	-385.21922									
•P	-690.86096		-691.16953	563.4392	642.6184	0.01801	0.02844	0.25777	-690.95773	-690.97955	-9.389
Me_2NO• (c)	-209.31173	-209.47574									
TEMPO•	-482.68690		-482.85091	436.0087	501.4818	0.01291	0.02154	0.25852	-482.62899	-482.64594	-7.751
MeCH=C(Me)COOMe (c)	-384.34704	-384.64731									
P(-H)	-690.29260		-690.59287	548.6295	626.0979	0.01759	0.02779	0.24761	-690.38997	-690.41123	-9.610
EtC(=CH_2)COOMe (c)	-384.34371	-384.64431									
P(-H) M	-690.29471		-690.59531	534.3112	611.1623	0.01708	0.02721	0.24825	-690.39065	-690.41137	-9.157
Me_2NOH (c)	-209.93491	-210.10521									
TEMPOH	-483.30194		-483.47224	428.5752	496.4265	0.01307	0.02202	0.27004	-483.23780	-483.25452	-7.366
TS2 (c)	-594.26206	-594.71801									
TS2	-1173.56100		-1174.01695	794.2262	941.1748	0.03066	0.05002	0.51368	-1173.56281	-1173.59418	-15.430
TS2 M (c)	-594.25940	-594.71744									
TS2 M	-1173.54631		-1174.00434	797.2464	943.8619	0.03048	0.04980	0.51377	-1173.55062	-1173.58211	-15.396
$Me_2NOC(Me)(Et)COOMe$ (c)	-594.31300	-594.77995									
TEMPOP	-1173.62149		-1174.08844	758.0933	904.4639	0.02966	0.04895	0.52190	-1173.62297	-1173.65303	-14.067
TS3a (c)	-594.21172	-594.67733									
TS3a	-1173.54334		-1174.00895	748.6206	893.0787	0.02916	0.04820	0.51855	-1173.54624	-1173.57592	-14.262
TS3a M (c)	-594.21068	-594.67621									
TS3a M	-1173.53691		-1174.00243	777.0865	921.6235	0.02963	0.04868	0.51819	-1173.54286	-1173.57357	-14.594
TS3b (c)	-594.25493	-594.71317									
TS3b	-1173.55601		-1174.01424	772.6940	918.7885	0.02992	0.04918	0.51629	-1173.55577	-1173.58635	-15.742
TS3b M (c)	-594.25450	-594.71416									
TS3b M	-1173.57106		-1174.03072	754.2706	899.5709	0.02939	0.04854	0.51690	-1173.57008	-1173.59998	-16.605
$Me_2NH{\rightarrow}O$ (c)	-209.90719	-210.07647									
TEMPH→O	-483.28088		-483.45015	424.3985	490.5982	0.01276	0.02149	0.27122	-483.21437	-483.23091	-10.331
$Me_2NH{\rightarrow}O$ (c)	-209.90723	-210.07647									
TEMPH→O	-483.28104		-483.45027	424.3985	490.5982	0.01276	0.02149	0.27122	-483.21449	-483.23102	-10.331
TS4 (c)	-209.86357	-210.03240									
TS4	-483.23658		-483.40542	425.0552	491.4887	0.01280	0.02156	0.26617	-483.17471	-483.19128	-8.205
TS5 (c)	-594.83209	-595.30991									
TS5	-1174.13271		-1174.61053	806.6180	955.1347	0.03095	0.05052	0.52490	-1174.14628	-1174.17813	-16.024
EtCH(Me)COOMe (c)	-385.56372	-385.87774									
PH	-691.51547		-691.82949	538.4124	617.8258	0.01759	0.02805	0.27162	-691.60142	-691.62233	-8.892
SG1-PMMA											
•CH(Et)(Me)COOMe (c)	-384.91070	-385.21922									
•P	-690.86104		-691.16956	563.4392	642.6184	0.01801	0.02844	0.25777	-690.95776	-690.97958	-9.389
Me_2NO• (c)	-209.31176	-209.47574									

SG1•	-1129.25885		-1129.42283	646.0508	753.0813	0.02310	0.03719	0.35903	-1129.11407	-1129.13938	-11.040
MeCH=C(Me)COOMe (c)	-384.34710	-384.64731									
P(-H)	-690.29271		-690.59292	548.6295	626.0979	0.01759	0.02779	0.24761	-690.39002	-690.41127	-9.610
Me_2NOH (c1)	-209.93115	-210.10132									
SG1H	-1129.86960		-1130.03977	638.1943	746.8886	0.02309	0.03740	0.37061	-1129.71855	-1129.74360	-10.135
•CH(Et)(Me)COOMe (c)	-384.91064	-385.21922									
•P	-690.86096		-691.16953	563.4392	642.6184	0.01801	0.02844	0.25777	-690.95773	-690.97955	-9.389
Me_2NO• (c)	-209.31173	-209.47574									
SG1•	-1129.25873		-1129.42274	646.0508	753.0813	0.02310	0.03719	0.35903	-1129.11397	-1129.13928	-11.040
MeCH=C(Me)COOMe (c)	-384.34704	-384.64731									
P(-H)	-690.29260		-690.59287	548.6295	626.0979	0.01759	0.02779	0.24761	-690.38997	-690.41123	-9.610
$EtC(=CH_2)COOMe$ (c)	-384.34371	-384.64431									
P(-H) M	-690.29471		-690.59531	534.3112	611.1623	0.01708	0.02721	0.24825	-690.39065	-690.41137	-9.157
Me_2NOH (c1)	-209.93110	-210.10132									
SG1H	-1129.86947		-1130.03969	638.1943	746.8886	0.02309	0.03740	0.37061	-1129.71846	-1129.74352	-10.135
TS2 (c)	-594.21633	-594.68355									
TS2	-1820.12241		-1820.58962	996.5921	1185.741	0.04114	0.06605	0.61352	-1820.04813	-1820.08761	-17.282
TS2 M (c)	-594.25941	-594.71744									
TS2 M	-1820.12660		-1820.58463	1003.724	1191.733	0.04076	0.06552	0.61484	-1820.04301	-1820.08272	-18.089
$Me_2NOC(Me)(Et)COOMe$	-594.31305	-594.78007									
SG1P	-1820.18578		-1820.65280	954.0577	1142.074	0.03972	0.06448	0.62246	-1820.09897	-1820.13688	-17.168
TS3b (c)	-594.25888	-594.71707									
TS3b	-1820.12796		-1820.58615	940.6070	1127.905	0.03946	0.06412	0.61781	-1820.03569	-1820.07310	-16.977
TS3b M (c)	-594.25834	-594.71775									
TS3b M	-1820.14036		-1820.59978	955.6496	1142.597	0.03947	0.06410	0.61748	-1820.05135	-1820.08930	-18.734
$Me_2NH{\rightarrow}O$ (c)	-209.90719	-210.07647									
SG1H→O	-1129.84634		-1130.01562	632.0318	739.7782	0.02292	0.03711	0.37180	-1129.69267	-1129.71749	-14.807
$Me_2NH{\rightarrow}O$ (c)	-209.90723	-210.07647									
SG1H→O	-1129.84648		-1130.01571	632.0318	739.7782	0.02292	0.03711	0.37180	-1129.69276	-1129.71757	-14.807
TS4 (c)	-209.86357	-210.03240									
TS4	-1129.79976		-1129.96860	640.5769	748.8012	0.02314	0.03739	0.36601	-1129.65220	-1129.67733	-11.664
TS5 (c)	-594.83059	-595.30839									
TS5	-1820.71588		-1821.19368	1022.417	1212.900	0.04143	0.06651	0.62478	-1820.64357	-1820.68401	-19.054
EtCH(Me)COOMe (c)	-385.56372	-385.87774									
PH	-691.51547		-691.82949	538.4124	617.8258	0.01759	0.02805	0.27162	-691.60142	-691.62233	-8.892
DPAIO-PMMA											
•CH(Et)(Me)COOMe (c)	-384.91064	-385.21922									
•P	-690.86096		-691.16953	563.4392	642.6184	0.01801	0.02844	0.25777	-690.95773	-690.97955	-9.389
•Iminopyrrol-*N*-oxyl (c)	-339.40379	-339.64623									
DPAIO•	-1184.38602		-1184.62846	689.9340	812.8981	0.02347	0.03970	0.37324	-1184.31009	-1184.33724	-20.580
TS2 (c)	-724.31013	-724.85529									

TS2	-1875.25128		-1875.79643	1029.915	1234.219	0.04118	0.06812	0.62892	-1875.24329	-1875.28421	-28.309
MeCH=C(Me)COOMe (c)	-384.34704	-384.64731									
P(-H)	-690.29260		-690.59287	548.6295	626.0979	0.01759	0.02779	0.24761	-690.38997	-690.41123	-9.610
EtC(=CH_2)COOMe (c)	-384.34371	-384.64431									
P(-H) M	-690.29471		-690.59531	534.3112	611.1623	0.01708	0.02721	0.24825	-690.39065	-690.41137	-9.157
Iminopyrrol-NOH (c)	-340.02497	-340.26998									
DPAIOH	-1185.00402		-1185.24903	683.2195	808.6065	0.02382	0.04036	0.38457	-1184.91823	-1184.94518	-21.999
Iminopyrrol-NOC(Me)(Et)COOMe (c)	-724.40378	-724.94529									
DPAIOP	-1875.33612		-1875.87763	1005.743	1209.572	0.04045	0.06733	0.63628	-1875.31511	-1875.35514	-28.500
Iminopyrrol-NH→O (c)	-339.98367	-340.22994									
DPAIH→O	-1184.96686		-1185.21313	679.9925	803.8378	0.02346	0.03981	0.38563	-1184.88126	-1184.90806	-23.181
EtCH(Me)COOMe (c)	-385.56372	-385.87774									
PH	-691.51547		-691.82949	538.4124	617.8258	0.01759	0.02805	0.27162	-691.60142	-691.62233	-8.892
•CH(Et)(Me)COOMe (c)	-384.76163	-385.21922									
•P	-690.59420		-691.05179	563.4392	642.6184	0.01801	0.02844	0.25777	-690.83999	-690.86180	-9.389
Iminopyrrol-NOH (c)	-339.89714	-340.26998									
DPAIOH	-1184.61839		-1184.99124	683.2195	808.6065	0.02382	0.04036	0.38457	-1184.66044	-1184.68739	-21.999
TS5 (c)	-724.64718	-725.47644									
TS5	-1875.20929		-1876.03855	1068.195	1274.577	0.04187	0.06908	0.63901	-1875.47898	-1875.52132	-29.567
•Iminopyrrol-*N*-oxyl (c)	-339.27958	-339.64623									
•DPAIO	-1184.00441		-1184.37106	689.9340	812.8981	0.02347	0.03970	0.37324	-1184.05270	-1184.07985	-20.580
EtCH(Me)COOMe (c)	-385.41260	-385.87774									
PH	-691.24690		-691.71203	538.4124	617.8258	0.01759	0.02805	0.27162	-691.48396	-691.50488	-8.892

[a] Calculated using G3(MP2)-RAD method or an ONIOM approximation to it in conjunction with optimized B3LYP/6-31G(d) geometries and scaled frequencies; [b] P• is a corresponding dimeric propagating radical (see Figure S10 below), (c) denotes the species used for a core layer in ONIOM approximation to the full compound in the next row, → denotes N^+–O^- bond in the *N*-oxides, 'M' denotes reactions of H-abstraction from methyl group of PMMA model; [c] 'Low' corresponds to a level of theory used for the full system in ONIOM approximation (R(O)MP2/6-311+G(3df,2p), RI-R(O)MP2/6-311+G(3df,2p), RI-R(O)MP2/6-31+G(2df,p) or B3LYP/6-31G(d)), 'high' stands for the G3(MP2)-RAD method applied to the core layer; [d] Gibbs free energy of solvation in bulk monomer solution at 120 °C, calculated using COSMO-RS method at the BP/TZVP level of theory in conjunction with optimized UAKS-CPCM/B3LYP/6-31G(d) geometries.

Figure S10. Structures of the various reactive species in five studied polymerization systems

	P•	PH	P(-H)	P(-H) M	R'R"NO-P	R'R"NO-P•
TEMPO-PS				n/a		
SG1-PBA				n/a		
TEMPO-PMMA						n/a
SG1-PMMA	-"-	-"-	-"-	-"-		n/a
DPAIO-PMMA	-"-	-"-	-"-	-"-		n/a

Appendix S2. Geometries of all the species in the present work

NOTE: All species had either zero imaginary frequencies, or one in the case of transition states, as determined from frequency calculations at the B3LYP/6-31G(d) level.

TEMPO-PS

•CH(Et)Ph (c)

1\1\GINC-X140\FOpt\UB3LYP\Gen\C9H11(2)\GXG501\04-Jun-2012\0\\#B3LYP/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\
\ps_rcore.freq\\0,2\C,-6.3106288372,2.4639494704,-0.0814381812\H,-5.63
4217894,1.6218859148,-0.2200729255\C,-5.8524148103,3.7400634719,-0.488
8793501\C,-6.6440001721,4.9183739693,-0.3593273455\C,-6.1620584678,6.1
535967606,-0.7696237396\C,-4.8808090311,6.2729454305,-1.3234439661\C,-
4.0816158758,5.1289662502,-1.4620758074\C,-4.5529032327,3.8907411906,-
1.0557615905\H,-7.639944454,4.8468529713,0.0676617349\H,-6.7870987488,
7.0363743842,-0.6591745192\H,-4.5097922782,7.2428022807,-1.6425766023\
H,-3.0860348161,5.2122161942,-1.8908007008\H,-3.9273912621,3.007762816
3,-1.166232787\C,-7.6528406983,2.1798352768,0.5258309882\H,-7.78888127
53,2.7822565691,1.4392418234\H,-8.4533218758,2.5137073998,-0.154940405
4\C,-7.8605868217,0.6984865345,0.8619639313\H,-8.8484433757,0.52692495
36,1.3026325415\H,-7.1078902177,0.3480807293,1.5778873874\H,-7.7810213
198,0.0760559196,-0.0369945232\\Version=EM64L-G09RevB.01\State=2-A\HF=
-349.5466276\S2=0.779757\S2-1=0.\S2A=0.750606\RMSD=4.964e-09\RMSF=5.31
2e-06\Dipole=-0.1074608,-0.0988349,0.063174\Quadrupole=1.1958502,1.600
2614,-2.7961116,-0.1471273,-2.0512573,-0.853544\PG=C01 [X(C9H11)]\\@

•P

1\1\GINC-X105\FOpt\UB3LYP\Gen\C16H17(2)\GXG501\04-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\ps_r.freq\\0,2\C,-6.2658819492,2.4881206537,0.196510135\C,-5.2291028
844,1.3501470838,0.139686872\C,-3.9477612544,1.8187793028,-0.593158149
\C,-2.9436397105,0.7295909086,-0.8182148847\H,-7.1886241798,2.15449105
77,0.682862898\H,-6.5177261003,2.8365696124,-0.8122984381\H,-5.8836290
818,3.3466634704,0.7614707993\H,-5.6622082022,0.5367430581,-0.45830666
67\C,-4.9456090885,0.7878887409,1.5271695957\H,-3.4949955596,2.6476141
416,-0.0204618711\H,-4.2465346383,2.2656587906,-1.5526435277\H,-3.0125
997613,-0.1489440763,-0.1803889031\C,-1.8866762589,0.7662448905,-1.759
5458626\C,-4.3315948683,1.5663308039,2.5205487579\C,-4.0948505225,1.05
05233265,3.7942037364\C,-4.4682659559,-0.2595218022,4.103521787\C,-5.0
792087722,-1.0460941381,3.1273970771\C,-5.3136995983,-0.523893375,1.85
32886274\C,-0.9976609944,-0.3434180338,-1.8746691324\C,0.0457852741,-0
.3428135139,-2.78627947\C,0.2554312499,0.7617980217,-3.6245015455\C,-0
.6000821884,1.8671122067,-3.5305934673\C,-1.6486845065,1.8768101804,-2
.6213634696\H,-4.0331740167,2.5882389647,2.2984193925\H,-3.6167965806,
1.6723226517,4.5469243868\H,-4.2831075458,-0.6618540409,5.0959220944\H
,-5.3741851617,-2.0674491158,3.354413097\H,-5.792565475,-1.1442921367,
1.0985084503\H,-1.1537095023,-1.2033608805,-1.2273363063\H,0.705421885
7,-1.204635125,-2.8502692393\H,1.0741518227,0.7611182663,-4.3385192349
\H,-0.4419431015,2.7286935713,-4.1747225594\H,-2.2951327726,2.74729653
4,-2.5622479793\\Version=EM64L-G09RevB.01\State=2-A\HF=-619.9090768\S2
=0.779968\S2-1=0.\S2A=0.750615\RMSD=8.373e-09\RMSF=1.288e-06\Dipole=-0
.1611631,0.073385,0.0773106\Quadrupole=-2.2648335,2.2579102,0.0069233,
-0.0594196,-0.3913278,-1.9530433\PG=C01 [X(C16H17)]\\@

Me_2NO• (c)

1\1\GINC-X5\FOpt\UB3LYP\Gen\C2H6N1O1(2)\GXG501\01-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280

\\dmno_r.freq\\0,2\N,0.1133169818,-0.7476260729,-0.222995057\O,0.25868
37008,-2.0172658141,-0.0964932201\C,-0.0280321604,0.0417501064,0.99725
25746\C,-0.4987696703,-0.2564114627,-1.4543182282\H,0.2314989596,1.087
0015291,0.8019479214\H,0.649255583,-0.379671783,1.7415136426\H,-1.0580
938645,-0.0048754347,1.3817778987\H,-0.2325389705,0.7930834231,-1.6147
318986\H,-0.1220329661,-0.8682001012,-2.2753077234\H,-1.5949508858,-0.
3449166009,-1.4141390846\\Version=EM64L-G09RevB.01\State=2-A'\HF=-209.
7185634\S2=0.753314\S2-1=0.\S2A=0.750007\RMSD=6.261e-09\RMSF=8.840e-06
\Dipole=-0.3577638,1.1677133,-0.0733221\Quadrupole=0.03852,-2.071597,2
.0330771,0.6056015,0.3307864,0.3965186\PG=CS [SG(N1O1),X(C2H6)]\\@

TEMPO•

1\1\GINC-X107\FOpt\UB3LYP\Gen\C9H18N1O1(2)\GXG501\01-Jun-2012\0\\#B3LY
P/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177
280\\tempo.freq\\0,2\N,0.,-0.7435629979,-0.2018749548\O,0.,-2.01955837
26,-0.0452138765\C,0.,2.1287431572,0.022478889\H,0.,3.1643266531,-0.33
89095322\H,0.,2.1853670546,1.1183573257\C,1.2468109685,1.4016096686,-0
.4843632856\C,-1.2468109685,1.4016096686,-0.4843632856\C,1.332094799,-
0.0692232091,-0.0280357781\C,-1.332094799,-0.0692232091,-0.0280357781\
C,2.3390131141,-0.8257078879,-0.9101375173\C,-2.3390131141,-0.82570788
79,-0.9101375173\C,1.7656296787,-0.1817542896,1.4491795741\C,-1.765629
6787,-0.1817542896,1.4491795741\H,2.1614438326,1.9129009799,-0.1595530
52\H,-2.1614438326,1.9129009799,-0.159553052\H,1.2445020187,1.43111212
19,-1.5827455901\H,-1.2445020187,1.4311121219,-1.5827455901\H,2.020177
8627,-0.812821417,-1.9578535715\H,-2.0201778627,-0.812821417,-1.957853
5715\H,3.3215611799,-0.3455230276,-0.8413559353\H,-3.3215611799,-0.345
5230276,-0.8413559353\H,2.4275897199,-1.86604479,-0.5921891872\H,-2.42
75897199,-1.86604479,-0.5921891872\H,2.8058045224,0.1450721711,1.56066
76004\H,-2.8058045224,0.1450721711,1.5606676004\H,1.1483467193,0.43180
94881,2.1125277739\H,-1.1483467193,0.4318094881,2.1125277739\H,1.69017
89976,-1.2236114852,1.7728412125\H,-1.6901789976,-1.2236114852,1.77284
12125\\Version=EM64L-G09RevB.01\State=2-A'\HF=-483.7198066\S2=0.753696
\S2-1=0.\S2A=0.750009\RMSD=4.307e-09\RMSF=5.248e-06\Dipole=0.,1.137060
4,0.061192\Quadrupole=2.820864,-3.6092589,0.7883949,0.,0.,-0.4074767\P
G=CS [SG(C1H2N1O1),X(C8H16)]\\@

MeCH=CHPh (c)

1\1\GINC-X146\FOpt\RB3LYP\Gen\C9H10\GXG501\04-Jun-2012\0\\#B3LYP/gen 6
D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\ps
_dcore.freq\\0,1\C,-5.5713984199,3.093383524,0.8166024352\H,-4.8021064
98,2.3417311752,0.6321430624\C,-5.0524683743,4.4303976075,1.1450408077
\C,-5.8769765718,5.5386363736,1.4174302261\C,-5.3294356402,6.781070213
2,1.7226270992\C,-3.9425528976,6.9539670419,1.7649416874\C,-3.10988799
81,5.8672101023,1.4978293151\C,-3.6604748741,4.6233251663,1.1922762758
\H,-6.9572894559,5.4286336949,1.390730974\H,-5.9879176899,7.6210379522
,1.929083301\H,-3.5185765753,7.925577107,2.0036127291\H,-2.0298352828,
5.9862415909,1.5268049242\H,-3.004142087,3.7808408585,0.9852020173\C,-
6.8531184833,2.7093148209,0.7223909903\H,-7.6499588389,3.4317435152,0.
899638181\C,-7.3009284273,1.3188876095,0.380820678\H,-7.9198664392,0.8
913373832,1.1818345118\H,-7.9194528741,1.3110528396,-0.527507254\H,-6.
4493825309,0.6499591822,0.2167155348\\Version=EM64L-G09RevB.01\State=1
-A\HF=-348.9680409\RMSD=4.669e-09\RMSF=5.980e-06\Dipole=-0.122532,-0.1
032029,-0.0268389\Quadrupole=2.4744967,1.950183,-4.4246797,0.5914155,0
.1452382,1.6715921\PG=C01 [X(C9H10)]\\@

P(-H)

1\1\GINC-X93\FOpt\RB3LYP\Gen\C16H16\GXG501\04-Jun-2012\0\\#B3LYP/gen 6
D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\ps
_d.freq\\0,1\C,-5.5872427585,3.0802691375,0.7491614618\C,-4.50030602,2
.0073817662,0.5151073077\C,-3.1164793645,2.6024824241,0.6481025421\C,-
2.2289734735,2.6900860756,-0.3535370795\H,-6.5883451112,2.6462690901,0
.6493990329\H,-5.4833757627,3.8926184423,0.0218317258\H,-5.5101536238,

3.5182275535,1.7507844911\H,-4.6092625684,1.6439336677,-0.5148992397\C
,-4.6730692443,0.805881973,1.4437153954\H,-2.8634576072,2.9807077902,1
.6388394894\H,-2.5264119464,2.3071792129,-1.3311801189\C,-0.8730839281
,3.2594579402,-0.3079372137\C,-4.8075352838,-0.4833519133,0.9139654725
\C,-4.959891911,-1.5932619015,1.746890466\C,-4.9761310289,-1.431582674
7,3.1324345992\C,-4.8396136583,-0.1523146168,3.6753175391\C,-4.6902328
661,0.9536173303,2.8385403319\C,-0.1386297047,3.3567287667,-1.50296263
65\C,1.148218173,3.8926809262,-1.52180102\C,1.7350264337,4.3439497841,
-0.3394548152\C,1.021397982,4.2504902445,0.8593110926\C,-0.2630223355,
3.7151146631,0.8761141982\H,-4.7928558673,-0.6194792176,-0.165304595\H
,-5.065260434,-2.58372018,1.3114802071\H,-5.0940523965,-2.2933052955,3
.7839701589\H,-4.8503392599,-0.0142813195,4.7535688017\H,-4.5877020301
,1.9421506273,3.2800026416\H,-0.5895492962,3.0071718294,-2.4291982648\
H,1.6920115883,3.9565487712,-2.4607808491\H,2.7383003572,4.7611979259,
-0.3485282656\H,1.4712593226,4.5941943638,1.7873134498\H,-0.795024376,
3.6434728132,1.8203866934\\Version=EM64L-G09RevB.01\State=1-A\HF=-619.
3295699\RMSD=4.393e-09\RMSF=9.531e-07\Dipole=-0.0875133,0.0177069,0.01
46569\Quadrupole=-1.733084,-1.8631402,3.5962242,2.5993677,-0.3287431,1
.2487478\PG=C01 [X(C16H16)]\\@

Me_2NOH (c)

1\1\GINC-X107\FOpt\RB3LYP\Gen\C2H7N1O1\GXG501\01-Jun-2012\0\\#B3LYP/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\
\dmnoh.freq\\0,1\N,-0.0284705719,-0.0532326366,-0.1208525404\O,1.42352
75475,-0.0309015674,-0.075432617\C,-0.4485588091,1.3370134444,0.024098
9673\C,-0.445811943,-0.8642851726,1.0185724006\H,1.659230205,-0.418232
8194,-0.9334537208\H,-0.0783274572,1.9115320379,-0.8289319964\H,-0.075
6700429,1.7990814792,0.9533975891\H,-1.5435488921,1.370143656,0.021760
6543\H,-0.0735920246,-1.8833747604,0.8854805616\H,-0.0728365882,-0.471
6079396,1.9792194766\H,-1.5407283368,-0.8902083798,1.0429124564\\Versi
on=EM64L-G09RevB.01\State=1-A'\HF=-210.3325559\RMSD=4.524e-09\RMSF=3.8
41e-05\Dipole=-0.2617274,-0.0643008,-0.1416089\Quadrupole=-0.518899,0.
2970903,0.2218087,-1.0012626,-2.2140108,-0.0469111\PG=CS [SG(H1N1O1),X
(C2H6)]\\@

TEMPOH

1\1\GINC-X134\FOpt\RB3LYP\Gen\C9H19N1O1\GXG501\01-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\tempoh.freq\\0,1\N,0.0016567883,0.0014023048,0.\O,1.4513717938,0.003
2114167,0.\C,-2.5405938696,1.3341742704,0.\H,-3.6373076341,1.298208162
7,0.\H,-2.2698645361,2.3974116652,0.\C,-1.9957063877,0.6405217959,-1.2
510556892\C,-1.9957063877,0.6405217959,1.2510556892\C,-0.4516051865,0.
5858881081,-1.295029624\C,-0.4516051865,0.5858881081,1.295029624\C,-0.
0271021407,-0.40896686,-2.3931613177\C,-0.0271021407,-0.40896686,2.393
1613177\C,0.1510779631,1.9680389483,-1.6368070891\C,0.1510779631,1.968
0389483,1.6368070891\H,-2.3509409854,1.1374234399,-2.162646513\H,-2.35
09409854,1.1374234399,2.162646513\H,-2.3801066069,-0.3881204196,-1.278
0978223\H,-2.3801066069,-0.3881204196,1.2780978223\H,-0.3752709074,-1.
4183173348,-2.1476879161\H,-0.3752709074,-1.4183173348,2.1476879161\H,
-0.4589936765,-0.1182775796,-3.3576764082\H,-0.4589936765,-0.118277579
6,3.3576764082\H,1.0611606779,-0.4318803093,-2.5028814721\H,1.06116067
79,-0.4318803093,2.5028814721\H,-0.0330471696,2.1999910984,-2.69251188
84\H,-0.0330471696,2.1999910984,2.6925118884\H,-0.2780324502,2.7801963
884,-1.0452786519\H,-0.2780324502,2.7801963884,1.0452786519\H,1.232156
8156,1.9581331705,-1.4751482525\H,1.2321568156,1.9581331705,1.47514825
25\H,1.6594075659,-0.9439187121,0.\\Version=EM64L-G09RevB.01\State=1-A
'\HF=-484.3259647\RMSD=5.700e-09\RMSF=4.675e-06\Dipole=-0.2408706,-0.1
856637,0.\Quadrupole=-0.4446223,0.5199738,-0.0753515,-2.2221345,0.,0.\
PG=CS [SG(C1H3N1O1),X(C8H16)]\\@

TS2 (c)

1\1\GINC-X97\FTS\RB3LYP\6-31G(d)\C11H17N1O1\GXG501\23-Jul-2012\0\\#B3L

YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_stcore.freq\\0,1\N,-
1.6112825396,-2.7262169675,-1.2766998845\C,-1.7650237175,-1.7494452887
,-0.2079187486\C,-0.6233155184,-2.405864901,-2.2963998913\O,-1.4963044
556,-3.9811244494,-0.8191548654\H,-2.3446634091,-5.1563755137,-0.85092
1931\C,-2.2764770259,-6.32487336,-0.507622458\C,-2.2033330202,-7.13832
90647,-1.8006337817\H,-1.3024553984,-6.8786113045,-2.3679933789\H,-3.0
684837528,-6.9339333137,-2.4402761745\H,-2.1803617018,-8.2167800464,-1
.6018975764\C,-1.0925312411,-6.2279458785,0.2829585197\H,-0.1433579894
,-6.371053418,-0.2304335141\C,-1.002153347,-5.9413089152,1.6886709611\
C,-2.133077,-5.6945507199,2.504723239\C,-1.9904672339,-5.4385206869,3.
8626012218\C,-0.7225471099,-5.4262275108,4.4550353786\C,0.4078114777,-
5.6702108468,3.6684388714\C,0.2707769817,-5.9201702994,2.3088963463\H,
-3.1246566562,-5.6962413355,2.063566597\H,-2.872820066,-5.2479186167,4
.4681415601\H,-0.6176802263,-5.2289039987,5.5182962812\H,1.3968620787,
-5.6624657181,4.1190103929\H,1.1528200627,-6.1038134998,1.699920181\H,
-0.680650874,-3.1657186337,-3.0798716783\H,-0.8411933499,-1.4235906268
,-2.7292899497\H,0.403025984,-2.3976290933,-1.8890713692\H,-0.85009211
35,-1.6569112526,0.4025737817\H,-2.5812316677,-2.0787635655,0.43998112
14\H,-2.0100585155,-0.7698470415,-0.6324744788\H,-3.1948556552,-6.5019
221326,0.061133227\\Version=EM64L-G09RevB.01\State=1-A\HF=-559.2394791
\RMSD=9.787e-09\RMSF=1.847e-06\Dipole=0.1671356,0.1104861,0.2191122\Qu
adrupole=0.2692404,-1.245554,0.9763135,0.2039997,-1.1042015,0.1131096\
PG=C01 [X(C11H17N1O1)]\\@

TS2

1\1\GINC-X100\FTS\RB3LYP\6-31G(d)\C25H35N1O1\GXG501\20-Jul-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigente
st,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_st.freq\\0,1\C,-1.5
099749054,-2.6592617452,-1.3439534152\C,-1.8954425497,-1.6219122039,-0
.2731657181\C,-1.2078378848,-0.2673989753,-0.5505259773\C,-1.186176342
6,0.6963003486,0.5018303742\H,-1.9715185295,-3.6297690237,-1.132721942
5\H,-0.4230802064,-2.7913948953,-1.3780296846\H,-1.8420466024,-2.34411
07925,-2.3404723443\H,-1.5103510603,-1.9817118276,0.6906683419\C,-3.40
84993153,-1.492362255,-0.1373791709\H,-1.4597662206,0.1355432309,-1.53
75937499\H,-0.0200765884,-0.5203439919,-0.6204681537\H,-1.2235570467,0
.3111177502,1.5196454054\C,-1.0757865189,2.1212912235,0.383637244\C,-4
.2014352968,-1.0316338005,-1.1992831012\C,-5.5854004078,-0.923360964,-
1.0687664152\C,-6.2089834242,-1.2764220368,0.1303221753\C,-5.434491792
4,-1.7377938983,1.1943221142\C,-4.0485130542,-1.843464757,1.0576791571
\C,-1.0103546867,2.9101397265,1.5601746254\C,-0.9191357979,4.294441003
9,1.498815434\C,-0.8874355971,4.9433462118,0.2599630746\C,-0.952352245
2,4.1861226159,-0.9156522397\C,-1.0481515376,2.8018414941,-0.860337452
\H,-3.7333742593,-0.7512503214,-2.1400596021\H,-6.1788603683,-0.561944
055,-1.9049266512\H,-7.2876354267,-1.1918284455,0.2325534826\H,-5.9067
170348,-2.0168660179,2.1329730825\H,-3.4531293892,-2.2062581099,1.8931
477554\H,-1.0307432628,2.4105784177,2.5258124756\H,-0.8711862668,4.873
0119551,2.4176591843\H,-0.8154320119,6.0262120669,0.2100863403\H,-0.93
1600206,4.6837613718,-1.8818225788\H,-1.1040507092,2.2349871384,-1.784
2836506\O,1.2504649576,-0.3149059254,0.0621135984\N,2.4960822681,-0.71
3371558,-0.1956293326\C,3.334318695,0.3525606062,-0.8199634268\C,3.020
790877,-1.6877508776,0.8060279999\C,4.718791294,-0.2289572886,-1.17540
64205\C,2.6273159694,0.7835358492,-2.1178987751\C,3.4569248293,1.58466
15872,0.1067220715\C,4.4226088229,-2.1647970157,0.3711247787\C,3.04600
50122,-1.0722771597,2.2246132618\C,2.0646837683,-2.8941974492,0.811720
5821\H,5.3685139582,0.5968564894,-1.491421677\C,5.3562421083,-1.022613
5908,-0.0335605218\H,4.6078631086,-0.8939125045,-2.0432094634\H,4.8545
389256,-2.755948783,1.1885285846\H,4.3111916462,-2.8439978111,-0.48546
10118\H,6.3248073942,-1.4269793583,-0.3534236508\H,5.5642799389,-0.369
5015499,0.8234244292\H,3.8859163158,2.4303272806,-0.4438704972\H,2.463
617232,1.8700315171,0.4635575931\H,4.0956363416,1.3948748881,0.9743527
355\H,3.2544799046,1.497972018,-2.6634493811\H,2.4483069647,-0.0835376

597,-2.7630486219\H,1.6685744951,1.2595719652,-1.9003597245\H,3.213393
811,-1.8535225929,2.975526527\H,3.8342836709,-0.3232592164,2.342068980
9\H,2.0835411879,-0.5937451151,2.4268342088\H,2.4543251712,-3.67715317
44,1.4724415727\H,1.0726614321,-2.6026468202,1.1642099721\H,1.96615444
52,-3.3099161892,-0.1970068116\\Version=EM64L-G09RevB.01\State=1-A\HF=
-1103.6003448\RMSD=8.997e-09\RMSF=3.254e-07\Dipole=0.2992944,0.1925745
,0.0233276\Quadrupole=-0.4874969,-0.7880657,1.2755626,-1.5654166,-0.17
74356,-1.9619996\PG=C01 [X(C25H35N1O1)]\\@

Me_2NOCH(Et)Ph (c)

1\1\GINC-X142\FOpt\RB3LYP\Gen\C11H17N1O1\GXG501\15-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\st_core.freq\\0,1\N,-1.864883509,-0.2019912291,-0.1672143129\O,-0.9
940134288,-0.0827166423,0.9893788915\C,0.3449629076,0.2066579125,0.563
8729299\H,0.6134728729,-0.4863297054,-0.2464728863\C,0.4902094406,1.63
13609584,0.0529554497\C,1.1102867961,1.8949473935,-1.172293087\C,1.272
6500381,3.2061809448,-1.625994091\C,0.8076776461,4.2734625015,-0.85770
32335\C,0.1801137403,4.0216654468,0.3655506279\C,0.025029118,2.7115659
499,0.8167842188\H,1.4639556713,1.0652848348,-1.7804748716\H,1.7553749
918,3.3914333524,-2.5821900089\H,0.9288247721,5.2946426127,-1.20956438
51\H,-0.1884580417,4.8481224842,0.9680968268\H,-0.4726087996,2.5173445
805,1.7633463076\C,1.2258429938,-0.0930082573,1.7876789305\H,0.9485799
843,0.59231048,2.5986407037\H,0.974593143,-1.1037153633,2.1316095766\C
,2.7273110247,0.0101086176,1.5044263799\H,3.0094954357,1.0205406135,1.
1907270924\H,3.3061151671,-0.2380250789,2.4007117986\H,3.0318675275,-0
.6832105254,0.7105805059\C,-2.2869745833,-1.5998452913,-0.1919188923\C
,-2.9882417718,0.6953983687,0.0838395899\H,-2.8031954756,-1.9060955357
,0.7329531297\H,-2.9614543725,-1.741847419,-1.0433770378\H,-1.41014166
72,-2.2374527901,-0.335432568\H,-3.5127136958,0.4659692467,1.026612202
\H,-3.694521049,0.5990134943,-0.7479044451\H,-2.6232348765,1.723770044
9,0.1170016577\\Version=EM64L-G09RevB.01\State=1-A\HF=-559.3270057\RMS
D=5.640e-09\RMSF=2.203e-06\Dipole=-0.0764942,-0.0699065,-0.1499217\Qua
drupole=-0.1790386,1.8706613,-1.6916227,0.1611214,-0.4605389,0.8539109
\PG=C01 [X(C11H17N1O1)]\\@

TEMPOP

1\1\GINC-X121\FOpt\RB3LYP\Gen\C25H35N1O1\GXG501\15-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\st.freq\\0,1\N,1.1600335233,-0.115748255,-0.2839656981\O,0.17671110
76,0.5491332353,0.5553746664\C,-0.9094135538,1.158528977,-0.1854196055
\C,3.7509555381,-1.4150152496,-0.5617244422\H,4.5020424295,-1.91894169
7,-1.1832263606\H,4.1679179719,-1.3764333808,0.4523760547\C,-1.2380655
524,2.4528554331,0.5831070229\C,-2.1235991055,0.2514445072,-0.31103567
88\C,1.5306351663,-1.6605706154,1.7382693747\C,2.9041319408,1.21280994
59,1.0657097324\C,1.2969412873,-1.5270664238,0.2150195366\C,2.38806753
33,0.7539886094,-0.3178702232\C,0.0034555353,-2.2843432647,-0.13329696
3\C,2.0567999795,2.0132708254,-1.1428695218\C,2.4414828971,-2.19920399
36,-0.5803823372\C,3.4879217251,-0.0088897593,-1.0938498638\H,2.115266
0979,-2.3145616173,-1.6230180081\H,3.1805080814,-0.083891815,-2.145855
4913\H,2.581103036,-3.2105631392,-0.1785430343\H,4.4002793348,0.600505
2302,-1.0728369668\H,0.161657366,-3.3600478618,0.0101805041\H,2.978599
6131,2.5726023161,-1.3419289991\H,-0.2767399471,-2.110704121,-1.176456
8111\H,1.6075441475,1.7425718964,-2.1035182283\H,-0.8304491275,-1.9803
065439,0.5005509849\H,1.3755185388,2.6853212441,-0.616423367\H,1.36950
58505,-2.701950196,2.0410589086\H,3.6142072747,2.0383900921,0.93738038
67\H,2.5416168497,-1.3849773466,2.0467166069\H,3.4211196101,0.42264889
72,1.6144901182\H,0.8213561824,-1.0348188704,2.2852464943\H,2.07332674
09,1.5696556361,1.6790178415\H,-0.314142047,3.034094943,0.6841632766\C
,-2.3449207101,3.3339431112,-0.0399284131\H,-1.5387828416,2.1817564291
,1.6033612479\H,-0.5493878071,1.4001303002,-1.1874988575\C,-2.62614506
6,-0.0893711283,-1.5716503266\C,-3.7578948726,-0.8992712107,-1.6987201
208\C,-4.402700097,-1.3820879999,-0.5602177285\C,-3.9096537941,-1.0497

066414,0.7048633309\C,-2.7824165557,-0.2384713229,0.8265898221\H,-2.12
57393162,0.2837238151,-2.4619612488\H,-4.1311448788,-1.1549966649,-2.6
871649666\H,-5.282103601,-2.0136289294,-0.6551504294\H,-4.4046472971,-
1.4245366185,1.5972146755\H,-2.3976878471,0.0035246125,1.8140604497\H,
-3.2415060841,2.7117426985,-0.1499501029\C,-1.9830357589,3.8551786432,
-1.4262343711\C,-2.7035787998,4.4897298136,0.9153550301\C,-2.772861656
6,3.5318304501,-2.5377443297\C,-2.4643857579,4.0178363186,-3.810364692
4\C,-1.3540047763,4.8415015881,-3.9952910241\C,-0.5578801895,5.1751939
771,-2.8974055832\C,-0.8713264236,4.6878053756,-1.6285283212\H,-3.6394
585922,2.8887659707,-2.4030263707\H,-3.093880819,3.7522391839,-4.65601
07855\H,-1.1107492802,5.2214401399,-4.9840168067\H,0.3087171831,5.8183
415901,-3.028510935\H,-0.2428996797,4.9637267502,-0.785028813\H,-3.040
0904434,4.1016581908,1.8840519849\H,-3.505353048,5.1080330414,0.497610
7018\H,-1.8411312149,5.1416238778,1.0983320751\\Version=EM64L-G09RevB.
01\State=1-A\HF=-1103.6726439\RMSD=7.919e-09\RMSF=8.439e-07\Dipole=-0.
0080376,0.0191783,-0.1406674\Quadrupole=2.1933329,-2.7628599,0.569527,
3.2752815,-0.4399387,-0.3575064\PG=C01 [X(C25H35N1O1)]\\@

TS3a (c)

Single point\\0,1\N,0,1.131684,1.245181,-0.131462\O,0,0.299336,0.12359
6,0.342332\C,0,0.392601,-1.227951,-0.365779\C,0,-0.776936,-1.693674,0.
483895\H,0,-0.666969,-0.563455,0.835836\C,0,1.908738,1.771253,1.039083
\C,0,0.245727,2.185635,-0.90172\H,0,1.308977,2.037355,1.906965\H,0,2.6
16382,1.003833,1.345759\H,0,2.482685,2.62351,0.68133\H,0,-0.641651,2.5
31922,-0.375992\H,0,-0.086923,1.67391,-1.802401\H,0,0.867715,3.022781,
-1.211656\H,0,0.121947,-1.047073,-1.406004\C,0,1.740311,-1.888642,-0.3
14078\C,0,2.607788,-1.746425,-1.409816\C,0,3.866708,-2.34814,-1.412348
\C,0,4.279881,-3.107967,-0.321976\C,0,3.430728,-3.261301,0.775119\C,0,
2.173633,-2.658472,0.777771\H,0,2.286567,-1.154943,-2.263667\H,0,4.518
005,-2.231181,-2.277625\H,0,5.257754,-3.58202,-0.324017\H,0,3.740977,-
3.850173,1.634616\H,0,1.521973,-2.785061,1.638674\H,0,-0.490551,-2.401
458,1.260024\C,0,-2.077859,-2.106629,-0.238556\H,0,-1.881373,-2.165598
,-1.315123\H,0,-2.89301,-1.397967,-0.107898\H,0,-2.394471,-3.09966,0.0
73519\\Version=EM64L-G09RevB.01\State=1-A\HF=-555.7519669\PG=C01 [X(C1
1H17N1O1)]\\@

TS3a

1\1\GINC-X114\Freq\RB3LYP\6-31G(d)\C25H35N1O1\GXG501\28-Jul-2012\0\\#B
3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17=4
) maxdisk=1342177280\\ts2_st.freq\\0,1\N,1.139331,1.238112,-0.130997\O
,0.300132,0.121644,0.342797\C,0.385121,-1.230449,-0.365314\C,1.910263,
4.023933,-0.188241\H,2.561015,4.817802,-0.573654\H,1.214552,4.510311,0
.506562\C,-0.787245,-1.689003,0.48436\C,1.728761,-1.899378,-0.313613\C
,1.069002,2.143056,2.273766\C,-0.999777,2.684153,-0.153604\C,1.919591,
1.759417,1.039548\C,0.259148,2.183972,-0.901255\C,2.912693,0.669108,1.
472819\C,-0.216294,1.462294,-2.176572\C,2.742606,2.965513,0.531158\C,1
.150183,3.368023,-1.341637\H,3.514206,2.588662,-0.157476\H,1.87719,2.9
9569,-2.076063\H,3.27401,3.399745,1.389673\H,0.517249,4.097515,-1.8646
52\H,3.61768,1.089187,2.204705\H,-0.654529,2.191098,-2.867386\H,3.4746
02,0.288449,0.619772\H,0.621537,0.970979,-2.684654\H,2.401936,-0.17111
8,1.946446\H,-0.9935,0.719653,-1.95801\H,1.733998,2.283625,3.13961\H,-
1.676964,3.167189,-0.86995\H,0.509857,3.069592,2.14623\H,-0.772931,3.4
21345,0.619466\H,0.362519,1.346338,2.52371\H,-1.54012,1.853119,0.30529
1\H,-0.670361,-0.559479,0.836301\C,-2.090672,-2.093986,-0.238091\H,-0.
505199,-2.398527,1.260489\H,0.11558,-1.047917,-1.405539\C,2.597092,-1.
762475,-1.409351\C,3.852305,-2.371886,-1.411883\C,4.260819,-3.134228,-
0.321511\C,3.410743,-3.28236,0.775584\C,2.157362,-2.671847,0.778236\H,
2.279499,-1.169037,-2.263202\H,4.504306,-2.258916,-2.27716\H,5.235771,
-3.614258,-0.323552\H,3.717381,-3.873121,1.635081\H,1.504939,-2.794444
,1.639139\H,-1.894551,-2.154157,-1.314658\C,-3.22724,-1.093613,-0.0549
36\C,-2.550159,-3.505224,0.206287\C,-4.017408,-0.701843,-1.150644\C,-5
.088351,0.175472,-0.993845\C,-5.396971,0.686461,0.27113\C,-4.624868,0.

309408,1.368955\C,-3.554653,-0.57006,1.206324\H,-3.783357,-1.097203,-2
.138065\H,-5.683662,0.469058,-1.857866\H,-6.231092,1.374192,0.39854\H,
-4.857255,0.697976,2.361335\H,-2.949288,-0.848165,2.071707\H,-1.767625
,-4.243049,0.013626\H,-3.457979,-3.813232,-0.326739\H,-2.779091,-3.519
085,1.28252\\Version=EM64L-G09RevB.01\State=1-A\HF=-1103.5911346\RMSD=
4.708e-09\RMSF=9.865e-03\ZeroPoint=0.5480608\Thermal=0.5741404\Dipole=
0.4272749,0.181811,-0.1720221\PG=C01 [X(C25H35N1O1)]\NImag=1\\@

$Me_2NH \rightarrow O$ (c)

1\1\GINC-X5\FOpt\RB3LYP\Gen\C2H7N1O1\GXG501\01-Jun-2012\0\\#B3LYP/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\d
mno_x.freq\\0,1\N,0.0641880278,-0.8326361048,0.019665735\O,-1.06081256
04,-0.1325879772,0.2559178465\C,0.9712783593,-0.095209984,-0.922576019
1\C,-0.2529125501,-2.2049354248,-0.5005952342\H,0.6211548939,-0.982341
2395,0.8869967984\H,1.9090921969,-0.6373125561,-1.0930979048\H,0.41158
95398,0.0345775622,-1.8493987127\H,1.1531195641,0.8791466902,-0.469618
4647\H,0.6544016443,-2.7995999565,-0.6606038386\H,-0.8045108193,-2.061
2049228,-1.4302067548\H,-0.9049964075,-2.6677344309,0.2398177731\\Vers
ion=EM64L-G09RevB.01\State=1-A'\HF=-210.3007619\RMSD=4.828e-09\RMSF=8.
018e-05\Dipole=1.475934,-0.9342613,-0.3891405\Quadrupole=-1.4883164,0.
4650634,1.0232531,2.4590647,1.7641309,-1.2473134\PG=CS [SG(H1N1O1),X(C
2H6)]\\@

TEMPH→O

1\1\GINC-X107\FOpt\RB3LYP\Gen\C9H19N1O1\GXG501\01-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\tempo_x.freq\\0,1\N,0.0078304227,-0.818275129,-0.0727605046\C,-1.305
1640293,-0.0030557763,0.19321025\C,-1.2031119746,1.3694955983,-0.49602
11467\C,0.0807806156,2.1367511608,-0.1635776699\C,1.3063412778,1.30548
44924,-0.5566558964\C,1.3715066288,-0.0714324539,0.1284713354\C,1.6915
283521,-0.0003364899,1.6223297237\O,-0.0077244548,-2.0162367122,0.5427
312217\C,2.3975167265,-0.9767636717,-0.5656059944\C,-2.4080610593,-0.8
543218176,-0.4494612857\C,-1.5484543831,0.0824159943,1.7006962733\H,0.
0919921081,3.0901327702,-0.7055991942\H,0.1129752536,2.3903668777,0.90
26521249\H,2.2345598267,1.8448456554,-0.3291927234\H,-2.0905588891,1.9
552498318,-0.2247370636\H,1.2977402477,1.1618058328,-1.6479736456\H,-1
.2545038376,1.2268509869,-1.5862849724\H,2.1782270798,-1.0790027187,-1
.6371466714\H,-2.2462366736,-0.9662217585,-1.5302179522\H,3.4010242386
,-0.5486575661,-0.471857551\H,-3.3828770986,-0.3759904401,-0.307911630
4\H,2.3749249474,-1.9690955737,-0.1113686283\H,-2.4139081563,-1.847043
5411,0.0044191844\H,2.7667092014,0.1586476588,1.7568495457\H,-2.606348
6383,0.2958668558,1.8869281694\H,1.1705442248,0.8101198612,2.137367909
2\H,-0.9624767891,0.8645965012,2.1889485231\H,1.4115403906,-0.95490446
75,2.0746422953\H,-1.2958825142,-0.8857236454,2.1401089485\H,-0.020412
8842,-0.9442338588,-1.103890661\\Version=EM64L-G09RevB.01\State=1-A\HF
=-484.3058121\RMSD=4.868e-09\RMSF=2.427e-05\Dipole=0.021883,1.4749952,
-0.6359991\Quadrupole=3.5495873,-5.3624352,1.8128478,-0.1834774,0.0038
671,1.8034743\PG=C01 [X(C9H19N1O1)]\\@

CH_2(Et)Ph (c)

1\1\GINC-X108\FOpt\RB3LYP\6-31G(d)\C9H12\GXG501\01-Jul-2012\0\\#B3LYP/
6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342
177280\\ps_core.freq\\0,1\C,-5.7118198812,3.0987314087,0.4765912249\C,
-4.6179056368,2.061595092,0.3365755083\C,-3.2667482996,2.4337835312,0.
3555304776\C,-2.2568403845,1.4855057825,0.1874824867\C,-2.582585967,0.
1413867942,-0.0025865429\C,-3.9240340093,-0.2446564312,-0.021809713\C,
-4.9294431566,0.7082976397,0.146802989\H,-3.0042605065,3.478792965,0.5
085266459\H,-1.2152244701,1.7959928664,0.2098258048\H,-1.7977277048,-0
.5994802288,-0.1300440692\H,-4.1885117473,-1.2895787424,-0.1634152878\
H,-5.9725932054,0.398332947,0.1359038994\H,-6.5832491206,2.6524575092,
0.9746002161\H,-5.3671993999,3.9146021252,1.1263267537\C,-6.1598504047

,3.692713353,-0.8742355625\H,-6.502531678,2.8782503805,-1.5262942619\H
,-5.2894305612,4.1371455203,-1.3750773558\C,-7.2663200724,4.7411114677
,-0.7255751286\H,-8.159678644,4.3122366618,-0.2548105746\H,-6.93625379
08,5.581589667,-0.1025385001\H,-7.5647744873,5.1456091299,-1.69940814\
\Version=EM64L-G09RevB.01\State=1-A\HF=-350.1942634\RMSD=9.119e-09\RMS
F=9.667e-06\Dipole=-0.0826531,0.0829763,-0.0290657\Quadrupole=1.593602
9,1.5282046,-3.1218075,0.259866,-0.0421777,0.6428071\PG=C01 [X(C9H12)]
\\@

PH

1\1\GINC-X93\FOpt\RB3LYP\Gen\C16H18\GXG501\04-Jun-2012\0\\#B3LYP/gen 6
D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\ps
.freq\\0,1\C,-5.7092587974,3.101867168,0.4933569561\C,-4.5990946819,2.
0437994259,0.3397654345\C,-3.2037446865,2.7055423372,0.398560839\C,-2.
0396413933,1.7511126687,0.0661994506\H,-6.7020297954,2.645091852,0.418
5771188\H,-5.6251932875,3.8684730259,-0.2860603818\H,-5.6473071891,3.6
062607263,1.4648369347\H,-4.70637603,1.5981893718,-0.6598291739\C,-4.7
612932562,0.9171317911,1.3530277137\H,-3.0416340586,3.1391444344,1.394
7952795\H,-3.1853059224,3.5487930539,-0.3051859353\H,-2.0584659484,0.9
05028072,0.7632729251\C,-0.6897073303,2.4339302271,0.1253174466\C,-5.0
26261719,-0.3922536807,0.9314744818\C,-5.1906749738,-1.430161922,1.851
3914763\C,-5.091205006,-1.1749479023,3.2189303953\C,-4.8267298067,0.12
50010759,3.656152985\C,-4.6644451083,1.1574587232,2.7326796402\C,-0.15
10522686,3.0667763664,-1.0033185896\C,1.076173208,3.7281756725,-0.9403
356628\C,1.7897085868,3.7679267718,0.2588973588\C,1.2665973087,3.14042
21714,1.3909996743\C,0.0390901711,2.4802980743,1.3218060874\H,-5.10599
80387,-0.6014355821,-0.1332941801\H,-5.395694796,-2.4372946476,1.49725
65582\H,-5.2181527434,-1.9796742578,3.9381975862\H,-4.7475191526,0.336
0495657,4.7196908241\H,-4.4617151178,2.1636705891,3.0920845052\H,-0.69
83794662,3.0356212559,-1.9434965919\H,1.4772348578,4.2084366373,-1.829
3884532\H,2.7473089494,4.2793922029,0.3095584054\H,1.8170716993,3.1601
492661,2.3282817601\H,-0.3595404644,1.988401892,2.2068550098\H,-2.1984
877427,1.3330895735,-0.9371748786\\Version=EM64L-G09RevB.01\State=1-A\
HF=-620.5566477\RMSD=1.470e-09\RMSF=1.766e-06\Dipole=-0.1388413,0.0136
834,-0.0229089\Quadrupole=-2.9436055,-0.4677582,3.4113637,2.2147593,1.
2192879,-0.9457031\PG=C01 [X(C16H18)]\\@

TS5 (c)

1\1\GINC-X101\FTS\UB3LYP\6-31G(d)\C11H18N1O1(2)\GXG501\27-Jul-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_stcore.freq\\0,2
\N,1.5877199022,-1.7299061835,2.080416469\O,0.6380685686,-0.8893855252
,2.6184791411\C,1.8633275931,-2.8240515798,3.0034435201\C,2.7628344174
,-0.9665114841,1.6740573353\H,-0.2345425943,-0.8548429121,1.8474978424
\C,-1.2981568628,-0.9408685973,0.9301561362\H,-1.8338769835,-0.0232405
571,1.1949290561\C,-2.0025391752,-2.2085546046,1.3758500512\C,-0.60916
8595,-0.8636679833,-0.3543167305\C,-0.1347444327,-2.0074939737,-1.0367
942007\C,0.55506934,-1.8909207788,-2.2408229446\C,0.8035267115,-0.6337
743876,-2.7974757708\C,0.3505864647,0.5129200004,-2.1342711308\C,-0.34
16527358,0.3995992507,-0.9349394764\H,-0.6932863608,1.2946179138,-0.42
64401865\H,0.5347140691,1.4960504462,-2.5601287953\H,1.3418095045,-0.5
465323056,-3.737339682\H,0.9021552121,-2.7872551646,-2.7487893936\H,-0
.3157932733,-2.9930372457,-0.6206747374\H,-1.2973604622,-3.0506657537,
1.3654331476\H,-2.789791743,-2.4686447814,0.6492996378\C,-2.6144534358
,-2.0827922792,2.7756564566\H,-3.3585295177,-1.2776987902,2.8109286248
\H,-1.8388148546,-1.8559746082,3.514887927\H,2.4495001125,-0.199409473
,0.963037797\H,3.4723826323,-1.63898381,1.1810708648\H,3.259747993,-0.
4824785933,2.5311796905\H,2.5565610799,-3.5260638528,2.5284872624\H,2.
3045465835,-2.4699875923,3.9501246777\H,0.9271234388,-3.3416936606,3.2
247003057\H,-3.1134045964,-3.0114071338,3.0744621056\\Version=EM64L-G0
9RevB.01\State=2-A\HF=-559.8692932\S2=0.76406\S2-1=0.\S2A=0.750161\RMS
D=7.477e-09\RMSF=7.670e-07\Dipole=0.3454607,-0.3325308,-0.25555\Quadru

pole=0.7210569,1.7041413,-2.4251982,-1.0841689,-1.0597922,-2.3998132\P
G=C01 [X(C11H18N1O1)]\\@

TS5

1\1\GINC-X88\FTS\UB3LYP\6-31G(d)\C25H36N1O1(2)\GXG501\25-Jul-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_st.freq\\0,2\C,1.
7526387194,-0.5250414883,3.2765193277\C,1.5495205328,-0.4138657441,1.7
519140887\C,1.2374835006,1.0470392403,1.3571156721\C,0.8636258287,1.23
62371621,-0.1008481767\H,1.94521261,-1.5614561541,3.5737982051\H,0.865
5066975,-0.1728856003,3.8169859624\H,2.607723958,0.0787582271,3.604000
5444\H,0.6711107877,-1.0170663577,1.4861054387\C,2.7432830642,-1.00752
18518,1.0114398856\H,2.104802946,1.6822516514,1.6019161247\H,0.4277857
35,1.4069219671,2.0065510299\H,1.3482693754,0.5300742857,-0.7800029269
\C,0.7288196347,2.5798123787,-0.659418103\C,3.9737125201,-0.3377281558
,0.931978594\C,5.0685729313,-0.9170964648,0.2903227138\C,4.9582087514,
-2.184441618,-0.285590441\C,3.7433041581,-2.865786089,-0.2118596191\C,
2.6507926336,-2.2799850516,0.4308282673\C,0.7767325143,2.7678109806,-2
.0603353778\C,0.6140288883,4.0261987845,-2.6274171504\C,0.3939299832,5
.1424175877,-1.8133762844\C,0.3380323907,4.9794893297,-0.4263285425\C,
0.4990535246,3.7197456281,0.1435945871\H,4.0819848742,0.6492937736,1.3
745516243\H,6.0102297123,-0.3762271302,0.2393329866\H,5.8107491599,-2.
6346983007,-0.7870992887\H,3.6426021132,-3.8530198376,-0.6557334733\H,
1.7087716039,-2.8213606571,0.4885749765\H,0.9499967267,1.9048342557,-2
.6992261459\H,0.6616445282,4.1413747636,-3.7073279812\H,0.2678170818,6
.1270876584,-2.2552102723\H,0.1678774785,5.84097154,0.2146840411\H,0.4
497919415,3.6143328185,1.2233403706\N,-1.9508289894,-0.7360385998,-0.1
235716734\O,-1.587077385,0.5245042965,-0.5335436895\C,-3.6570723463,-3
.0346240091,0.1940137283\H,-3.8554004957,-4.0484160206,0.5637885852\H,
-4.5689134257,-2.7151872775,-0.3259096366\C,-2.4672968281,-3.054181862
8,-0.7682648902\C,-3.3518444907,-2.1025811355,1.3687333866\C,-2.082686
2416,-1.6553824602,-1.2963639501\C,-3.0030874494,-0.661715827,0.936690
2723\C,-0.6991311504,-1.7413428784,-1.9657644827\C,-2.3937194162,0.080
8147421,2.139225632\C,-3.0939933743,-1.1499957722,-2.3516733678\C,-4.2
618972406,0.1147829639,0.4838021297\H,-2.6687822694,-3.7052096042,-1.6
282111745\H,-4.1986545777,-2.0591071541,2.0651550265\H,-1.5996186316,-
3.4793430929,-0.2449394234\H,-2.5006748987,-2.5128329758,1.9294363958\
H,0.0709953415,-2.0215644902,-1.2400189382\H,-1.4775860239,-0.41467859
73,2.4768087678\H,-0.7166363062,-2.4971288379,-2.7592105712\H,-3.10616
01076,0.0885420375,2.9718918633\H,-0.4199724625,-0.7838227084,-2.41321
37415\H,-2.1578499506,1.1158807099,1.8792235343\H,-2.9778061134,-1.720
9803399,-3.2803612888\H,-4.8981447012,0.329576862,1.3503647946\H,-4.13
34274012,-1.2540037912,-2.0309167593\H,-4.8667512559,-0.439573588,-0.2
377756574\H,-2.9039270964,-0.0957659525,-2.5708425141\H,-3.9679241942,
1.0649314645,0.0295265021\H,-0.4927784232,0.7476163673,-0.2634235172\\
Version=EM64L-G09RevB.01\State=2-A\HF=-1104.2236587\S2=0.763285\S2-1=0
.\S2A=0.750145\RMSD=6.686e-09\RMSF=2.500e-06\Dipole=-0.1515118,-0.3958
853,0.16403\Quadrupole=-1.2517407,1.9868258,-0.7350851,2.6740089,-2.21
58732,2.3415072\PG=C01 [X(C25H36N1O1)]\\@

•CH(Me)CH=CH$_2$ (c1)

1\1\GINC-X118\FOpt\UB3LYP\Gen\C4H7(2)\GXG501\04-Jun-2012\0\\#B3LYP/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\
ps_rcore1.freq\\0,2\C,-6.1614213406,2.505735921,0.2489390343\H,-5.4111
362226,1.7272421786,0.3896326176\C,-5.7919523916,3.6582893817,-0.43208
97478\C,-4.5353061043,3.9119190568,-0.9573111167\H,-6.5578683474,4.425
3564139,-0.5622094132\H,-3.7281936551,3.1902070448,-0.8625043471\H,-4.
3145227023,4.8367050198,-1.4795888632\C,-7.5239776814,2.249023667,0.80
9489524\H,-7.4901283584,2.0846917803,1.8968348244\H,-8.2041340697,3.08
62945797,0.618158666\H,-7.975383031,1.3433269438,0.3777313507\\Version
=EM64L-G09RevB.01\State=2-A\HF=-156.5806349\S2=0.780022\S2-1=0.\S2A=0.
750184\RMSD=8.227e-09\RMSF=1.097e-05\Dipole=-0.137629,-0.0852042,0.085

5609\Quadrupole=0.5132088,0.5745353,-1.0877441,-0.3251408,-0.5745128,-
1.0478602\PG=C01 [X(C4H7)]\\@

•CH(Me)Ph (c2)

1\1\GINC-X130\FOpt\UB3LYP\6-31G(d)\C8H9(2)\GXG501\16-Aug-2012\0\\#B3LY
P/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13
42177280\\ps_ru.freq\\0,2\C,0.8293424629,0.0699302649,-0.2803694942\H,
0.2462042097,-0.7507635552,-0.6916209845\C,2.2178936961,-0.1441062496,
-0.1063486327\C,0.111292821,1.3388930097,0.0597998298\H,-0.9562900649,
1.2600522045,-0.1645221959\C,2.8041043634,-1.3937034188,-0.463395993\C
,4.1605974398,-1.6268194617,-0.3023137327\C,4.9950415758,-0.6284357532
,0.2208089847\C,4.445179775,0.6090134361,0.5799811072\C,3.0879334785,0
.8529764858,0.4227896664\H,0.2065716103,1.5956696724,1.1257771349\H,0.
5039028367,2.2002041,-0.5017303331\H,2.1628661583,-2.1726826398,-0.869
7629823\H,4.5788556316,-2.5900382606,-0.5836698268\H,6.0582028301,-0.8
129237607,0.3463967155\H,5.0863275856,1.3875375059,0.9861625601\H,2.68
04246119,1.8187177172,0.7070450511\\Version=EM64L-G09RevB.01\State=2-A
\HF=-310.2333488\S2=0.779924\S2-1=0.\S2A=0.750613\RMSD=8.357e-09\RMSF=
7.251e-07\Dipole=-0.1287488,0.0782641,0.0055594\Quadrupole=2.101424,1.
0985094,-3.1999334,-0.5914437,0.9000994,1.7972721\PG=C01 [X(C8H9)]\\@

$Me_2NOCH(Me)CH=CH_2$ (c1)

1\1\GINC-X92\FOpt\RB3LYP\Gen\C6H13N1O1\GXG501\15-Jun-2012\0\\#B3LYP/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\
\st_core1.freq\\0,1\N,-1.8548628013,-0.3956018976,-0.217993394\O,-1.02
3521391,-0.1457816359,0.9429461844\C,0.3155148214,0.1837320506,0.53085
17886\C,0.389956081,1.580336079,-0.0307713133\H,0.0983434119,2.3734311
474,0.6598886023\C,0.7845977994,1.8800676982,-1.2678515955\H,1.0711665
263,1.1054172694,-1.976141294\H,0.8362922632,2.905978132,-1.6234035767
\H,0.6344537479,-0.5347985529,-0.2359342386\C,1.1707158215,0.026772565
5,1.7884926181\H,1.0828135183,-0.9906371273,2.1827758178\H,0.842798723
1,0.7250984581,2.5666030924\H,2.2218990414,0.2317130577,1.5616371963\C
,-2.9429509366,0.5752465351,-0.1542042211\C,-2.3388709294,-1.763188222
3,-0.0554011011\H,-3.5126167027,0.5149127823,0.7880397805\H,-3.6212222
878,0.3869162181,-0.9936976095\H,-2.529001009,1.5804637875,-0.25962408
87\H,-2.8976464662,-1.9099917506,0.8838705175\H,-2.9926292257,-2.00103
9805,-0.9015794429\H,-1.4869240059,-2.4482977893,-0.0705667227\\Versio
n=EM64L-G09RevB.01\State=1-A\HF=-366.3548947\RMSD=4.617e-09\RMSF=1.619
e-05\Dipole=-0.0618644,-0.0400853,-0.1459315\Quadrupole=0.9757829,0.92
6843,-1.9026259,0.2838975,0.7244858,0.372614\PG=C01 [X(C6H13N1O1)]\\@

TEMPOCH(Me)Ph (c2)

1\1\GINC-X133\FOpt\RB3LYP\6-31G(d)\C17H27N1O1\GXG501\16-Aug-2012\0\\#B
3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk
=1342177280\\stu.freq\\0,1\N,-1.9870509393,-0.4629895505,-0.1591826424
\O,-1.1124057757,0.0854355269,0.8631224423\C,0.2226071911,0.3774219889
,0.3882004714\C,-4.5151655733,-1.7042891033,-0.8928186927\H,-5.1860459
692,-2.1245455594,-1.6527892224\H,-5.0463113888,-1.7853562288,0.063748
214\C,1.1755406057,-0.0190157297,1.521999856\C,0.4251167457,1.83809574
06,0.0141178421\C,-3.8824510675,0.7066157332,1.1245698342\C,-2.5729366
38,-2.2458353126,1.6012693236\C,-3.2049713211,0.413949758,-0.234576436
3\C,-2.1703871595,-1.9252803321,0.1434364063\C,-2.7842360006,1.7582320
99,-0.8547925526\C,-0.8362173787,-2.6407470481,-0.1494751384\C,-4.2011
646716,-0.2460868034,-1.2174844125\C,-3.2075576111,-2.4907399879,-0.85
55766419\H,-3.7740407488,-0.1948142311,-2.2283217393\H,-2.7630232289,-
2.4789843288,-1.8601710675\H,-5.1145150731,0.3616876687,-1.2285894527\
H,-3.3842873092,-3.5430090501,-0.5994306732\H,-3.679284512,2.325828689
4,-1.136594951\H,-0.9878691981,-3.7260928677,-0.1196466912\H,-2.179296
9224,1.5963327296,-1.7521152349\H,-0.4647120746,-2.3750474625,-1.14454
65805\H,-2.2068925448,2.3666912473,-0.1576307664\H,-0.0693952379,-2.39
85710898,0.5898670094\H,-4.5888437332,1.5369524256,1.0078049362\H,-2.4
302991187,-3.3155413302,1.7952022705\H,-4.4426518297,-0.1434269104,1.5

208484468\H,-3.6176268915,-2.0128092302,1.8183222332\H,-3.1336671647,0
.9999396336,1.86418516\H,-1.9441381624,-1.6860556411,2.2976054293\H,1.
0842993527,-1.0824551041,1.7613434911\H,2.212177219,0.1910364785,1.238
1489209\H,0.9513245589,0.5536765675,2.4281161478\H,0.4095837015,-0.238
8719111,-0.4948584241\C,0.9500016748,2.183043163,-1.2352565454\C,1.189
1252448,3.5185363243,-1.5691192337\C,0.9009472145,4.5294077021,-0.6526
366555\C,0.3747897504,4.1967455625,0.5990024661\C,0.1435217599,2.86249
93307,0.9296131784\H,1.1723140364,1.3988458092,-1.9559535453\H,1.59586
05589,3.7669970241,-2.5460885427\H,1.0830398917,5.5695539978,-0.909732
5042\H,0.1456406647,4.9792510313,1.3180097027\H,-0.2749799264,2.610641
5812,1.9007115643\\Version=EM64L-G09RevB.01\State=1-A\HF=-793.9974365\
RMSD=4.379e-09\RMSF=3.779e-06\Dipole=0.0226846,-0.1007784,-0.1457403\Q
uadrupole=-0.8434376,1.9431264,-1.0996888,1.0728684,-0.7497485,0.48071
21\PG=C01 [X(C17H27N1O1)]\\@

TS6 (c1)

1\1\GINC-X154\FTS\UB3LYP\6-31G(d)\C10H20N1O1(2)\GXG501\10-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200,MaxStep=5) IOP(2/17=4) maxdisk=1342177280\\ts3_stcore
.freq\\0,2\N,-0.8513093416,-1.8494165727,-0.0505260955\O,0.4946894514,
-1.5667183527,0.4191777675\C,0.9662161757,-0.3103102855,-0.0019816563\
C,-1.6245978911,-2.1117253656,1.1625774655\C,-0.733069826,-3.054340979
3,-0.8712836482\H,-2.6468559728,-2.3708176761,0.8670856601\H,-1.202642
4784,-2.9346893825,1.7615175852\H,-1.6544682308,-1.2063772788,1.772280
2129\H,-0.284389301,-3.8966627092,-0.3209115094\H,-0.1198437861,-2.836
1919988,-1.7482753228\H,-1.7363351765,-3.3380471567,-1.2063584119\C,2.
1884230329,0.0372476193,0.7363028151\H,2.7037198269,0.9195323896,0.360
0557018\C,1.0094076716,-0.1090781743,-1.5086682273\H,1.7153997383,-0.8
068810769,-1.9795067364\C,2.6687677561,-0.5967327323,1.8198798011\H,3.
5663285606,-0.2461273874,2.3207346857\C,-0.8252908021,1.6168422583,0.8
198122336\C,-2.0057991728,1.541767497,-0.1315284034\H,-2.8699182371,2.
100909974,0.2561073785\C,-0.0671951232,2.8609684267,0.8712086926\C,0.6
71817933,3.2925204229,1.9142337109\H,1.24740702,4.2122362948,1.8635902
237\H,-0.0694266804,3.4596976506,-0.0427036327\H,2.1853114664,-1.47994
28975,2.2234028985\H,0.019867666,-0.2625061519,-1.9473156487\H,1.33519
40067,0.9106946177,-1.7413512722\H,0.0697975999,0.6470581604,0.3881557
581\H,-1.0212489725,1.1867227102,1.8078918756\H,0.7165101044,2.7382531
955,2.8489361482\H,-2.3171900712,0.5058873231,-0.2975401213\H,-1.75230
89465,1.9741796381,-1.1074829287\\Version=EM64L-G09RevB.01\State=2-A\H
F=-522.9025242\S2=0.773494\S2-1=0.\S2A=0.750407\RMSD=5.945e-09\RMSF=3.
396e-07\Dipole=-0.3903204,-0.3658875,-0.3018439\Quadrupole=-0.5078452,
0.3441183,0.1637268,4.0077568,-0.3069864,-0.5836957\PG=C01 [X(C10H20N1
O1)]\\@

TS6 (c2)

1\1\GINC-X138\FTS\UB3LYP\6-31G(d)\C25H36N1O1(2)\GXG501\18-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts3_stu.freq\\0,2\N,
-0.9219029716,-1.8931948514,0.1525570275\O,0.5203854099,-1.6435169712,
0.1749005485\C,0.9858075535,-0.3028339999,0.0792076905\C,-3.1812295292
,-3.7254623247,0.3748547267\H,-4.2675043219,-3.8793434221,0.357379996\
H,-2.736811388,-4.7117393035,0.5566659965\C,1.3137503252,0.1208954377,
-1.3492286935\C,2.1100222416,-0.0908636194,1.0503525978\C,-0.484720083
9,-3.6155658658,2.0392295498\C,-0.331684023,-4.0842419866,-1.078155727
7\C,-1.2997527684,-2.4017899707,1.5244196446\C,-1.2046108934,-2.808628
1809,-1.0127272422\C,-1.1248033028,-1.2488260635,2.5274305655\C,-0.976
8893178,-2.0359166519,-2.3232935839\C,-2.8076791604,-2.7478710111,1.48
65551851\C,-2.7123391519,-3.1608052595,-0.9636281314\H,-3.3750429633,-
1.8179864853,1.3463469298\H,-3.2846511825,-2.2489040302,-1.1819052707\
H,-3.0876239146,-3.143803935,2.4710161656\H,-2.9177917453,-3.864912544
4,-1.7796282822\H,-1.4841872183,-1.5687279286,3.5122737101\H,-1.410803
8938,-2.6033896855,-3.154752079\H,-1.7126552182,-0.3806715182,2.221525

5281\H,-1.4613800939,-1.0557251499,-2.2903111967\H,-0.0802973112,-0.94
8818213,2.6347312031\H,0.085021457,-1.9029515344,-2.5350217236\H,-0.56
03693158,-3.6672508346,3.1311186803\H,-0.4237933423,-4.5333963322,-2.0
738761125\H,-0.8427043054,-4.569921069,1.6480656343\H,-0.6175723292,-4
.8463701358,-0.3516687505\H,0.5709488387,-3.5200039525,1.7807223789\H,
0.7193799288,-3.830681861,-0.9187734534\H,0.0128333414,0.6477324492,0.
3930500444\C,2.7754494777,1.1510573255,1.1100888595\C,3.8151834816,1.3
704670777,2.0105802611\C,4.232957963,0.3546713115,2.8729821348\C,3.592
6224441,-0.8836219445,2.8206642744\C,2.5459836812,-1.1030364467,1.9256
010937\H,2.470356344,1.9636702503,0.4608196241\H,4.3001075507,2.342998
1425,2.0363444853\H,5.0471024622,0.5257265377,3.5722444286\H,3.9111686
174,-1.6902161822,3.4765976534\H,2.0713558234,-2.0739657359,1.88478732
27\C,-0.8805619063,1.7031778531,0.5574326158\C,-2.0298405717,1.3941541
39,-0.3858003558\C,-0.1646622396,2.9856391137,0.4061276327\C,0.3604324
944,3.6371092186,1.5432596425\C,1.0530372639,4.8395845122,1.4371917577
\C,1.2488023011,5.4314851647,0.1857552172\C,0.7386514218,4.8038347719,
-0.9535205378\C,0.0416250062,3.6016347813,-0.8464058658\H,0.2164482701
,3.183574877,2.5211092049\H,1.4388218119,5.3194215648,2.3332040331\H,1
.78837968,6.3707570809,0.1000999551\H,0.8807487784,5.2557965956,-1.932
1330065\H,-0.3494958261,3.1359077285,-1.7461507559\H,-1.1403795459,1.5
186773324,1.6022142027\H,-1.7297539736,1.4439011334,-1.4384308729\H,-2
.4079723577,0.3851738857,-0.2034542555\H,-2.8529584074,2.1106977595,-0
.2503788219\H,1.8037622336,1.0967941063,-1.3618743604\H,1.996283805,-0
.6058635349,-1.8092819814\H,0.416566567,0.1917943854,-1.9655171413\\Ve
rsion=EM64L-G09RevB.01\State=2-A\HF=-1104.1906527\S2=0.764631\S2-1=0.\
S2A=0.75019\RMSD=6.153e-09\RMSF=4.375e-06\Dipole=-0.3824545,-0.2427989
,-0.0702049\Quadrupole=-2.2119527,1.2695978,0.9423549,5.757898,1.83245
2,-0.8555092\PG=C01 [X(C25H36N1O1)]\\@

TS6

1\1\GINC-X83\FTS\UB3LYP\6-31G(d)\C41H52N1O1(2)\GXG501\31-Jul-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts3_st.freq\\0,2\N,-0
.8647755972,-1.8609687758,0.1447366643\O,0.5886012733,-1.6493505119,0.
1013723145\C,1.0868931935,-0.3147467926,0.1142430911\C,-3.171047706,-3
.6411925136,0.3387520633\H,-4.2608848198,-3.7639763799,0.3629769645\H,
-2.7465509371,-4.6492205426,0.4248168748\C,1.5055614155,0.1832703773,-
1.2756381679\C,2.1169228133,-0.1468965471,1.1939519226\C,-0.398464762,
-3.7107555524,1.8931790254\C,-0.414473286,-3.9686507781,-1.2717336273\
C,-1.2021821801,-2.4476134253,1.4945511227\C,-1.2360514069,-2.67380574
03,-1.0688570713\C,-0.9681836335,-1.3647838349,2.5629441897\C,-1.04836
62634,-1.803816017,-2.3239388378\C,-2.7198156123,-2.757754106,1.498382
2495\C,-2.750805173,-2.9856868683,-0.9735321545\H,-3.2725704862,-1.810
4903288,1.4522824407\H,-3.3072322787,-2.046837568,-1.0931982307\H,-2.9
62070272,-3.2195752956,2.4641202943\H,-3.013062465,-3.6195056475,-1.83
00159735\H,-1.3316419904,-1.7301734419,3.5305266485\H,-1.5481921593,-2
.2842540243,-3.1730406283\H,-1.521955377,-0.4549722521,2.3183386452\H,
-1.4909122254,-0.81344262,-2.1847263388\H,0.0871424713,-1.1137795545,2
.6782636845\H,0.003977774,-1.6923601516,-2.5853928724\H,-0.4285260786,
-3.8335978903,2.981670624\H,-0.5682162399,-4.3381907331,-2.2923357491\
H,-0.7993229457,-4.6274303616,1.4552863455\H,-0.6974465471,-4.77245266
67,-0.5899602894\H,0.647241396,-3.6236667584,1.5943595013\H,0.65211965
42,-3.7683437566,-1.1426291904\H,1.9172174311,1.1926118358,-1.17340377
14\C,2.5094253079,-0.7065260786,-2.0623322339\H,0.6029911401,0.2917539
665,-1.885269854\H,0.0924956546,0.6399225948,0.3897544829\C,2.67928231
74,1.1199466881,1.4450578738\C,3.6164669122,1.3063160185,2.4582741141\
C,4.0325070099,0.2303754152,3.2449436144\C,3.4994779487,-1.0349576976,
2.9981709283\C,2.5548107329,-1.220782859,1.9896992986\H,2.3766097861,1
.9744413996,0.8509426066\H,4.0248035364,2.2990008847,2.6307036347\H,4.
766339966,0.375512021,4.0332833639\H,3.8237078851,-1.8879303723,3.5894
027412\H,2.1632066562,-2.210792506,1.7980652264\H,2.1647139186,-1.7429
989601,-1.9692762267\C,3.9449309454,-0.6624565045,-1.5530269873\C,2.46

93267916,-0.3321145031,-3.5597977492\C,4.5894359193,-1.8371085462,-1.1
460846908\C,5.9245615975,-1.8263535413,-0.7379798544\C,6.6443502348,-0
.631938397,-0.7319404602\C,6.0164593484,0.5482810036,-1.1359186708\C,4
.6831176767,0.530510941,-1.5429213132\H,4.0360079061,-2.7737188194,-1.
1476384097\H,6.4002545828,-2.7523353366,-0.4245426554\H,7.6838491513,-
0.6188017291,-0.4148188196\H,6.566844354,1.4858948294,-1.1344922535\H,
4.2125342902,1.4596383572,-1.8562662834\H,1.4617713575,-0.4602570407,-
3.9728718373\H,3.1577771525,-0.9588751449,-4.1368646464\H,2.7624044563
,0.712945695,-3.7155468862\C,-0.7953946019,1.6989247807,0.6297854576\C
,-2.0944033814,1.3024239188,-0.0633104593\C,-0.1419495634,2.9792122831
,0.280686843\C,0.4329968045,3.7812164977,1.2908576224\C,1.063824474,4.
9867587987,0.993022523\C,1.1483322066,5.42953467,-0.3297338544\C,0.592
0877411,4.6490475154,-1.3468983682\C,-0.0422130228,3.4454157669,-1.047
9704384\H,0.3741895347,3.4460954184,2.3237112067\H,1.4873637547,5.5848
37449,1.7960390228\H,1.6393478894,6.3698392517,-0.5647940508\H,0.65187
63564,4.9812183864,-2.3804183175\H,-0.463119496,2.8549199508,-1.856690
1025\H,-0.8583129651,1.570405361,1.7150689639\H,-2.0612879159,1.571437
8283,-1.1269001486\H,-2.1790227211,0.2130053312,-0.0256259764\C,-3.381
2670284,1.9084643345,0.5723451651\C,-4.619732963,1.2035889777,0.033450
0572\H,-3.3347383493,1.6938432628,1.6497759983\C,-3.4868433314,3.43598
46887,0.410392269\H,-4.4085894179,3.8093182902,0.8707114877\H,-2.63919
0465,3.9445927868,0.8786714787\H,-3.5019457073,3.7249181865,-0.6471893
524\C,-5.4449533046,0.4578109371,0.8862499867\C,-6.5787497036,-0.20089
55619,0.4047073521\C,-6.9093593646,-0.1259524175,-0.9483770297\C,-6.09
81589361,0.6140496407,-1.8117365325\C,-4.9679816557,1.2710630094,-1.32
46924315\H,-5.1982416894,0.3972696133,1.9443432907\H,-7.2033103141,-0.
7699175961,1.0888822054\H,-7.7907401314,-0.6364459357,-1.3274142475\H,
-6.3471942187,0.6817111504,-2.867883091\H,-4.3510469173,1.8458295847,-
2.0112243465\\Version=EM64L-G09RevB.01\State=2-A\HF=-1723.5350498\S2=0
.764704\S2-1=0.\S2A=0.750192\RMSD=4.281e-09\RMSF=3.833e-07\Dipole=-0.3
207745,-0.1489468,-0.0156206\Quadrupole=-3.1574933,2.5829799,0.5745134
,7.9034675,3.8785606,-2.0226024\PG=C01 [X(C41H52N1O1)]\\@

EtCH=CH$_2$ (c1)

1\1\GINC-X118\FOpt\RB3LYP\Gen\C4H8\GXG501\04-Jun-2012\0\\#B3LYP/gen 6D
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\ps_
core1.freq\\0,1\C,-5.7037459605,2.9494511895,0.407367092\H,-4.98231428
58,2.1359197626,0.2590217801\H,-5.1155206317,3.8526076267,0.6294140585
\C,-6.5876024392,2.6317437011,1.5832020445\C,-6.546029223,1.5077896796
,2.2994173763\H,-7.3233970853,3.3963965861,1.8414525128\H,-5.833065787
6,0.7156612303,2.0776511626\H,-7.218439258,1.3343029412,3.1355088565\C
,-6.4993576451,3.1857609152,-0.8877848696\H,-7.2179375683,4.0054576595
,-0.766839176\H,-7.0623733288,2.2893125062,-1.1701755364\H,-5.83249678
66,3.445964202,-1.7175673014\\Version=EM64L-G09RevB.01\State=1-A\HF=-1
57.2210722\RMSD=3.151e-09\RMSF=2.411e-05\Dipole=0.0263353,0.0877663,-0
.0957003\Quadrupole=-0.1198601,0.4768744,-0.3570142,-0.5153686,-0.8205
041,-0.2778337\PG=C01 [X(C4H8)]\\@

CH$_2$CH$_2$Ph (c2)

1\1\GINC-X142\FOpt\RB3LYP\6-31G(d)\C8H10\GXG501\16-Aug-2012\0\\#B3LYP/
6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342
177280\\psu.freq\\0,1\C,-0.8017393859,0.3003945266,0.7185224082\C,-2.2
310385044,-0.0854508223,0.3980712863\C,-3.3024117463,0.7209997317,0.80
54183543\C,-4.6177339487,0.3887864718,0.4783218084\C,-4.8853922932,-0.
7622468587,-0.2648863692\C,-3.8284253782,-1.57653358,-0.6755661388\C,-
2.5152434858,-1.2390161529,-0.3453580691\C,-0.1660799421,1.1917260036,
-0.3638667936\H,0.8660135766,1.4519394326,-0.101327056\H,-0.1524019303
,0.6816373123,-1.3336252633\H,-0.7311530437,2.1224727661,-0.4870304282
\H,-0.1950059211,-0.6060647782,0.8394544788\H,-3.1026958154,1.61729021
48,1.3895468375\H,-5.4339292157,1.0266243532,0.808239392\H,-5.90919034
34,-1.0249480051,-0.5177630342\H,-4.0263017644,-2.4783049421,-1.249598
0401\H,-1.697334311,-1.8819221005,-0.6649270561\H,-0.7704136089,0.8264

18531,1.6811799387\\Version=EM64L-G09RevB.01\State=1-A\HF=-310.8802276
\RMSD=8.887e-09\RMSF=1.900e-05\Dipole=0.1037603,0.0353375,0.01082\Quad
rupole=1.6968726,0.2617569,-1.9586295,-0.2258277,0.3790223,2.303185\PG
=C01 [X(C8H10)]\\@

$Me_2NOC•(Me)CH=CH_2$ (c1)

1\1\GINC-X138\FOpt\UB3LYP\6-31G(d)\C6H12N1O1(2)\GXG501\12-Jul-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdi
sk=1342177280\\st_rcore1.freq\\0,2\N,-1.7449115266,-0.8771889832,-0.00
93279828\O,-1.2783582955,0.4105795475,0.5057625226\C,-0.8240541456,-1.
2176318365,-1.0924076433\C,-3.091400012,-0.6066907629,-0.5009718166\H,
-0.8026774831,-0.4562902924,-1.8884922201\H,-1.1385082974,-2.176882257
3,-1.5175756631\H,0.1816759045,-1.332570817,-0.6798101887\H,-3.1149498
792,0.1893136564,-1.2628494511\H,-3.4834884094,-1.5312293603,-0.936927
2935\H,-3.7271769971,-0.3156433375,0.3385487881\C,-0.6147957306,0.3034
55851,1.7090473156\C,0.3876434469,1.2551340221,1.9010913248\C,1.128046
5456,1.4819427707,3.0449868215\H,0.9929393663,0.9078944413,3.956049380
3\H,1.8874155953,2.2557467234,3.0634380452\C,-1.0892932286,-0.70770247
94,2.7024199569\H,-0.587488213,-0.5680140449,3.6625755448\H,-0.9074469
013,-1.7325385539,2.3606236143\H,-2.1719654498,-0.6169227083,2.8624747
672\H,0.5822547103,1.8856044213,1.0342491779\\Version=EM64L-G09RevB.01
\State=2-A\HF=-365.7208256\S2=0.775519\S2-1=0.\S2A=0.750146\RMSD=9.274
e-09\RMSF=4.753e-06\Dipole=-0.3159102,-0.506225,-0.4151254\Quadrupole=
0.0235213,-1.5925484,1.5690271,0.8422637,0.6072182,0.6616763\PG=C01 [X
(C6H12N1O1)]\\@

TEMPOC•(Me)Ph (c2)

1\1\GINC-X129\FOpt\UB3LYP\6-31G(d)\C17H26N1O1(2)\GXG501\16-Aug-2012\0\
\#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=1342177280\\st_ru.freq\\0,2\N,-1.8418662361,-0.8260589273,-0.24109
84948\O,-1.5472849112,0.52790613,0.1758526669\C,-0.2789190145,1.004417
8161,-0.0966131153\C,-3.6767853015,-3.0108933301,-0.5991983667\H,-3.87
25827493,-4.0446956857,-0.9098065882\H,-4.6386473175,-2.6065372497,-0.
2604673972\C,0.8413737694,0.0812266672,-0.4531819669\C,-0.1361243518,2
.408169399,0.0802355736\C,-4.0317583378,0.1169474824,-1.2147024599\C,-
3.393413697,-0.9083565941,1.8088045898\C,-2.7671023428,-0.748059064,-1
.4193974263\C,-2.2591118274,-1.5697530074,0.9915218841\C,-1.9668890169
,-0.1488712324,-2.5923275317\C,-1.0205826925,-1.6765810763,1.901763510
4\C,-3.1392299967,-2.204686431,-1.7831218282\C,-2.6536117286,-2.994302
5473,0.5382416895\H,-2.2417330531,-2.7043671894,-2.1717618047\H,-1.746
3379029,-3.5150608821,0.2036054949\H,-3.8674748032,-2.1760143724,-2.60
31038012\H,-3.0287478071,-3.5395360515,1.4131641106\H,-2.5596852749,-0
.2135566133,-3.5119044466\H,-1.2474190701,-2.3204672633,2.7589638211\H
,-1.0330990801,-0.698029656,-2.7482955493\H,-0.174640964,-2.1123368055
,1.3615246445\H,-1.7272178046,0.90474989,-2.4226306013\H,-0.7218113113
,-0.6973917043,2.2868263196\H,-4.5117113093,0.2900395856,-2.1847734697
\H,-3.4638463044,-1.3942444069,2.7887394994\H,-4.773552826,-0.35003900
5,-0.5638253075\H,-4.3727583338,-0.9927021179,1.3335719323\H,-3.767613
4881,1.0901550653,-0.7934846689\H,-3.1800894654,0.1508011924,1.9733679
304\H,1.3923920587,0.4480324287,-1.3283381002\H,1.5704962916,-0.016343
0926,0.3659287855\H,0.4505779593,-0.9097893081,-0.6814375051\C,-1.2406
310132,3.2455826928,0.4163726082\C,-1.0764032569,4.6132655492,0.577516
5723\C,0.1804149668,5.212210417,0.4180023898\C,1.2797565083,4.40717026
04,0.0939068898\C,1.1341385228,3.0370593808,-0.0704115893\H,-2.2195962
993,2.7992425603,0.5479607036\H,-1.9383624646,5.2258086019,0.831890140
1\H,0.3008930771,6.2841775534,0.5459214537\H,2.2625466982,4.8560635438
,-0.0293695707\H,2.0049005013,2.4368373973,-0.3146586203\\Version=EM64
L-G09RevB.01\State=2-A\HF=-793.362722\S2=0.774407\S2-1=0.\S2A=0.750419
\RMSD=8.645e-09\RMSF=2.740e-06\Dipole=-0.3300058,-0.9206452,-0.1723081
\Quadrupole=2.0231817,0.1644245,-2.1876062,0.4881188,-0.4851929,0.0350
506\PG=C01 [X(C17H26N1O1)]\\@

TEMPOP•

1\1\GINC-X87\FOpt\UB3LYP\6-31G(d)\C25H34N1O1(2)\GXG501\11-Jul-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdi
sk=1342177280\\st_r.freq\\0,2\N,-1.8836577384,-0.8586854722,-0.0468156
501\O,-0.8570488821,-0.7872007966,0.9957048034\C,0.3235825601,-0.16131
00932,0.6507660455\C,-4.6499822358,-1.1889951703,-0.8194230445\H,-5.41
16062656,-1.2782462196,-1.6040413201\H,-5.1854925642,-1.2539276752,0.1
358082838\C,0.8856984252,-0.284694459,-0.736095328\C,0.9492419731,0.54
06433825,1.7274407992\C,-3.343046214,0.6110478468,1.4956010919\C,-2.96
12122844,-2.6217951119,1.4922614827\C,-2.7826893772,0.3430355563,0.081
1814832\C,-2.476868857,-2.2317095638,0.0753064568\C,-1.9838086413,1.58
76798809,-0.3555488139\C,-1.3934915553,-3.239808071,-0.3445546978\C,-3
.9264504022,0.1508846136,-0.9449127654\C,-3.6320187165,-2.3213753108,-
0.9481874306\H,-3.5006587453,0.2280955433,-1.9543270501\H,-3.202455322
3,-2.2958242903,-1.9587273502\H,-4.6247591494,0.9891124013,-0.83005565
17\H,-4.1124805342,-3.3006817645,-0.8314673251\H,-2.6706472074,2.43448
19355,-0.4702650084\H,-1.8273223742,-4.2442666003,-0.4078589632\H,-1.4
90577284,1.4159112006,-1.3171005509\H,-0.9856306957,-2.9816171468,-1.3
270436326\H,-1.2284397808,1.8731482959,0.3809274068\H,-0.5746414354,-3
.2687810913,0.3773306972\H,-3.7978517347,1.6081197545,1.5182395185\H,-
3.1553706321,-3.7001578851,1.521769292\H,-4.1107882225,-0.1029949795,1
.7997849226\H,-3.8838246964,-2.1182547009,1.7870010779\H,-2.541375095,
0.5934167003,2.237618428\H,-2.1936879558,-2.3983604752,2.2371159996\H,
1.0283873881,0.7161896875,-1.1694848913\C,2.2535668741,-1.0367993872,-
0.8503402647\H,0.1365974174,-0.7776483552,-1.3597189292\C,0.4480687052
,0.4645554445,3.059652589\C,1.0589846037,1.1547505262,4.0967451695\C,2
.1857133346,1.9534730039,3.8637471939\C,2.6891236982,2.052316697,2.561
3628246\C,2.0922311761,1.3638696479,1.5137398551\H,-0.4154649446,-0.15
88179954,3.2601901461\H,0.6551910951,1.0693388457,5.1028557555\H,2.659
3372848,2.4913015953,4.6800538331\H,3.5532493142,2.680919988,2.3601605
899\H,2.4880640078,1.4858972103,0.5110980796\H,2.9761245675,-0.5003813
915,-0.2254722552\C,2.7680663585,-0.9751283562,-2.2820345957\C,2.19427
17799,-2.4789717067,-0.3212458433\C,2.085584531,-1.6044967683,-3.33451
91608\C,2.5610255755,-1.5357060522,-4.643760558\C,3.7337047727,-0.8331
297391,-4.9302710882\C,4.4236204237,-0.2016616605,-3.8955178863\C,3.94
19470451,-0.273655971,-2.5867273192\H,1.1716345098,-2.1573402077,-3.13
02754938\H,2.0152782935,-2.0323337157,-5.4422116484\H,4.1051618136,-0.
7799309055,-5.9502287796\H,5.3384284349,0.3473133506,-4.1043326108\H,4
.4891717282,0.2198415324,-1.7860292587\H,1.8421649747,-2.4961041755,0.
7160908892\H,3.1890836723,-2.936951415,-0.350588478\H,1.5227902051,-3.
1047809611,-0.9176280704\\Version=EM64L-G09RevB.01\State=2-A\HF=-1103.
0334328\S2=0.773065\S2-1=0.\S2A=0.750375\RMSD=3.706e-09\RMSF=4.692e-06
\Dipole=-0.6745189,-0.1172261,-0.347719\Quadrupole=3.7164446,-2.851519
8,-0.8649247,4.3250731,-0.4777532,0.5922072\PG=C01 [X(C25H34N1O1)]\\@

SG1-PBA

•CH(Et)COOMe (c)

1\1\GINC-X146\FOpt\UB3LYP\Gen\C5H9O2(2)\GXG501\04-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\pba_rcore.freq\\0,2\C,-3.8982725564,2.2010411932,0.2898047362\H,-3.2
189306339,1.3560977687,0.2146366304\C,-3.3445879413,3.5320177051,0.137
8989317\O,-3.9845808535,4.5752221384,0.1873596596\O,-1.9981219809,3.49
58283854,-0.0719737152\C,-1.376120366,4.7760197222,-0.2320413207\H,-1.
5218612958,5.3930369262,0.659597061\H,-1.7920827457,5.3049705599,-1.09
4755774\H,-0.3157434743,4.5709585022,-0.3852217122\C,-5.3497161275,1.9
768157056,0.5274966633\H,-5.4829794485,1.50413232,1.5145806787\H,-5.85
57835873,2.9462650141,0.5659818695\C,-6.0014537503,1.067998594,-0.5353
280268\H,-5.5079121485,0.0903548634,-0.5817095765\H,-7.0579711633,0.90
17503685,-0.2986523875\H,-5.9428219268,1.523050233,-1.5295727175\\Vers
ion=EM64L-G09RevB.01\State=2-A\HF=-346.3616838\S2=0.756697\S2-1=0.\S2A

=0.750028\RMSD=7.705e-09\RMSF=7.267e-06\Dipole=0.2751924,-0.5739462,-0
.0380806\Quadrupole=1.6449938,-0.8528511,-0.7921427,4.2067003,-0.43371
26,-0.9451296\PG=C01 [X(C5H9O2)]\\@

•P

1\1\GINC-X118\FOpt\UB3LYP\Gen\C8H13O4(2)\GXG501\04-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\pba_r.freq\\0,2\C,-3.8738307064,2.2139145137,0.2489655958\C,-2.8568
517188,1.0608349844,0.1243584524\C,-1.4127960705,1.6028989612,-0.02637
77935\C,-0.3946937546,0.5472971682,-0.2783905165\H,-4.8935759581,1.827
5631393,0.3347609418\H,-3.8214433803,2.8582862142,-0.6346431336\H,-3.6
604400202,2.8282038809,1.1313893605\H,-3.1165296277,0.4693150985,-0.76
14912071\H,-1.1606186277,2.1364173802,0.9000328679\H,-1.3991830311,2.3
161767055,-0.8558627518\H,-0.1193766202,-0.1450594351,0.5097569263\C,0
.2240354414,0.4015736832,-1.5812941335\C,-2.9732329509,0.1449417528,1.
3357917762\O,-2.1920621022,0.0960796494,2.2633358884\O,-4.0950398989,-
0.6056835139,1.2708271568\C,-4.3244346912,-1.4743009215,2.3933303924\O
,-0.015547604,1.099369381,-2.5599137241\O,1.1222373608,-0.6222196584,-
1.6021147232\C,1.7782437464,-0.8272991676,-2.8586793503\H,-5.256519412
9,-1.9956459866,2.1738137593\H,-4.415429818,-0.8947033737,3.3158114499
\H,-3.5016914206,-2.1859261045,2.5014917489\H,2.4571537234,-1.66665849
3,-2.7025220449\H,2.3356776944,0.0658614507,-3.1561496151\H,1.05203244
76,-1.063093309,-3.6423723229\\Version=EM64L-G09RevB.01\State=2-A\HF=-
613.548489\S2=0.756633\S2-1=0.\S2A=0.750028\RMSD=9.307e-09\RMSF=3.706e
-06\Dipole=-0.5622485,-0.4920597,0.2166296\Quadrupole=4.0875553,0.7741
965,-4.8617518,-0.8495385,-4.95436,1.8686749\PG=C01 [X(C8H13O4)]\\@

SG1•

1\1\GINC-X123\FOpt\UB3LYP\Gen\C11H25N1O4P1(2)\GXG501\05-Jun-2012\0\\#B
3LYP/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342
177280\\sg1_r.freq\\0,2\C,-3.6535499731,3.8640803043,0.017319589\N,-3.
0853720504,2.4882532458,0.2852046475\C,-3.8612172543,1.2630732753,0.56
09189413\O,-1.8079244713,2.4144982378,0.4087270103\C,-5.1863945507,3.8
489591926,-0.0180919145\C,-3.0870350967,4.3241393201,-1.3383007648\C,-
3.1661583054,4.7951039903,1.1437782603\C,-3.4447363605,0.0399017337,-0
.3426668464\H,-4.9018978589,1.4898615072,0.3208056171\P,-3.9061658583,
1.1017051991,2.4201848927\H,-5.5781717287,3.219633998,-0.8256884072\H,
-5.5362112638,4.8695255811,-0.2061273209\H,-5.6059127888,3.523268764,0
.9383630447\H,-3.4616833351,3.700802866,-2.157479078\H,-1.9956528672,4
.2672731687,-1.3285224118\H,-3.3833625718,5.360551718,-1.5329943833\H,
-3.5652483178,4.4670767423,2.1072183014\H,-3.5042907849,5.8186071012,0
.9474381513\H,-2.0742523811,4.7907419023,1.1884548127\C,-3.2034059736,
0.5577875219,-1.7768940335\C,-4.6210672355,-0.9596764627,-0.3917135816
\C,-2.1776836428,-0.6876926512,0.145861135\O,-2.4694655843,0.629020006
3,2.9888646009\O,-4.7809582548,-0.2421024418,2.6249915952\O,-4.4436614
879,2.3342701942,3.0627823763\C,-1.5149459367,1.5865619374,3.496355487
8\C,-5.1633791468,-0.6188140778,3.9630475473\H,-4.0756785585,1.1003837
891,-2.1633216216\H,-3.0231419713,-0.2925777223,-2.4445954879\H,-2.334
324266,1.2182060386,-1.8259464587\H,-5.5289946994,-0.4898489626,-0.791
9262422\H,-4.8546018946,-1.3661930635,0.5941651678\H,-4.3623953514,-1.
7941608559,-1.0538044205\H,-1.3364249223,0.0036188357,0.2251861472\H,-
1.9168751748,-1.4778890056,-0.5688364634\H,-2.3300504627,-1.1557261445
,1.1224625311\H,-0.9939661567,2.0581951466,2.6609346865\H,-0.814960993
8,1.0169476338,4.1106968359\H,-2.0197885022,2.3420846412,4.1034770377\
H,-5.8480387651,-1.4620470995,3.8597140009\H,-5.6658906862,0.212917187
4,4.4645178544\H,-4.2818565138,-0.9235422928,4.5348691636\\Version=EM6
4L-G09RevB.01\State=2-A\HF=-1131.2159172\S2=0.754214\S2-1=0.\S2A=0.750
012\RMSD=4.521e-09\RMSF=1.057e-05\Dipole=-0.4094107,-0.3638698,-0.0225
707\Quadrupole=-2.5805344,0.5131979,2.0673364,1.629283,3.2316167,-4.98
51161\PG=C01 [X(C11H25N1O4P1)]\\@

MeCH=CHCOOMe(c)

1\1\GINC-X135\FOpt\RB3LYP\Gen\C5H8O2\GXG501\04-Jun-2012\0\\#B3LYP/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\p
ba_dcore.freq\\0,1\C,-3.4092946229,2.2830855306,0.2359159884\H,-2.7593
441846,1.4319956461,0.0512497674\C,-2.7760138779,3.5136748023,0.758892
496\O,-3.343773391,4.5564029436,1.0224810959\O,-1.4398849348,3.3346588
228,0.9150236222\C,-0.7273187589,4.4725842193,1.4192632042\H,-0.833591
368,5.3254129517,0.7428917023\H,-1.1034520822,4.7575154687,2.405831685
2\H,0.3162115952,4.161762003,1.4824464105\C,-4.7272164465,2.2359039814
,0.0055408999\H,-5.304905673,3.1350340945,0.2185032446\C,-5.4717914246
,1.0499577638,-0.5202928869\H,-4.8102620985,0.1974300613,-0.7032529659
\H,-5.9847841254,1.2984646157,-1.4590968725\H,-6.2528982587,0.73758530
7,0.1857300142\\Version=EM64L-G09RevB.01\State=1-A\HF=-345.7898203\RMS
D=2.165e-09\RMSF=2.857e-05\Dipole=0.1139315,-0.599549,-0.1861237\Quadr
upole=3.1764226,-1.8396122,-1.3368103,4.4082672,2.3427442,0.7642004\PG
=C01 [X(C5H8O2)]\\@

P(-H)

1\1\GINC-X121\Freq\RB3LYP\Gen\C8H12O4\GXG501\05-Jun-2012\0\\#B3LYP/gen
6D IOP(2/17=4) SCF=Tight guess=read geom=check INT(Grid=Ultrafine) Fr
eq=noraman maxdisk=1342177280\\pba_d.freq\\0,1\C,-3.4069669049,2.03840
42007,0.0683474268\C,-2.3319886442,0.9313923029,-0.0056028068\C,-0.966
3077302,1.4929033264,0.292844042\C,0.0475074738,1.5318035882,-0.579079
3313\H,-4.3959904425,1.6337513196,-0.1727917838\H,-3.175939562,2.83652
39656,-0.6435170265\H,-3.445894049,2.4630678508,1.0754936722\H,-2.3342
155432,0.4724369182,-0.9986629632\H,-0.8147876289,1.9026546526,1.29049
13961\H,-0.0393387012,1.1332375975,-1.5862686271\C,1.3492005563,2.1301
789501,-0.2018266277\C,-2.6531631594,-0.1484818643,1.0282987682\O,-2.8
093463194,0.060828134,2.2115642484\O,-2.7372398198,-1.3690347758,0.461
2340021\C,-3.0208103354,-2.4497893176,1.3688831346\O,1.6236423722,2.62
57989921,0.8733503978\O,2.2242587266,2.0551605901,-1.2349017055\C,3.52
3017898,2.6072136046,-0.9749860351\H,-3.0536467282,-3.347710572,0.7515
515294\H,-3.9798799428,-2.288626782,1.8678369909\H,-2.2353852293,-2.52
90823292,2.1248214503\H,4.091245156,2.4669320228,-1.8951612842\H,4.003
7215149,2.0854601697,-0.1428280345\H,3.4474570426,3.6697534549,-0.7277
908333\\Version=EM64L-G09RevB.01\State=1-A\HF=-612.973402\RMSD=3.278e-
09\RMSF=3.538e-07\ZeroPoint=0.1961637\Thermal=0.2100743\Dipole=-0.2063
302,-0.6164609,-0.9981923\PG=C01 [X(C8H12O4)]\\@

Me_2NOH (c1)

1\1\GINC-X93\FOpt\RB3LYP\Gen\C2H7N1O1\GXG501\06-Jun-2012\0\\#B3LYP/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\
dmno1_r.freq\\0,1\N,-2.5674628504,-0.8485270405,-0.2634161504\O,-1.572
4428897,-0.1105422483,0.4444790461\C,-2.1615842306,-0.944342649,-1.656
0683068\C,-3.8450904687,-0.1766797552,-0.0900348456\H,-1.5464037482,0.
7832492553,0.0334417536\H,-2.888809731,-1.5563971558,-2.1997277772\H,-
1.1824842212,-1.4260885955,-1.7058647189\H,-2.0989502714,0.0462181806,
-2.1516110501\H,-4.0674596472,-0.1112193357,0.97742166\H,-4.6278134122
,-0.7629882315,-0.5826287457\H,-3.8512278696,0.8455939594,-0.520716804
3\\Version=EM64L-G09RevB.01\State=1-A\HF=-210.3293027\RMSD=3.994e-09\R
MSF=2.441e-05\Dipole=-0.4184723,0.5321438,-0.7102834\Quadrupole=0.2250
789,0.6505836,-0.8756625,0.7894005,-1.3951629,1.0965321\PG=C01 [X(C2H7
N1O1)]\\@

SG1H

1\1\GINC-X112\FOpt\RB3LYP\Gen\C11H26N1O4P1\GXG501\06-Jun-2012\0\\#B3LY
P/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177
280\\sg1h.freq\\0,1\C,-2.5295536028,-0.7204183196,-0.3218144566\N,-1.4
96281294,0.1007110662,0.3907763861\C,-0.245425143,0.4934532068,-0.2784
434609\O,-1.2254977066,-0.4214536831,1.6974011809\C,-2.9831099904,0.04
20859367,-1.5808787828\C,-3.7344765265,-0.8211104053,0.6337087652\C,-2
.0741033583,-2.1373786024,-0.7311983185\C,0.0696034805,2.0261490224,-0
.0752319925\H,-0.3782180865,0.3486446409,-1.3566370489\P,1.1524416748,

-0.6996266431,0.0960121463\H,-3.3356701005,1.0462260021,-1.3311929149\
H,-3.8093790885,-0.5044311096,-2.0478842777\H,-2.1923980596,0.12939677
34,-2.3338254555\H,-4.056849589,0.1775787353,0.9454082205\H,-3.4865021
343,-1.3912128514,1.5310579184\H,-4.5689169682,-1.3168225241,0.1254750
878\H,-1.2530330833,-2.1105990563,-1.4548717977\H,-2.9129917427,-2.666
4882905,-1.1984551559\H,-1.738430982,-2.7289507148,0.123633082\C,-1.08
57521228,2.8291167192,-0.7078112716\C,1.3734935882,2.4194912222,-0.800
3039922\C,0.155503115,2.4087011996,1.4139788506\O,2.2454133247,-0.0480
410086,1.1096126283\O,1.9506183006,-0.6672709055,-1.3093552615\O,0.701
1917767,-2.0490366651,0.5619618155\C,2.2703887473,-0.4730129902,2.4884
016636\C,3.1306674247,-1.4787908656,-1.4681940628\H,-1.187365979,2.618
9700182,-1.7797798787\H,-0.8930609519,3.9027339446,-0.5976792289\H,-2.
0348990104,2.6000719424,-0.2173872182\H,1.3485978961,2.1344516178,-1.8
588180302\H,2.2568639231,1.9635763156,-0.3461931102\H,1.5011176597,3.5
073458805,-0.7518866661\H,-0.7453701784,2.0989980799,1.9499212858\H,0.
2554434341,3.4970887076,1.5070763178\H,1.0228977707,1.9557493215,1.899
8547232\H,1.3619457937,-0.1494657376,3.004884292\H,3.1426711712,0.0084
915372,2.9339615202\H,2.3619572065,-1.5594111733,2.5528075539\H,3.4302
195038,-1.3817437517,-2.5128195869\H,2.9086578497,-2.5253246668,-1.240
1179015\H,3.9305911598,-1.1149241167,-0.8167093953\H,-0.7880781018,-1.
2919998088,1.5485798281\\Version=EM64L-G09RevB.01\State=1-A\HF=-1131.8
217611\RMSD=5.992e-09\RMSF=4.883e-06\Dipole=0.7790273,0.0134923,-0.434
2441\Quadrupole=4.1541127,-4.5881727,0.4340601,-1.5680764,2.7492052,0.
7438449\PG=C01 [X(C11H26N1O4P1)]\\@

TS2 (c)

1\1\GINC-X85\FTS\RB3LYP\6-31G(d)\C7H15N1O3\GXG501\19-Aug-2012\0\\#B3LY
P/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest
,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_bscore.freq\\0,1\N,-1
.8629898262,1.2007384893,0.7829420529\C,-0.4331669627,1.0435048291,0.9
96777641\C,-2.7351523298,0.0774235289,1.0951727876\O,-2.2000147917,1.8
789972574,-0.2869440819\H,-2.3985057477,1.6411752788,-1.7407422942\C,-
3.0336371671,2.2140169829,-2.6127037882\H,-2.2625980567,2.5313848438,-
3.3234981647\C,-3.9788918055,1.1589238415,-3.1937162671\C,-3.510697273
6,3.302166409,-1.8252588452\H,-4.6667529452,0.7885494733,-2.4334672299
\H,-3.4033289383,0.320967578,-3.6016909443\H,-4.5743763456,1.585271418
2,-4.0100395573\H,-2.9137978376,4.2048288327,-1.752567533\C,-4.7041146
344,3.2695810913,-0.9879682191\O,-5.4741891344,2.3326156055,-0.8237718
394\O,-4.8871884908,4.4781236464,-0.3768505735\C,-6.0268641328,4.55378
93497,0.4830079859\H,-5.9404915797,3.8390822816,1.3074441833\H,-6.0405
356328,5.5753710133,0.8661910506\H,-6.9475105763,4.3391458428,-0.06800
15591\H,0.0412205796,2.017776846,0.8621798533\H,-0.246402864,0.6799187
738,2.0118404632\H,0.0041423913,0.3320331741,0.2753980229\H,-2.5721280
926,-0.2472362397,2.1274787011\H,-2.5462200083,-0.7733534211,0.4175570
377\H,-3.7659647971,0.4098142733,0.9646121172\\Version=EM64L-G09RevB.0
1\State=1-A\HF=-556.0553615\RMSD=3.880e-09\RMSF=1.270e-06\Dipole=0.824
2358,-0.3460266,0.5034013\Quadrupole=-0.6026578,-0.1535962,0.756254,-4
.7801244,-0.2146197,-1.6113825\PG=C01 [X(C7H15N1O3)]\\@

TS2

1\1\GINC-X121\FTS\RB3LYP\6-31G(d)\C19H38N1O8P1\GXG501\12-Aug-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(grid=ultrafine)
OPT=(TS,readfc,MaxStep=10,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=
1342177280\\ts1_bs.freq\\0,1\N,1.2991600067,0.3576169538,1.2601518297\
O,0.1998614532,-0.3225714343,1.0294473778\H,-0.8513840487,-0.266494674
5,0.0256550428\C,-1.9432019318,-0.7963667228,-0.191822134\C,-2.0195553
219,-1.6422026032,0.9456829353\C,-1.5503063546,-3.0175467928,0.9851665
74\O,-1.6732462879,-3.5368475563,2.2412254978\C,-1.2653134428,-4.90108
84373,2.37535108\C,1.0886320636,1.7366997566,1.8174183387\C,0.16444437
31,2.5344111701,0.8751829381\C,2.5152256444,-0.149068733,0.6298742445\
P,2.2938083544,-0.1569218008,-1.2289135314\O,1.4108757364,0.9350863671
,-1.7282329821\C,-1.8497048585,-1.3513820833,-1.6163381566\C,-3.013842

234,-2.2880365958,-1.9256896929\O,-2.7652338165,-2.9895118922,-3.05843
32432\C,-3.8037207918,-3.8959507332,-3.4553401994\C,2.416220543,2.4882
920429,1.9861262876\C,0.4142467713,1.5626699053,3.1924150541\C,3.09680
5981,-1.439437436,1.332888609\C,2.074396077,-2.5865580888,1.4400439054
\C,3.5243062489,-1.0293267908,2.7583544262\C,4.3515441612,-1.933883057
3,0.5836936472\O,1.8900222153,-1.6665723468,-1.6097031111\C,1.73071265
48,-2.0407130803,-2.9943668978\O,3.8036800231,-0.0725117523,-1.8474303
708\C,4.3350918717,1.1902182801,-2.2798148551\C,-1.8060386096,-0.20843
07134,-2.6515925103\O,-1.1099886348,-3.6709965898,0.0460537484\O,-4.04
37220456,-2.3936041599,-1.2964019358\H,3.2839797888,0.6205152404,0.746
817106\H,3.1301613807,1.9361972608,2.6059177799\H,2.2131006395,3.44006
38355,2.4876220664\H,2.8831844851,2.7245274516,1.0236077863\H,1.097657
3231,1.0992609456,3.9124406683\H,-0.4702941579,0.9282863359,3.09828785
28\H,0.1070286568,2.536940075,3.5882068777\H,0.5884100482,2.5925983056
,-0.1302836663\H,0.0243137774,3.5471572629,1.269846127\H,-0.8171653493
,2.0589086018,0.8038376731\H,4.3122142256,-0.2649747199,2.7430106522\H
,3.921128742,-1.9001546658,3.2927148055\H,2.6774552143,-0.6431997682,3
.3341810382\H,5.0942521625,-1.13745577,0.4566196492\H,4.1111555061,-2.
3325450325,-0.4045812951\H,4.820688515,-2.7374607366,1.1631551194\H,1.
2318479193,-2.3118802738,2.0786623975\H,2.5699935329,-3.4593341362,1.8
847709154\H,1.6753030264,-2.878170319,0.4670199346\H,2.708259894,-2.08
12540237,-3.4832805567\H,1.080143714,-1.3311023174,-3.5126256585\H,1.2
691569911,-3.0285353774,-2.9884394065\H,4.737845026,1.7487184177,-1.42
61053557\H,3.5670370596,1.7869904199,-2.7774131475\H,5.147480944,0.964
8215542,-2.9739300905\H,-1.7323288739,-0.6098691667,-3.6669038007\H,-0
.9399686685,0.4339381935,-2.4646327063\H,-2.7142979087,0.4044939079,-2
.5954094457\H,-0.9421061162,-1.9514886039,-1.7065824902\H,-2.625650349
8,0.0579864113,-0.1171132564\H,-2.3975906511,-1.2404943325,1.878946239
\H,-3.4454783786,-4.3719403834,-4.3692695699\H,-4.7372977778,-3.358263
9157,-3.6438714052\H,-3.9774988074,-4.6437192897,-2.6768256861\H,-1.46
50941118,-5.1674720835,3.4144464451\H,-0.1999098818,-5.0124737698,2.15
1513541\H,-1.8341193399,-5.5456879348,1.6986399467\\Version=EM64L-G09R
evB.01\State=1-A\HF=-1744.7333771\RMSD=8.283e-09\RMSF=5.143e-07\Dipole
=1.7551614,0.5313418,-0.0829927\Quadrupole=-5.5763907,1.8617537,3.7146
37,4.8909433,0.7755539,3.9128766\PG=C01 [X(C19H38N1O8P1)]\\@

$Me_2NOCH(Et)COOMe$ (c)

1\1\GINC-X142\FOpt\RB3LYP\6-31G(d)\C7H15N1O3\GXG501\01-Jul-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
1342177280\\bs_core.freq\\0,1\N,1.0025207834,2.4065831459,0.8285133194
\C,1.3494293369,1.3509603888,1.7750435899\C,1.9875979142,2.5164933389,
-0.2453825836\O,1.0989900551,3.6420856046,1.5923352695\C,-0.0122044853
,4.4679226708,1.2866330627\C,-1.360462413,3.8197594133,1.6070193749\O,
-2.3652424012,4.0082615726,0.9554694062\O,-1.3280413628,3.0843127884,2
.7379329639\C,-2.5827117608,2.4928172128,3.1141342699\H,-2.38252147,1.
9412709369,4.0332583517\H,-2.9390992489,1.8194652397,2.3301706685\H,-3
.3362355269,3.2661508514,3.2858191521\H,-0.0434051844,4.6947350203,0.2
120119671\C,0.1847939656,5.7648706582,2.0886202015\H,0.1381787838,5.51
87094811,3.1561230994\H,1.2067982054,6.1073295967,1.88768344\C,-0.8207
323225,6.8671787065,1.7411680015\H,-0.7521502573,7.1482418376,0.683900
4131\H,-0.6243338065,7.7631972108,2.3394873946\H,-1.852354385,6.553697
6853,1.9300803373\H,2.3577251694,1.4808598757,2.201653662\H,0.61533908
37,1.3508281256,2.5817764653\H,1.3072205748,0.3926982681,1.2465181038\
H,1.9521083436,1.5966882528,-0.8387917041\H,1.7216944495,3.3541257389,
-0.8962568787\H,3.0117949594,2.6658033785,0.1325726522\\Version=EM64L-
G09RevB.01\State=1-A\HF=-556.1469536\RMSD=4.029e-09\RMSF=6.827e-06\Dip
ole=0.3932074,-0.3611044,0.3444083\Quadrupole=-2.5380266,2.8956454,-0.
3576188,0.7777001,-5.966261,-0.2473446\PG=C01 [X(C7H15N1O3)]\\@

SG1P

1\1\GINC-X142\FOpt\RB3LYP\6-31G(d)\C19H38N1O8P1\GXG501\02-Jul-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdi

sk=1342177280\\bs.freq\\0,1\C,-2.220224949,-1.0103075836,-0.4992970993
\N,-1.3977153232,-0.0292446578,0.3083491691\C,-0.2111640941,0.55197072
33,-0.3698709644\O,-0.9249824888,-0.6971656557,1.5122528564\C,-2.84155
10155,-0.2553050408,-1.690515095\C,-3.3756844869,-1.4987475898,0.38973
19515\C,-1.4381944533,-2.2310806392,-1.0188533285\C,-0.1702312773,2.13
69632965,-0.297635168\H,-0.28095814,0.3083615104,-1.4339747096\P,1.432
9874517,-0.2228255959,0.1221596254\H,-3.4506413788,0.5880688536,-1.354
9018484\H,-3.4899261577,-0.9466453366,-2.2389878105\H,-2.0965608511,0.
1163049491,-2.4000182353\H,-3.8926185225,-0.6594836787,0.8659931863\H,
-3.0191720734,-2.1836714353,1.1603498509\H,-4.1029126833,-2.0404507463
,-0.2246280426\H,-0.6305082594,-1.951569766,-1.7023612294\H,-2.1217605
906,-2.889484721,-1.5677742508\H,-1.002525186,-2.8000050332,-0.1962051
784\C,-1.4703038213,2.6919832796,-0.9135686415\C,1.0123353249,2.681256
4845,-1.1302373535\C,-0.0501149946,2.6871479624,1.135311424\O,2.140666
0307,-0.1265731882,-1.3401872172\O,1.3248192102,-1.8342888286,0.245513
0053\O,2.1802316146,0.4140851739,1.2455499916\C,3.5128109995,-0.533975
9958,-1.4638072855\C,1.4458960727,-2.5119447259,1.5097178696\H,-1.5751
136874,2.4143163612,-1.9687153433\H,-1.4594360693,3.7869774705,-0.8607
61098\H,-2.3497087182,2.3358464923,-0.3712127559\H,1.0147620161,2.2789
351742,-2.149266547\H,1.9783649412,2.4537156457,-0.6724586851\H,0.9274
102888,3.7721100142,-1.199303584\H,-0.9183237996,2.4148179414,1.742353
6675\H,-0.0153221839,3.7828086227,1.097887213\H,0.8590943994,2.3328225
485,1.6247835796\H,4.1375131891,-0.0167628294,-0.729136251\H,3.8269568
076,-0.2627166545,-2.4734786276\H,3.6012158263,-1.6166468737,-1.328101
7477\H,1.9095913471,-3.4780049594,1.2955298586\H,0.455364546,-2.653905
9802,1.9461792361\H,2.0769774647,-1.9385825274,2.1928671089\C,-1.45983
37142,-0.1336551245,2.7256343141\C,-2.4790859496,-1.0613654925,3.38899
46788\H,-1.9896017094,0.7873883128,2.4790901103\C,-0.2862826235,0.1341
622086,3.6933594116\O,-3.5191781509,-0.671124344,3.8786862856\O,-2.051
4786679,-2.3355551534,3.4364963776\C,-2.8671606451,-3.2327775474,4.213
3022299\H,-2.4054146398,-4.2141429589,4.1024387209\H,-3.8928049414,-3.
2433746786,3.8362265503\H,-2.8591423007,-2.9176124836,5.2589550712\H,0
.1069121266,-0.8218753487,4.0541116672\C,-0.6315314767,1.0228732418,4.
9027790787\H,0.5065332885,0.6101898003,3.111740479\C,0.6571614329,1.49
22886413,5.6122611248\C,-1.4906908856,0.2883096258,5.9245399554\H,-1.1
88159613,1.906954743,4.572264284\O,-1.3447219032,-0.8755760946,6.24432
7675\O,-2.4082679118,1.103871173,6.4769269256\C,-3.2882867573,0.487673
6332,7.4320228779\H,1.2312569654,0.6326362858,5.9742129179\H,0.4228508
531,2.1351981203,6.4673646133\H,1.2862252152,2.0580645934,4.917688411\
H,-3.9263143649,1.2908402666,7.8018398937\H,-2.7189716842,0.0383700436
,8.2498317809\H,-3.8874822671,-0.2823299245,6.9394850694\\Version=EM64
L-G09RevB.01\State=1-A\HF=-1744.8100898\RMSD=9.289e-09\RMSF=4.613e-06\
Dipole=-0.1817695,-0.4759696,-0.4008013\Quadrupole=-3.4870856,0.217619
5,3.2694661,-0.0464028,-4.5470492,1.3689504\PG=C01 [X(C19H38N1O8P1)]\\
@

TS3a (c)

Single Point\\0,1\N,0,1.958923,1.943853,-1.311635\O,0,1.317319,1.15143
8,-0.212677\C,0,2.137389,0.074731,0.415353\C,0,0.997929,-0.17058,1.394
167\H,0,0.542832,0.660323,0.688875\C,0,1.610854,3.389931,-1.046476\C,0
,1.615447,1.363951,-2.636548\H,0,0.544139,3.599479,-1.002268\H,0,2.065
631,3.664574,-0.097006\H,0,2.06105,4.020212,-1.810552\H,0,1.272909,2.1
80392,-3.281082\H,0,2.477186,0.932299,-3.14135\H,0,0.746735,0.709335,-
2.612858\H,0,1.212454,0.207093,2.394404\C,0,0.365186,-1.557976,1.40990
5\H,0,0.165679,-1.884129,0.386988\H,0,-0.559324,-1.55808,1.983513\H,0,
1.048597,-2.269737,1.868261\H,0,2.295185,-0.714975,-0.31363\C,0,3.4837
93,0.524642,0.952653\O,0,4.54166,0.117949,0.517723\O,0,3.382518,1.3715
42,1.992317\C,0,4.627866,1.78196,2.575557\H,0,5.247396,2.300286,1.8368
86\H,0,4. 360154,2.452802,3.392737\H,0,5.174136,0.914559,2.954301\\Ver
sion=EM64L-G09RevB.01\State=1-A\HF=-552.8548311\ PG=C01 [X(C7H15N1O3)]
\\@

TS3a

1\1\GINC-X104\Freq\RB3LYP\6-31G(d)\C19H38N1O8P1\GXG501\26-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17
=4) maxdisk=1342177280\\ts2_bs.freq\\0,1\C,1.93536,1.96678,-1.31184\N,
1.29834,1.16048,-0.20428\C,2.10009,0.08939,0.4435\O,0.03347,0.5932,-0.
77488\C,3.24289,2.60276,-0.80269\C,0.97388,3.12042,-1.65192\C,2.23711,
1.1699,-2.59563\C,2.19507,0.26478,2.02774\H,3.12796,0.17047,0.07439\P,
1.61932,-1.63758,-0.09871\H,3.07091,3.22476,0.08031\H,3.64434,3.24207,
-1.59554\H,4.01841,1.86655,-0.56454\H,0.76322,3.72185,-0.76232\H,0.026
04,2.75426,-2.05016\H,1.43598,3.76932,-2.40457\H,2.94886,0.36084,-2.42
618\H,2.66318,1.84435,-3.34613\H,1.32473,0.73795,-3.01473\C,2.56601,1.
7273,2.34882\C,3.32353,-0.62651,2.60258\C,0.88716,-0.06025,2.77519\O,2
.97468,-2.42571,0.33307\O,1.7581,-1.67673,-1.71391\O,0.35256,-2.23553,
0.40985\C,3.04314,-3.84489,0.10757\C,0.72576,-2.1988,-2.56803\H,3.5606
1,1.98916,1.9698\H,2.5852,1.85648,3.43718\H,1.83214,2.42261,1.9357\H,4
.25987,-0.51225,2.04326\H,3.06341,-1.6853,2.60433\H,3.51475,-0.32725,3
.63797\H,0.11106,0.68554,2.57834\H,1.08245,-0.03459,3.85498\H,0.50064,
-1.05128,2.52729\H,2.17101,-4.34755,0.53417\H,3.95171,-4.19051,0.60418
\H,3.10922,-4.05405,-0.96345\H,1.19901,-2.90594,-3.25462\H,0.28256,-1.
37641,-3.13579\H,-0.04457,-2.70457,-1.98157\C,-1.18584,0.65609,0.08277
\C,-1.53959,2.04067,0.59435\H,-1.05151,-0.00905,0.931\C,-1.98401,0.071
63,-1.07393\O,-1.54229,2.33236,1.77272\O,-1.90315,2.88924,-0.38348\C,-
2.30418,4.19615,0.05317\H,-2.56381,4.74037,-0.85562\H,-1.48526,4.69434
,0.58165\H,-3.16821,4.12587,0.71857\H,-2.61748,0.81082,-1.5653\C,-2.69
695,-1.25628,-0.84187\H,-0.88439,0.06557,-1.50492\C,-3.20084,-1.85246,
-2.17204\C,-3.90076,-1.04413,0.07001\H,-2.01787,-1.95953,-0.35522\O,-4
.74018,-0.17359,-0.07348\O,-3.94059,-1.95814,1.07002\C,-5.05529,-1.836
93,1.9695\H,-3.91841,-1.17646,-2.64959\H,-3.69038,-2.81991,-2.01617\H,
-2.36116,-2.00196,-2.86112\H,-4.92419,-2.63277,2.70625\H,-6.00084,-1.9
6226,1.43178\H,-5.05041,-0.85653,2.45535\\Version=EM64L-G09RevB.01\Sta
te=1-A\HF=-1744.7277844\RMSD=9.817e-09\RMSF=1.013e-02\ZeroPoint=0.5750
39\Thermal=0.6111409\Dipole=1.0013002,-0.2309297,-0.8597483\PG=C01 [X(
C19H38N1O8P1)]\NImag=1\\@

SG1H→O

1\1\GINC-X141\FOpt\RB3LYP\Gen\C11H26N1O4P1\GXG501\06-Jun-2012\0\\#B3LY
P/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177
280\\sg1_x.freq\\0,1\C,-2.5319111948,-0.729479735,-0.2506955047\N,-1.3
660707986,0.0970540003,0.3907121238\C,-0.1698569254,0.4903042122,-0.45
54529146\O,-0.8650228309,-0.4782385511,1.5318653794\C,-3.1346284248,0.
0583430582,-1.4201389392\C,-3.5535479977,-0.8676453637,0.885585523\C,-
2.0372508607,-2.1012588261,-0.6962894413\C,0.1238895391,2.0287004501,-
0.2775522887\H,-0.368752603,0.3034099129,-1.5163137327\P,1.1458875683,
-0.7643512594,0.0586613664\H,-3.4964228144,1.0469127852,-1.1149708801\
H,-3.9954374991,-0.4964432313,-1.8079175048\H,-2.431627812,0.185327963
9,-2.2495244187\H,-3.9284960496,0.1126003351,1.2101067088\H,-3.0914099
162,-1.3623145193,1.7405864163\H,-4.4109311359,-1.4529039528,0.5385221
952\H,-1.3614262398,-2.0418637701,-1.5537840374\H,-2.9052404953,-2.702
1545394,-0.9907349649\H,-1.5019821545,-2.5986579766,0.1117088761\C,-1.
0521091972,2.832618138,-0.887901405\C,1.3920618901,2.4534924059,-1.047
0148805\C,0.2864155986,2.4238100898,1.2067532895\O,1.978545375,-0.2683
654225,1.3573605705\O,2.207511784,-0.3093552641,-1.1026624774\O,0.8570
469638,-2.2210123705,-0.029921061\C,1.7133437354,-0.8415771123,2.65258
58143\C,3.3779275811,-1.1146364423,-1.2953527459\H,-1.2181235647,2.573
1387741,-1.9398624204\H,-0.8216851355,3.9023796779,-0.8406887343\H,-1.
9999979147,2.6967267214,-0.3528218031\H,1.3420760033,2.1648596486,-2.1
025313138\H,2.2935646078,2.0106703036,-0.6245313038\H,1.4847436499,3.5
448415231,-0.9975813768\H,-0.544888075,2.0833627792,1.8332909421\H,0.3
473467244,3.5154883677,1.2858472601\H,1.1983127995,1.9941670361,1.6247
792029\H,0.8703800765,-0.3267018711,3.1152282777\H,2.6274185893,-0.702
5539193,3.2350649942\H,1.4839063345,-1.9053665663,2.5582579755\H,3.887
9068069,-0.7188281613,-2.1767411429\H,3.1023816207,-2.1602336713,-1.45

99365236\H,4.041379515,-1.0426385573,-0.4266096823\H,-1.8377630653,0.9
775822657,0.6448489921\\Version=EM64L-G09RevB.01\State=1-A\HF=-1131.79
69143\RMSD=7.395e-09\RMSF=4.166e-06\Dipole=-0.7224279,1.25551,-0.65419
\Quadrupole=6.3645033,-5.2862942,-1.0782091,-1.08682,2.2040201,0.28005
31\PG=C01 [X(C11H26N1O4P1)]\\@

EtCH$_2$COOMe (c)

1\1\GINC-X92\FOpt\RB3LYP\6-31G(d)\C5H10O2\GXG501\01-Jul-2012\0\\#B3LYP
/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134
2177280\\pba_core.freq\\0,1\C,-3.8195619336,2.252574383,0.1221540504\C
,-2.6636791495,1.2712906466,0.1304851064\O,-1.4960934749,1.5519159379,
0.2945088092\O,-3.103460024,0.0066241715,-0.0730936812\C,-2.0834625333
,-1.0045569634,-0.0835139906\H,-1.3595914652,-0.814186924,-0.880687850
6\H,-2.6056766131,-1.9460133252,-0.2575718696\H,-1.5554784086,-1.02986
56191,0.8736674163\H,-4.5386574421,1.9321912262,0.888474498\H,-4.34732
59467,2.1429336204,-0.835097637\C,-3.3812106596,3.7010379894,0.3480613
588\H,-2.8450984058,3.7684452808,1.3018718136\H,-2.6537645474,3.979485
3778,-0.4235264259\C,-4.5612321834,4.6769177325,0.336387921\H,-5.09347
80569,4.6504809405,-0.6225682479\H,-4.2225210592,5.7058472898,0.499898
3123\H,-5.2870523251,4.436961202,1.1234452879\\Version=EM64L-G09RevB.0
1\State=1-A\HF=-347.0168735\RMSD=9.495e-09\RMSF=1.216e-05\Dipole=-0.51
74648,-0.328398,-0.0957367\Quadrupole=-3.4251229,3.3683612,0.0567617,-
2.3506777,-0.6822267,0.1450506\PG=C01 [X(C5H10O2)]\\@

PH

1\1\GINC-X112\FOpt\RB3LYP\Gen\C8H14O4\GXG501\06-Jun-2012\0\\#B3LYP/gen
 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\
pba.freq\\0,1\C,-3.8382688349,2.2379168379,0.1356456909\C,-2.648513957
9,1.254401834,0.102907817\C,-1.307144202,1.9903016522,0.228729951\C,-0
.0883791598,1.0820607437,0.0520413928\H,-4.7902466095,1.7102588991,0.0
251508711\H,-3.7487161327,2.9630899898,-0.6800692002\H,-3.857098976,2.
7925332401,1.0807388233\H,-2.6875980216,0.7100525537,-0.8500253997\H,-
1.2540157417,2.4783454882,1.2075648692\H,-1.2726696001,2.7885960445,-0
.5207434473\H,-0.1405821593,0.5255089562,-0.894653521\H,-0.0414983001,
0.3279966952,0.8453106045\C,1.216637971,1.8531772066,0.0554276929\C,-2
.8296240564,0.2254513343,1.2120375013\O,-2.2495469784,0.2211636353,2.2
779262403\O,-3.765748846,-0.6924077156,0.8765582732\C,-4.0522189377,-1
.6782442314,1.8821956418\O,1.3284725739,3.059585659,0.0933548331\O,2.2
735171011,1.0091289747,0.0008444462\C,3.5637718358,1.639893159,-0.0093
974604\H,-4.815912971,-2.3250428292,1.4491809345\H,-4.4232182908,-1.20
20973678,2.7937793292\H,-3.1538855409,-2.2526131143,2.1238325534\H,4.2
8771255,0.8255075655,-0.0544849927\H,3.7096681734,2.2331471809,0.89737
38187\H,3.6670471116,2.2938746081,-0.8797062634\\Version=EM64L-G09RevB
.01\State=1-A\HF=-614.2031429\RMSD=4.517e-09\RMSF=1.251e-05\Dipole=-0.
3360802,-0.7798747,-0.4404158\Quadrupole=7.2302397,-3.586267,-3.643972
7,0.3956366,-1.5877664,-0.9820621\PG=C01 [X(C8H14O4)]\\@

TS5 (c)

1\1\GINC-X113\Freq\UB3LYP\6-31G(d)\C7H16N1O3(2)\GXG501\11-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(Grid=Ultrafine)
 Freq=noraman maxdisk=1342177280\\ts4_bscore.freq\\0,2\N,-2.4386673238
,-0.1718411597,-0.2611159018\C,-3.6352762835,0.6542304768,-0.346733449
6\C,-2.6671964179,-1.6109353371,-0.2056808078\O,-1.670005911,0.2283175
851,0.810600396\H,-0.663660337,0.4650511361,0.4173646263\C,0.633358137
1,0.8106109432,-0.2183843421\H,0.2216631525,0.6980920557,-1.2240429231
\C,1.4916142877,-0.2978417363,0.2255441225\O,2.347391936,-0.2278256191
,1.0922617174\O,1.1978296928,-1.4576859577,-0.4290686507\C,1.974731687
5,-2.593101207,-0.0248820746\H,1.8242889639,-2.8083434019,1.036988573\
H,1.6222877849,-3.4240032638,-0.6376288158\H,3.0398465495,-2.415382096
6,-0.1987046596\C,0.9785134566,2.2003547263,0.2445900062\H,1.232650307
1,2.1673599876,1.3095353916\H,0.0983755762,2.846186158,0.134803169\C,2
.1617986868,2.8115699214,-0.5343409055\H,2.3712198869,3.8270561146,-0.

1786889484\H,1.9465465892,2.8662603996,-1.6078875672\H,3.0638877565,2.
2078691878,-0.3941925009\H,-4.2906824855,0.5327728574,0.5312052868\H,-
4.1914228708,0.3792563958,-1.2484801717\H,-3.3331439225,1.7016651957,-
0.4181694143\H,-3.2335715758,-1.9088160296,0.6915194527\H,-1.695424372
4,-2.109691644,-0.1995605929\H,-3.2211339512,-1.9166836883,-1.09899001
54\\Version=EM64L-G09RevB.01\State=2-A\HF=-556.6873955\S2=0.756925\S2-
1=0.\S2A=0.750033\RMSD=3.501e-09\RMSF=3.416e-07\ZeroPoint=0.2275162\Th
ermal=0.2422836\Dipole=-0.8971681,-0.3383926,-0.8190421\PG=C01 [X(C7H1
6N1O3)]\NImag=1\\@

TS5

1\1\GINC-X81\FTS\UB3LYP\6-31G(d)\C19H39N1O8P1(2)\GXG501\07-Aug-2012\0\
\#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_bs.freq\\0,2\N,
1.0552632635,-0.7525719337,-0.8215468988\O,0.3092054993,-0.463299671,0
.2923520417\H,-0.543418597,0.1304752218,0.0506790355\C,-2.0614862885,0
.7478295209,0.1033216332\C,-1.8877353867,2.1778036448,0.3524573147\O,-
1.7556584547,2.8832384607,-0.8075011546\C,-1.55433325,4.2922469871,-0.
6422947633\C,0.738519457,-2.0993260209,-1.4090392103\C,0.6250825677,-3
.1779875753,-0.3129230894\C,2.3582188621,-0.0892807951,-0.8235643021\P
,3.3472825763,-0.640235044,0.6736851815\O,3.4755944801,-2.1230811216,0
.7575676752\C,-2.5780527205,-0.104581946,1.2282825229\C,-4.1211074369,
-0.1278326841,1.3346337268\C,-4.7415098751,-0.7723136223,0.1024626456\
O,-6.0539983349,-0.465839237,0.0013679047\C,-6.74731456,-1.0660295579,
-1.1054405971\C,1.8244360613,-2.5089706906,-2.4156156493\C,-0.61029459
16,-1.9659446863,-2.1468171004\C,2.2888336791,1.4502654474,-1.17959834
72\C,1.9667244593,2.3500575583,0.0297103758\C,1.2130465145,1.641943651
,-2.2692419974\C,3.6388330122,1.893852893,-1.7870845695\O,2.7927386987
,0.0517241272,2.0285800347\C,1.9745175076,-0.6775508751,2.9641346083\O
,4.7413507225,0.1603273416,0.470100729\C,5.8299632761,-0.1214345842,1.
3704275625\C,-4.5855867836,-0.8835247114,2.5972460671\O,-1.8472570937,
2.7081967018,1.4539523052\O,-4.1678808595,-1.495193088,-0.6872349337\H
,2.9188304015,-0.5512643195,-1.6385810218\H,1.9499299282,-1.7678261795
,-3.2136106147\H,1.5190656945,-3.4478960888,-2.8882545522\H,2.78527032
2,-2.683853304,-1.9224193912\H,-0.5591135307,-1.1923329396,-2.92082312
24\H,-1.4290326273,-1.7251248449,-1.4627835707\H,-0.863068187,-2.91694
44009,-2.628751956\H,1.5742764519,-3.2960001022,0.2137117609\H,0.35013
30415,-4.1328975733,-0.7753150555\H,-0.1524134085,-2.9158887891,0.4090
193029\H,1.3902587673,0.9827980258,-3.1277257311\H,1.2472447959,2.6758
231578,-2.6332103526\H,0.2023648724,1.4580582278,-1.8994215305\H,3.879
3824451,1.3122044864,-2.6865946092\H,4.4640039929,1.7870276063,-1.0817
123694\H,3.5758643578,2.9473465528,-2.084138483\H,1.0467422933,2.04990
15149,0.5364416508\H,1.8487634782,3.3863992445,-0.3102777067\H,2.77124
26464,2.3327776799,0.7702206407\H,2.3188694499,-1.7110986698,3.0502202
675\H,0.9340248838,-0.6564065727,2.6342697958\H,2.0783143343,-0.164115
2422,3.9222138945\H,6.6934668098,0.4261033386,0.9890161703\H,6.0438458
234,-1.1937894504,1.3872536191\H,5.5857804982,0.2267699093,2.378684284
8\H,-5.6768824531,-0.8841155772,2.6750150448\H,-4.1759428292,-0.403740
644,3.4920679509\H,-4.2389949875,-1.9233631475,2.5791674534\H,-4.49630
31156,0.9005821835,1.3950081814\H,-2.2299314989,-1.1366511283,1.108023
123\H,-2.1807821246,0.2829600748,2.1719287621\H,-2.3245280599,0.466521
3018,-0.9140170668\H,-7.7764060798,-0.7132526717,-1.0318261458\H,-6.70
86026719,-2.156576149,-1.0382410778\H,-6.3003660993,-0.7533788772,-2.0
528627473\H,-1.4671365437,4.6966064179,-1.6517265204\H,-0.6436638071,4
.4901234083,-0.0698252526\H,-2.4020716688,4.7460328303,-0.1207187763\\
Version=EM64L-G09RevB.01\State=2-A\HF=-1745.3605645\S2=0.757257\S2-1=0
.\S2A=0.750037\RMSD=5.982e-09\RMSF=5.377e-07\Dipole=-0.4025004,0.28153
64,-0.3824495\Quadrupole=11.2953611,-9.1309307,-2.1644305,6.3201734,3.
6612095,-3.8776494\PG=C01 [X(C19H39N1O8P1)]\\@

•CH(Me)COOH (c1)

1\1\GINC-X146\FOpt\UB3LYP\Gen\C3H5O2(2)\GXG501\04-Jun-2012\0\\#B3LYP/g

en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\pba_rcore1.freq\\0,2\C,-3.8756323897,2.18905255,0.2788139625\H,-3.20
62404422,1.3379448078,0.1973974425\C,-3.3098471837,3.5137957991,0.1296
485173\O,-3.9352771441,4.5643727454,0.1956801309\O,-1.964169648,3.4847
32193,-0.1001358858\H,-1.692382976,4.4169124778,-0.1834184175\C,-5.323
8128219,1.9907633503,0.5351253155\H,-5.4880573851,1.4466337236,1.47712
55549\H,-5.841218096,2.9514721027,0.58615175\H,-5.7852338352,1.3786369
283,-0.254004537\\Version=EM64L-G09RevB.01\State=2-A\HF=-267.7416359\S
2=0.757003\S2-1=0.\S2A=0.75003\RMSD=9.540e-09\RMSF=1.422e-05\Dipole=0.
1140166,-0.6334916,0.0055107\Quadrupole=0.7832456,-0.2824349,-0.500810
7,3.8120848,-0.3858383,-0.6670146\PG=C01 [X(C3H5O2)]\\@

$Me_2NOCH(Me)COOH$ (c1)

1\1\GINC-X92\FOpt\RB3LYP\6-31G(d)\C5H11N1O3\GXG501\01-Jul-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1
342177280\\bs_core1.freq\\0,1\N,1.1038067139,2.437169277,0.6747344691\
C,1.2947725562,1.2323634195,1.4772529768\C,2.2431230424,2.6882827877,-
0.2056159909\O,1.0891149553,3.5325690206,1.634882982\C,0.0332127787,4.
4171227351,1.3081146587\C,-1.3509941417,3.7715895439,1.3712622141\O,-2
.2801659666,4.1029271368,0.6695896085\O,-1.4647328346,2.8417050029,2.3
493697084\H,-2.3904716624,2.5346348308,2.310750434\H,0.1378968933,4.78
52505008,0.2792758116\C,0.1176142555,5.5841877825,2.2941901423\H,-0.00
20843961,5.2233814606,3.3201485949\H,1.0939933127,6.0693917644,2.20563
57732\H,-0.6645949075,6.3183534528,2.0792623938\H,2.2253250234,1.26179
73535,2.0675049673\H,0.4438677762,1.1218868531,2.1505112843\H,1.331629
096,0.374862302,0.7970941185\H,2.294400972,1.8767100033,-0.9390934084\
H,2.0850970062,3.6269696558,-0.7441108744\H,3.1975345273,2.7440791169,
0.3419541361\\Version=EM64L-G09RevB.01\State=1-A\HF=-477.5268658\RMSD=
8.959e-09\RMSF=1.263e-05\Dipole=0.4708352,-0.3255698,0.2077227\Quadrup
ole=-1.3472206,2.7253207,-1.3781001,1.7907424,-5.3167469,0.8439068\PG=
C01 [X(C5H11N1O3)]\\@

CH_3CH_2COOH (c1)

1\1\GINC-X93\FOpt\RB3LYP\Gen\C3H6O2\GXG501\06-Jun-2012\0\\#B3LYP/gen 6
D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\pb
a_core1.freq\\0,1\C,-3.8374490502,2.2122633515,0.147857909\C,-2.685216
6663,1.231034909,0.1173443624\O,-1.5138832977,1.499311568,0.2668663296
\O,-3.1186193821,-0.0372939916,-0.1047276692\H,-2.3191123649,-0.596530
5223,-0.1085539535\H,-4.3780373523,2.11807666,-0.802958744\H,-4.541693
1169,1.8724912598,0.9182791915\C,-3.3857814429,3.6498064422,0.39580040
12\H,-4.2481995734,4.3239273083,0.4105089465\H,-2.697760403,3.98503882
47,-0.3858403829\H,-2.8622403107,3.7367597623,1.3524764876\\Version=EM
64L-G09RevB.01\State=1-A\HF=-268.3966253\RMSD=3.971e-09\RMSF=2.286e-05
\Dipole=-0.5434484,-0.1601354,-0.0744708\Quadrupole=-2.5145844,2.27333
26,0.2412518,-2.4973906,-0.6231864,0.044825\PG=C01 [X(C3H6O2)]\\@

$Me_2NOC•(Me)COOH$ (c1)

1\1\GINC-V1303\FOpt\UB3LYP\6-31G(d)\C5H10N1O3(2)\GXG501\21-Jul-2012\0\
\#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=268435456\\bs_rcore1.freq\\0,2\N,0.7998255344,-1.5935278532,2.0108
461605\O,0.6716845453,-1.1103173667,0.6388014134\C,1.8602937256,-0.962
0749726,-0.0027259409\C,1.7713520056,-0.4858908362,-1.3619544761\C,3.1
699946811,-1.2640213855,0.635043172\O,0.4937867111,-0.2583791083,-1.79
00856058\H,0.5960460767,0.052824711,-2.7075576952\O,2.7444550932,-0.29
49397119,-2.088156419\H,3.2357272321,-2.3111413144,0.9563180195\H,3.33
84860029,-0.652534441,1.5304103391\H,3.956862297,-1.0607527558,-0.0931
422084\C,0.0366127197,-2.8410186897,2.0367174278\C,0.1772422839,-0.553
3056391,2.829209747\H,-1.0131316634,-2.7039418218,1.7352336312\H,0.072
3126647,-3.230178486,3.059245251\H,0.5111406246,-3.5647836766,1.369852
4891\H,0.216481798,-0.8841986516,3.8719244925\H,0.7530357954,0.3702342
257,2.7330121345\H,-0.8690064357,-0.3594748432,2.5473593602\\Version=E
M64L-G09RevB.01\State=2-A\HF=-476.8858009\S2=0.755675\S2-1=0.\S2A=0.75

0021\RMSD=3.667e-09\RMSF=7.555e-06\Dipole=-0.681481,-0.3906622,1.24702
86\Quadrupole=-2.8797732,1.1615791,1.7181942,-0.5153601,2.1791589,-0.3
821512\PG=C01 [X(C5H10N1O3)]\\@

SG1P•

1\1\GINC-X153\Freq\UB3LYP\6-31G(d)\C19H37N1O8P1(2)\GXG501\23-Jul-2012\
0\\#B3LYP/6-31G(d) 6D INT(grid=ultrafine) SCF=tight Freq=noraman maxdi
sk=1342177280\\bs_r.freq\\0,2\C,1.1883197467,2.1233822684,0.8159244252
\N,1.2942604199,0.6531903914,1.1671610767\C,2.5854974926,-0.0125420297
,0.8744716702\O,0.2370347011,-0.1042998429,0.4723380258\C,2.0853820761
,2.8742494879,1.8224907269\C,-0.2593538267,2.5826583472,1.0452445389\C
,1.5989104405,2.5099044756,-0.6174282064\C,3.0936117724,-0.9353529308,
2.0552323808\H,3.3222088484,0.7914901853,0.7990742605\P,2.7746682121,-
0.8652452254,-0.8061727432\H,1.8223034793,2.6209479097,2.8531653437\H,
1.9450164647,3.951679351,1.6855372316\H,3.1502711372,2.6672915388,1.67
83438606\H,-0.5689604184,2.4320232555,2.0825749242\H,-0.9562314215,2.0
614388353,0.384940219\H,-0.3297093055,3.6536921297,0.829668214\H,2.624
4178199,2.2154472474,-0.8562913737\H,1.5376473418,3.5997695793,-0.7177
267837\H,0.9392813077,2.0598064255,-1.3600107579\C,3.1553515151,-0.088
904932,3.3430438835\C,4.5279699289,-1.4282545646,1.7530701666\C,2.1958
431271,-2.1613180667,2.3073838542\O,4.2542158674,-0.2625686246,-1.1330
483425\O,1.9099814052,-0.1048228877,-1.942842439\O,2.6597837056,-2.348
6156206,-0.8585982281\C,4.9322299535,-0.7257621553,-2.3122549627\C,0.8
429259867,-0.7466644298,-2.6640357986\H,3.8536215108,0.7512313021,3.24
370365\H,3.5054287763,-0.7123614811,4.1738978654\H,2.1738350302,0.3104
01516,3.6107098856\H,5.2006172254,-0.6000943862,1.5024522066\H,4.54871
94821,-2.1502600492,0.9330784958\H,4.9273028981,-1.9270337717,2.643674
3689\H,1.2095792121,-1.8723770651,2.6794991422\H,2.6561139619,-2.79375
33121,3.0762506465\H,2.0731141325,-2.7596619356,1.4017925268\H,4.97853
21102,-1.8187970147,-2.3270234873\H,5.9416106393,-0.3120591094,-2.2723
873138\H,4.4217624347,-0.3644103761,-3.2111453386\H,-0.0992002909,-0.5
993177819,-2.1356994976\H,1.0396106523,-1.8156021192,-2.767307286\H,0.
8130058316,-0.2705357926,-3.6472369063\C,-0.6202954727,-0.7960931765,1
.2810990587\C,-1.1016168476,-2.0697650944,0.7721108706\C,-1.0450685468
,-0.3353393179,2.639502301\O,-1.8538354192,-2.7956502605,1.4156538454\
O,-0.6313854805,-2.3916991527,-0.4556113375\C,-0.9880153567,-3.7001302
444,-0.9188033536\H,-0.4609599366,-3.8274386177,-1.8645847821\H,-2.069
4530064,-3.7787586253,-1.0651343522\H,-0.6703034027,-4.4619386244,-0.2
025485957\H,-1.0773632249,-1.2039239937,3.3064070421\C,-2.4379283952,0
.3752495994,2.7345096687\H,-0.2864762478,0.3521969516,3.0199411086\C,-
2.5871101131,1.0461734898,4.1063373605\C,-3.5706378981,-0.6223625117,2
.5273676901\H,-2.5061650741,1.1236268857,1.940561971\O,-4.0688474959,-
1.2943691957,3.4033075316\O,-3.968259629,-0.6529400731,1.2358372869\C,
-4.9475210894,-1.6595723026,0.9267725234\H,-2.5510402723,0.2980055998,
4.9035066972\H,-3.5456598815,1.5695910946,4.1857971315\H,-1.7855006358
,1.7750254827,4.2707647559\H,-5.1909733825,-1.5167896343,-0.1271033691
\H,-5.838078167,-1.5335727104,1.5476839485\H,-4.5205684084,-2.65075330
94,1.0959148734\\Version=EM64L-G09RevB.01\State=2-A\HF=-1744.1625532\S
2=0.755594\S2-1=0.\S2A=0.750022\RMSD=8.068e-09\RMSF=3.045e-06\ZeroPoin
t=0.5648413\Thermal=0.6012144\Dipole=0.8217365,1.399142,-1.2701218\PG=
C01 [X(C19H37N1O8P1)]\\@

TS6 (c1)

1\1\GINC-X133\Freq\UB3LYP\6-31G(d)\C8H16N1O5(2)\GXG501\21-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(Grid=Ultrafine)
 Freq=noraman maxdisk=1342177280\\ts3_bscore1.freq\\0,2\N,-0.224960029
8,-1.9332309856,-1.6397610025\C,-0.5796910593,-2.6223177584,-0.3979508
157\C,-1.360827572,-1.9269036127,-2.5672051512\O,0.7698825544,-2.79246
33893,-2.2935720101\C,1.9342650838,-2.124149064,-2.6458606234\C,2.8942
716166,-1.7275291486,-1.5549179742\C,2.6035414117,-2.8583021843,-3.793
0620247\H,1.9183912536,-2.9149375412,-4.6433066256\H,2.8645818059,-3.8
81477812,-3.494971401\H,3.515905419,-2.3373662175,-4.0895392617\O,3.98

75141396,-1.2447340103,-1.7814627765\O,2.4396740611,-1.920584128,-0.29
45013934\H,3.1509905281,-1.5928016894,0.2882537161\H,1.6252136931,-0.9
290840146,-3.1691269704\C,1.3518823817,0.3164372506,-3.7501726135\C,1.
3238111719,0.0142248648,-5.1944637385\O,2.2158688998,0.2324441031,-5.9
929737309\O,0.1638802484,-0.6109832584,-5.5676834685\H,0.2599350761,-0
.7963514751,-6.5203019763\C,2.4340993593,1.2574678156,-3.281312027\H,2
.4806934678,1.2890703516,-2.188923922\H,3.4117225909,0.9570184798,-3.6
649643434\H,2.2353917951,2.2781812242,-3.637606494\H,-0.9643757146,-3.
6387697821,-0.5783703017\H,-1.3588471122,-2.0307799132,0.0942122451\H,
0.2955554366,-2.6692599461,0.2475455375\H,-2.1424314146,-1.2965403981,
-2.1292562666\H,-1.7675804819,-2.9360854143,-2.7385657428\H,-1.0546292
592,-1.499237649,-3.5233566306\H,0.3640486492,0.4694303025,-3.31583321
24\\Version=EM64L-G09RevB.01\State=2-A\HF=-745.2459134\S2=0.757388\S2-
1=0.\S2A=0.750039\RMSD=3.410e-09\RMSF=1.832e-06\ZeroPoint=0.2424393\Th
ermal=0.2595485\Dipole=-1.0758228,-0.3538485,0.767108\PG=C01 [X(C8H16N
1O5)]\NImag=1\\@

TS6

1\1\GINC-X113\FTS\UB3LYP\6-31G(d)\C27H51N1O12P1(2)\GXG501\03-Aug-2012\
0\\#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noe
igentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts3_bs.freq\\0,2\
C,-0.9871087114,-1.9990646396,-1.9063418659\N,-1.0718733238,-1.3844182
342,-0.5132466427\C,-2.2975068507,-1.7578210898,0.2581151003\O,-1.1252
484485,0.0770114097,-0.693060259\C,-0.970507578,-3.5361089127,-1.77903
32379\C,0.3594174887,-1.6003923074,-2.5308368284\C,-2.1302161103,-1.57
52128726,-2.8462462446\C,-1.9717143204,-2.3574627319,1.6915756093\H,-2
.7988690818,-2.5608136851,-0.2878287797\P,-3.6438958772,-0.4402551275,
0.3314842773\H,-0.1547768789,-3.8782810305,-1.1382506822\H,-0.80874689
88,-3.9538664882,-2.7781569652\H,-1.9096829148,-3.9551156146,-1.406837
7761\H,1.2025833113,-1.9381942853,-1.9232515179\H,0.4248326816,-0.5250
332027,-2.6939672323\H,0.4502624549,-2.0815083407,-3.5112213683\H,-3.1
128107458,-1.8833893081,-2.4778148743\H,-1.9808855622,-2.0477450093,-3
.8241030507\H,-2.1414624451,-0.4933387942,-2.9842209587\C,-1.030311528
,-3.568101604,1.5264218121\C,-3.26159625,-2.8673500448,2.3737108788\C,
-1.2862408424,-1.3523622598,2.630725818\O,-4.9071028086,-1.4692765804,
0.3415255794\O,-3.9009606399,0.252709974,-1.1063345693\O,-3.5895166477
,0.5286809648,1.4642237774\C,-6.2278031282,-0.9220951065,0.4727045564\
C,-3.6464719613,1.6552156939,-1.3329898102\H,-1.4950020679,-4.37557818
61,0.9494989294\H,-0.7837075254,-3.9698686693,2.5162865829\H,-0.094964
7187,-3.2822521974,1.0389896878\H,-3.8348984426,-3.5374621465,1.723972
6918\H,-3.9179579557,-2.0499565572,2.6820137844\H,-2.9844096153,-3.426
9970589,3.2749199263\H,-0.2911601208,-1.0926219421,2.2653601762\H,-1.1
547902782,-1.8166202672,3.6166247403\H,-1.8829904947,-0.446599871,2.75
51491693\H,-6.2936569982,-0.2751086249,1.3530229955\H,-6.9055147475,-1
.7705502629,0.5861500264\H,-6.4951047278,-0.3538823624,-0.4241556041\H
,-4.4300855932,1.9997441666,-2.0127656295\H,-2.6649793018,1.7797101163
,-1.7890886507\H,-3.6919772941,2.213904263,-0.3964248679\C,-0.04593742
38,0.8913187097,-0.3043365047\C,0.4320635492,1.7653685249,-1.442927314
3\H,1.0832092039,0.1709588965,-0.0176508271\C,-0.3399415426,1.63478333
48,1.0134321274\O,1.4339035728,2.45424467,-1.3694060017\O,-0.336172351
9,1.7097583828,-2.5491166998\C,0.0671273868,2.5895745389,-3.6130862655
\H,-0.6293441212,2.3939871907,-4.4286116427\H,1.0940525924,2.378252794
1,-3.9208804031\H,-0.0064649222,3.6287695554,-3.283600537\H,-1.4246207
243,1.778922264,1.0496946686\C,0.3587814916,2.9747495387,1.2995934799\
H,-0.1057355612,0.954121442,1.8357216937\C,0.1513224439,3.3711064972,2
.7782507791\C,-0.170886855,4.081684129,0.3989913932\H,1.4346538615,2.8
993227103,1.1180824013\O,-1.1202388508,3.9954075841,-0.3574577612\O,0.
5374303982,5.2195748294,0.5552090528\C,0.1181041438,6.3292762474,-0.25
13751239\H,-0.9145755836,3.4270953726,3.0285559314\H,0.6108141286,4.34
02926825,2.9886382503\H,0.6152299411,2.6250026917,3.4314987209\H,0.768
9447085,7.1580798525,0.0292941384\H,-0.9284476436,6.5777365981,-0.0556
936189\H,0.2356170556,6.0955530913,-1.3133211303\C,5.6497698684,-0.202

785863,-1.6530910486\C,4.6458150175,-0.7353047512,-0.6081901606\C,3.27
73720363,-0.0347928933,-0.7458481971\C,2.2802134697,-0.4362645548,0.32
36840089\H,6.6285311252,-0.6776216136,-1.5360873329\H,5.7728477422,0.8
783810866,-1.5334341863\H,5.2912311487,-0.3939712219,-2.6712315439\H,5
.0587691953,-0.5336669143,0.3871357471\H,2.8672128498,-0.2601935543,-1
.7347641043\H,3.4391695548,1.0443734303,-0.6921072365\H,1.9624430361,-
1.4770830641,0.3048140791\C,2.6040604137,0.0502965645,1.6885966838\C,4
.5244298777,-2.2452219747,-0.7561771479\O,3.6076025304,-2.8403314269,-
1.2868100059\O,5.6063044183,-2.8729418514,-0.2424352306\C,5.6148679975
,-4.3036578941,-0.3762103512\O,3.2215861422,1.0690922513,1.9513151118\
O,2.1242308437,-0.7840842072,2.6487513597\C,2.3852866361,-0.3845934492
,4.0019402013\H,6.5455223176,-4.6350710724,0.085354836\H,5.5842538364,
-4.5923379984,-1.4303121119\H,4.7542885981,-4.7420465381,0.1360970758\
H,1.9562650861,-1.1689848799,4.6260571232\H,1.9138690952,0.5776402442,
4.2210787123\H,3.4611848568,-0.297347232,4.1760819074\\Version=EM64L-G
09RevB.01\State=2-A\HF=-2358.3248365\S2=0.757366\S2-1=0.\S2A=0.750037\
RMSD=7.344e-09\RMSF=8.044e-07\Dipole=0.3864966,-0.450153,-0.6287162\Qu
adrupole=-1.8843698,3.0658987,-1.1815288,-7.2218285,2.5701581,-7.03712
86\PG=C01 [X(C27H51N1O12P1)]\\@

TEMPO-PMMA

- **CH(Et)COOMe(c)**

1\1\GINC-X135\FOpt\UB3LYP\Gen\C6H11O2(2)\GXG501\05-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\pmma_rcore.freq\\0,2\C,-2.9990669883,-0.8314803994,-0.3711283071\C,
-1.6436009996,-0.5565588015,0.1944686314\C,-3.2160952181,-1.7282365342
,-1.4956104832\H,-1.6487535121,-0.6662729615,1.2885697121\H,-0.8787101
174,-1.212897185,-0.2224876409\H,-1.3450648123,0.4852695431,-0.0039531
037\O,-4.3184906771,-1.9993585206,-1.9608531856\O,-2.0621359068,-2.255
8480612,-1.9987031674\C,-2.2385334545,-3.1489708269,-3.1036577298\H,-2
.8503647835,-4.0087348085,-2.8148866001\H,-1.2347735225,-3.4717811688,
-3.3839821906\H,-2.7249800176,-2.6402282308,-3.9410729538\C,-4.2097987
967,-0.2065805362,0.2547851859\H,-3.9314890497,0.7579139306,0.69957675
93\H,-4.9615576104,-0.0184908052,-0.5186067944\C,-4.8437594168,-1.1027
683024,1.343315552\H,-5.7073195012,-0.6013426798,1.7944184392\H,-4.129
1796903,-1.3304642669,2.1426615727\H,-5.1845819249,-2.0459583848,0.905
8283042\\Version=EM64L-G09RevB.01\State=2-A\HF=-385.6824852\S2=0.75638
5\S2-1=0.\S2A=0.750027\RMSD=7.410e-09\RMSF=1.006e-05\Dipole=0.6428771,
0.1530743,0.3203607\Quadrupole=-2.6319065,1.2222406,1.4096659,-1.29572
95,-2.325733,2.1673606\PG=C01 [X(C6H11O2)]\\@

- **P**

1\1\GINC-X57\FOpt\UB3LYP\Gen\C10H17O4(2)\GXG501\05-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\pmma_r.freq\\0,2\C,-3.027730848,-0.9055518939,-0.3312935153\C,-1.62
4366241,-0.6000360324,0.2389271975\C,-0.5701871938,-1.3784032071,-0.63
12504427\C,0.8538707251,-1.2899252357,-0.1762103217\H,-3.8003789462,-0
.3535726584,0.2163805146\H,-3.2424706251,-1.9749750769,-0.2284165067\H
,-3.0996456411,-0.6364500586,-1.3887564585\C,-1.5482848416,-1.03193202
5,1.7105401678\H,-0.6478622754,-1.0031580242,-1.659367557\H,-0.8730792
419,-2.4293468831,-0.6246167442\C,1.6650938164,-0.0572246845,-0.422389
3226\C,1.3976719745,-2.4305786109,0.5509525165\C,-1.3715439563,0.90850
82317,0.1442811583\O,-1.1095221983,1.6418371294,1.0743454575\O,-1.4783
382333,1.3579558529,-1.1308057241\C,-1.2752687835,2.7692740964,-1.3067
97918\O,0.7774815437,-3.458875161,0.8024008492\O,2.6923655916,-2.24901
28838,0.9358249533\C,3.2703629834,-3.3451907389,1.6541047514\H,-1.4142
853012,2.9544269679,-2.372465721\H,-0.2669989443,3.0553773584,-0.99522
8476\H,-2.0007536924,3.3379322103,-0.7192830868\H,4.2915710052,-3.0387
494097,1.8849162432\H,3.27124919,-4.2525625737,1.0430634744\H,2.712515
4414,-3.5432468033,2.5738761894\H,-1.6545681913,-2.1183950959,1.785945

573\H,-2.3422701643,-0.5561308378,2.2945309559\H,-0.5947932068,-0.7479
847115,2.1635745542\H,1.3883313388,0.4055981583,-1.3771193202\H,2.7362
082604,-0.2698733842,-0.4200548281\H,1.4825686554,0.697313985,0.359524
3872\\Version=EM64L-G09RevB.01\State=2-A\HF=-692.181122\S2=0.756539\S2
-1=0.\S2A=0.750028\RMSD=7.580e-09\RMSF=8.868e-06\Dipole=0.2285986,0.46
5701,-0.709814\Quadrupole=4.0660871,-2.9458168,-1.1202703,-2.7171436,2
.6718261,-5.3888703\PG=C01 [X(C10H17O4)]\\@

MeCH=C(Me)COOMe (c)

1\1\GINC-X135\FOpt\RB3LYP\Gen\C6H10O2\GXG501\04-Jun-2012\0\\#B3LYP/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\
pmma_dcore.freq\\0,1\C,-2.9185535715,-1.1120974566,-0.1633814026\C,-1.
5602498097,-0.6339760879,0.2848171221\C,-2.9815168887,-2.1133186656,-1
.2730857507\H,-1.0146959964,-0.1668728884,-0.5429814937\H,-1.632940271
2,0.0928424604,1.0970010836\H,-0.9427420792,-1.4708686164,0.6302405531
\O,-3.9937738991,-2.5944989694,-1.7463960454\O,-1.7421584866,-2.444218
2685,-1.716103475\C,-1.7111307764,-3.402334919,-2.783089725\H,-2.17375
86698,-4.3424890569,-2.4704493431\H,-0.6553172955,-3.5516539605,-3.012
5195963\H,-2.2450869406,-3.0219884614,-3.6582444584\C,-4.1038439521,-0
.7239631038,0.3412645227\H,-4.9845594111,-1.1782296204,-0.1097331667\C
,-4.3675174912,0.2530656268,1.4438384932\H,-4.9999440067,1.0747971692,
1.0812565287\H,-3.4603602675,0.6867786524,1.8714309954\H,-4.9286871867
,-0.2305548339,2.254967158\\Version=EM64L-G09RevB.01\State=1-A\HF=-385
.1057484\RMSD=2.011e-09\RMSF=2.563e-05\Dipole=0.5040402,0.2970297,0.29
97891\Quadrupole=-1.7791479,0.4479797,1.3311682,-3.1513063,-3.4878608,
2.3467941\PG=C01 [X(C6H10O2)]\\@

P(-H)

1\1\GINC-X107\FOpt\RB3LYP\Gen\C10H16O4\GXG501\04-Jun-2012\0\\#B3LYP/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\
\pmma_d.freq\\0,1\C,-2.9067682004,-1.1157442009,-0.1656670469\C,-1.509
2183716,-0.6948013402,0.3580256015\C,-0.4455630563,-1.4180388049,-0.45
46110318\C,0.8724819463,-1.1680051096,-0.5424414221\H,-3.7003271061,-0
.6061792741,0.3917169213\H,-3.0403782217,-2.1954007481,-0.0360965612\H
,-3.0181628966,-0.8770761367,-1.2269796044\C,-1.3849922244,-1.07341504
16,1.8492856733\H,-0.7995414138,-2.2837115083,-1.0112422044\C,1.624976
0861,-0.0452751626,0.1269009808\C,1.6475288708,-2.1125678854,-1.409734
2459\C,-1.4244026145,0.8331764869,0.2163425898\O,-1.411407555,1.623165
7899,1.1366306888\O,-1.4167520848,1.2106231357,-1.0803299745\C,-1.3928
631902,2.6288864495,-1.311498035\O,1.1940401153,-3.0715055676,-2.00506
91261\O,2.9593540915,-1.774040443,-1.464524008\C,3.7772284787,-2.62820
6369,-2.2768749677\H,-1.3852782683,2.7474209338,-2.3953234666\H,-0.498
1416364,3.0748207624,-0.869150481\H,-2.2768794734,3.1042104664,-0.8780
148363\H,4.7855676327,-2.2179245768,-2.2104389593\H,3.4272537543,-2.62
45374547,-3.3127537914\H,3.7536153931,-3.6547380018,-1.9010827982\H,-1
.4762055542,-2.1585022872,1.9638819732\H,-2.1731784565,-0.589050632,2.
4334241154\H,-0.4214029773,-0.7639959644,2.26201325\H,0.986662426,0.55
11212444,0.7808012156\H,2.0737452937,0.6223499749,-0.6180572541\H,2.45
27622131,-0.4384287351,0.7271908054\\Version=EM64L-G09RevB.01\State=1-
A\HF=-691.5993171\RMSD=6.361e-09\RMSF=3.267e-06\Dipole=0.2329695,0.357
6594,-0.3244256\Quadrupole=6.4354077,-2.6154426,-3.8199651,-1.373493,-
0.8653806,-6.7819585\PG=C01 [X(C10H16O4)]\\@

EtC(=CH_2)COOMe (c)

1\1\GINC-X105\FOpt\RB3LYP\6-31G(d)\C6H10O2\GXG501\09-Jul-2012\0\\#B3LY
P/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13
42177280\\pmma_d1core.freq\\0,1\C,2.0669131847,1.8579617319,-1.1453519
32\C,1.2382262412,1.2111837028,-0.3152750165\C,1.9338050253,1.82600307
73,-2.6511598248\C,3.2075802662,2.6689858796,-0.6175521512\H,0.4190585
473,0.6093275312,-0.7009007424\H,1.3523595518,1.2612725022,0.761685929
8\O,4.0358319755,3.212035259,-1.324747562\O,3.2393420281,2.7395842415,
0.7336944262\C,4.3289818213,3.4963433785,1.2802550134\H,5.2876786754,3

.0597186296,0.9871618221\H,4.2020786101,3.4511394864,2.3624723255\H,4.
2918150236,4.5320991434,0.9318159228\H,1.2642068051,1.0030725191,-2.92
68520433\H,2.9146655675,1.6112092595,-3.0907643559\C,1.4043455225,3.14
48080718,-3.2417648315\H,0.4119686316,3.3842396899,-2.8429338624\H,1.3
236000309,3.0707016627,-4.3320470816\H,2.0801904918,3.9723192335,-3.00
77980361\\Version=EM64L-G09RevB.01\State=1-A\HF=-385.0998834\RMSD=8.57
7e-09\RMSF=8.004e-06\Dipole=-0.3257973,-0.2061766,0.5240195\Quadrupole
=-0.7032204,-0.7107377,1.4139581,1.0310438,3.3080487,1.9975261\PG=C01
[X(C6H10O2)]\\@

P(-H) M

1\1\GINC-X109\FOpt\RB3LYP\6-31G(d)\C10H16O4\GXG501\09-Jul-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1
342177280\\pmma_d1.freq\\0,1\C,2.1020849735,1.9111672065,-1.1448110922
\C,1.1223886673,1.1822975326,-0.2040135718\C,0.0582530637,0.4472229233
,-1.0944236395\C,-1.0292197193,-0.3041573854,-0.3596471179\H,2.8948874
846,2.4095518555,-0.5760371778\H,1.5662878645,2.6784080036,-1.71608413
39\H,2.5746346998,1.2217627546,-1.8487016684\C,0.448033033,2.193349617
8,0.7368797959\H,0.5880629966,-0.2472245252,-1.7539695136\H,-0.4080903
021,1.2144584216,-1.7234397842\C,-2.2530693119,0.1972652777,-0.1461742
403\C,-0.6920577526,-1.6971326417,0.0718102681\C,1.8456355694,0.129154
5147,0.6452742241\O,1.537312067,-0.1668960664,1.7820621013\O,2.8507283
761,-0.4661383454,-0.0265977705\C,3.4698848199,-1.5756467274,0.6451518
356\O,0.2982389825,-2.2992422073,-0.3023451162\O,-1.6085570932,-2.2360
034111,0.9019939652\C,-1.327619555,-3.5735931812,1.3404505326\H,4.2731
249557,-1.9042171029,-0.0154668281\H,2.7377725905,-2.373388518,0.78793
5353\H,3.8696655759,-1.2649965234,1.6138745409\H,-2.1610720409,-3.8490
051778,1.987388965\H,-0.3858943928,-3.6016344511,1.8948282493\H,-1.260
6928718,-4.2542760821,0.4874296944\H,-0.1248125546,2.9249936579,0.1546
98498\H,1.1994521811,2.7382425893,1.3186138286\H,-0.2233942684,1.69897
20082,1.4410311563\H,-2.5205930501,1.1910373478,-0.4957093673\H,-3.017
1989885,-0.3664253648,0.3769000133\\Version=EM64L-G09RevB.01\State=1-A
\HF=-691.5980164\RMSD=9.223e-09\RMSF=5.298e-06\Dipole=-0.3588491,-0.04
79048,-0.2729855\Quadrupole=2.7079373,2.9098777,-5.617815,0.2663855,0.
01328,-4.4486398\PG=C01 [X(C10H16O4)]\\@

TS2 (c)

1\1\GINC-X148\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\24-Oct-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200,Cartesian,MaxStep=10) IOP(2/17=4) maxdisk=1342177280\\ts1
_mtcore.freq\\0,1\N,-0.8798281567,1.4163242226,-0.063851983\C,-1.26864
56023,1.9497093651,1.2460896183\C,0.1529310112,2.1993081606,-0.7546513
175\O,-1.9152754522,1.1493049671,-0.8378891995\H,-1.7332442161,-0.2207
584121,-0.9519552364\C,-1.185535517,-1.3058298855,-0.6990660758\H,-0.7
57015797,-1.5634262218,-1.6707927717\C,-2.3048219719,-2.2433290143,-0.
251101054\C,-0.1948083243,-0.8613341644,0.230315838\C,-0.3579428479,-1
.0555178788,1.7139222165\C,1.1558710004,-0.5992188242,-0.3115693382\O,
1.4567448916,-0.5951562165,-1.4945644259\O,2.072255091,-0.3450028969,0
.6661813684\C,3.4084105889,-0.114771881,0.2007009152\H,3.7741283814,-0
.974951886,-0.3667001175\H,4.0098491425,0.0357974281,1.0984063685\H,3.
4506047475,0.7699479528,-0.4412144901\H,0.3004723277,-0.4066441553,2.2
929480287\H,-0.1109476159,-2.0933154738,1.9848224361\H,-1.3920030116,-
0.8889382986,2.0295694084\H,-2.8722241011,-1.8391820186,0.594128624\H,
-1.9187641922,-3.2271543539,0.0464901883\H,-3.0134018948,-2.4001433139
,-1.0708377497\H,-1.6897067731,2.958054482,1.1325697965\H,-0.398272608
4,1.9903090528,1.9066321006\H,-2.0305704694,1.296515852,1.6719800585\H
,-0.2433022307,3.1887557298,-1.0182092609\H,1.0236738249,2.3128689882,
-0.1022198496\H,0.4386117753,1.6639176945,-1.6602810961\\Version=EM64L
-G09RevB.01\State=1-A\HF=-595.4035443\RMSD=6.318e-09\RMSF=6.447e-06\Di
pole=0.5633175,0.3532914,1.2182797\Quadrupole=0.7622554,2.6836986,-3.4
45954,2.7491153,-0.6266213,0.6772884\PG=C01 [X(C8H17N1O3)]\\@

TS2

1\1\GINC-X123\Freq\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\28-Oct-2012\0\\#B
3LYP/6-31G(d) 6D INT(grid=ultrafine) SCF=tight Freq=noraman maxdisk=13
42177280\\ts1_mt.freq\\0,1\N,1.493775,-0.666164,0.160092\C,1.932578,-1
.041251,-1.224972\C,2.455747,-0.696471,1.313189\O,0.320192,-1.273037,0
.489677\H,-0.567675,-0.34377,0.519495\C,-1.424208,0.595376,0.783023\C,
-1.210557,1.53077,-0.226427\C,-0.182483,2.569461,0.051649\O,0.15253,3.
267711,-1.065536\C,1.119946,4.306543,-0.865542\C,-2.74211,-0.166245,1.
06064\C,-3.342503,-0.892058,-0.151223\O,-2.467857,-1.755835,-0.711018\
C,-2.984839,-2.549203,-1.791822\C,3.255981,-0.307334,-1.535347\C,4.315
184,-0.458624,-0.442631\C,3.74677,0.035077,0.888571\C,0.858411,-0.5407
48,-2.202685\C,2.073676,-2.571002,-1.407135\C,1.813326,0.0747,2.479272
\C,2.756103,-2.134291,1.800015\C,-2.477941,-1.242631,2.145869\C,-3.778
276,0.84862,1.584344\C,-1.941517,1.585237,-1.538526\O,0.296254,2.82587
5,1.144843\O,-4.484318,-0.766001,-0.541852\H,-3.402691,-1.781762,2.381
686\H,-2.127558,-0.758447,3.064927\H,-1.721665,-1.960262,1.82245\H,-0.
946719,0.890916,1.721715\H,-2.159893,-3.191629,-2.101376\H,-3.308252,-
1.911691,-2.619811\H,-3.83537,-3.146953,-1.45416\H,1.249707,4.778074,-
1.841516\H,2.067503,3.888132,-0.513755\H,0.761558,5.032699,-0.131051\H
,-3.378449,1.368962,2.46139\H,-4.703495,0.338172,1.870083\H,-4.028617,
1.592098,0.822769\H,-1.250518,1.536379,-2.382493\H,-2.484571,2.539693,
-1.628469\H,-2.675349,0.783605,-1.640332\H,5.208818,0.120722,-0.707007
\H,4.640173,-1.503495,-0.360939\H,3.631428,-0.669794,-2.501448\H,4.483
84,-0.071636,1.694314\H,3.03614,0.761873,-1.662215\H,3.523366,1.107505
,0.802961\H,0.733606,0.541825,-2.108418\H,1.513273,1.079834,2.171435\H
,1.157537,-0.764795,-3.232894\H,2.534084,0.162489,3.299711\H,-0.100709
,-1.023743,-2.004996\H,0.933931,-0.454114,2.858307\H,2.168228,-2.81382
3,-2.472041\H,3.259216,-2.097572,2.772907\H,2.95014,-2.980532,-0.89854
9\H,3.401433,-2.694077,1.118431\H,1.183389,-3.069925,-1.015523\H,1.819
208,-2.686765,1.919023\\Version=EM64L-G09RevB.01\State=1-A\HF=-1175.88
09278\RMSD=6.443e-09\RMSF=3.990e-03\ZeroPoint=0.5234702\Thermal=0.5531
94\Dipole=0.5826787,0.034929,-0.7078238\ PG=C01 [X(C19H35N1O5)]\NImag=
1\\@

TS2 M (c)

1\1\GINC-X115\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\28-Oct-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200,MaxStep=5) IOP(2/17=4) maxdisk=1342177280\\ts1_mt1core.fr
eq\\0,1\N,-1.5969312358,-0.1299629175,-1.2616679176\O,-1.1795101678,-1
.2300453684,-0.657072406\C,-0.7637270122,1.044127965,-0.9812027835\C,-
3.0332214866,0.1090275276,-1.0618502799\H,-0.9384762495,-2.0019003636,
-1.7787980169\C,-0.9190264853,-2.1985469876,-3.0103295311\C,-1.1231876
059,-0.8790617387,-3.5007354782\H,0.0647121996,-2.6328433316,-3.190227
3027\H,-1.7350164682,-2.9010237905,-3.1748404468\C,0.0231444264,0.0073
172619,-3.9446649987\C,-2.44526447,-0.4186108294,-3.9796899183\O,-2.65
46066991,0.6772161328,-4.4765556505\O,-3.4292795776,-1.346352514,-3.82
78077307\C,-4.7194122013,-0.9495567797,-4.3107792075\H,-5.0883898268,-
0.0749941175,-3.7670541313\H,-5.3716155449,-1.8072286343,-4.140993603\
H,-4.674231471,-0.705858764,-5.3756712513\H,-0.1640376795,1.0365351959
,-3.6224006527\H,-0.0190801869,0.0641894401,-5.0433872649\C,1.42615363
46,-0.4404173913,-3.5221395825\H,1.4999967808,-0.6049524397,-2.4417802
058\H,2.1617342579,0.3221674955,-3.7997588551\H,-0.892155959,1.3549513
132,0.0648870136\H,-1.0524391936,1.8673766017,-1.6404900982\H,0.280314
7405,0.7805286501,-1.1454485331\H,-3.5664228329,-0.8038689741,-1.32562
70278\H,-3.2288909332,0.3541165295,-0.0092154424\H,-3.3618083905,0.934
0718821,-1.700275037\H,1.7209316378,-1.3726530536,-4.0161026602\\Versi
on=EM64L-G09RevB.01\State=1-A\HF=-595.4014902\RMSD=4.483e-09\RMSF=3.25
6e-06\Dipole=-0.2559641,0.2659008,-0.0406291\Quadrupole=5.8135954,-1.8
678799,-3.9457155,2.1306608,-1.304467,6.3431602\PG=C01 [X(C8H17N1O3)]\
\@

TS2 M

1\1\GINC-X152\Freq\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\24-Oct-2012\0\\#B
3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17=4
) maxdisk=1342177280\\ts1_mt1.freq\\0,1\N,-2.117217,-0.387022,-0.16703
6\O,-1.057834,-0.983024,-0.729085\H,-0.113948,-0.175092,-1.090564\C,0.
824085,0.484595,-1.761724\C,1.838858,1.089861,-1.00514\C,1.639856,2.42
8704,-0.411905\O,0.375948,2.907321,-0.579386\C,0.160433,4.232872,-0.07
7602\C,-2.093637,-0.347796,1.32575\C,-2.317195,-1.743104,1.956137\C,-3
.384308,-0.434616,-0.954884\C,-4.018805,-1.849417,-0.976083\C,-3.15636
6,0.664727,1.811831\C,-0.705083,0.16155,1.744539\C,-3.061237,-0.033975
,-2.401513\H,-2.406854,-0.769441,-2.87453\H,-2.570996,0.944503,-2.4352
15\H,-3.993216,0.023196,-2.973745\C,3.229018,0.513728,-0.846041\C,3.52
548,-0.409316,0.387227\C,2.648869,-1.666177,0.327554\O,2.682165,-2.243
679,-0.896283\C,1.854354,-3.407866,-1.059893\C,5.004375,-0.862285,0.30
2276\C,3.292091,0.307401,1.725978\O,2.510228,3.079116,0.148587\O,2.014
023,-2.127606,1.252446\C,-4.377118,0.59177,-0.356667\H,-2.797737,1.678
226,1.582796\H,-3.222771,0.592643,2.904293\C,-4.528334,0.482897,1.1621
81\H,-0.462544,1.079388,1.200479\H,0.064966,-0.585166,1.543417\H,-0.70
3012,0.380155,2.817531\H,-3.347426,-2.096133,1.859723\H,-2.083137,-1.7
0657,3.026456\H,-1.65093,-2.473113,1.486437\H,5.246223,-1.543232,1.126
286\H,5.665761,0.008137,0.382796\H,5.219282,-1.374461,-0.641035\H,3.47
577,-0.056631,-1.746351\H,3.930478,1.354595,-0.777232\H,2.036963,-3.74
6272,-2.079461\H,0.802447,-3.145309,-0.922882\H,2.127586,-4.183867,-0.
34126\H,-0.864636,4.486652,-0.352068\H,0.864673,4.936949,-0.528634\H,0
.285091,4.259259,1.008921\H,3.927849,1.195609,1.790249\H,3.525203,-0.3
5956,2.560869\H,2.25321,0.626813,1.839575\H,1.157403,-0.323174,-2.4219
38\H,0.11529,1.170161,-2.231791\H,-4.857082,-1.870726,-1.683926\H,-3.2
79846,-2.589281,-1.296088\H,-4.408915,-2.152262,-0.001363\H,-5.347411,
0.468943,-0.855289\H,-4.022549,1.603088,-0.599416\H,-5.220376,1.253288
,1.525919\H,-4.972555,-0.480511,1.443938\\Version=EM64L-G09RevB.01\Sta
te=1-A\HF=-1175.8781385\RMSD=5.856e-09\RMSF=2.528e-03\ZeroPoint=0.5235
598\Thermal=0.5531088\Dipole=-0.8559673,0.0403073,-0.6364709\PG=C01 [X
(C19H35N1O5)]\NImag=1\\@

Me_2NOC(Me)(Et)COOMe (c)

1\1\GINC-X151\FOpt\RB3LYP\Gen\C8H17N1O3\GXG501\12-Jun-2012\0\\#B3LYP/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\\mt_core.freq\\0,1\N,2.5611848702,-2.8204292258,0.4020447087\O,2.4539
260016,-1.3731546866,0.2811343765\C,1.4052768248,-0.8362112425,1.08620
5378\C,1.606520314,-1.1553590835,2.574905096\C,0.0331564385,-1.3314722
782,0.5817826421\C,1.485975771,0.693840474,0.8486373264\H,2.5841520487
,-0.7791084623,2.8938071077\H,1.5692241817,-2.2342155962,2.7455425052\
H,0.8327945278,-0.6813336947,3.1826832258\O,-0.1998466708,-1.798952483
5,-0.5105094877\O,-0.9336478267,-1.1040189971,1.5021321861\C,-2.265480
8771,-1.4607336974,1.0962147997\H,-2.3231099878,-2.528107927,0.8679277
57\H,-2.9054396997,-1.2138743199,1.9439009979\H,-2.5627150653,-0.89264
04095,0.21061735\H,2.4549284751,1.019969238,1.2463821374\H,0.711868688
3,1.1668829431,1.4644632161\C,1.3527434267,1.1377902323,-0.6118951619\
H,2.1300089921,0.6800058546,-1.2290421191\H,1.4502782461,2.2267763563,
-0.6838063092\H,0.3833702965,0.8580249468,-1.0374231223\C,3.8849705588
,-3.0683910512,0.9733607685\C,2.4857247765,-3.3320049907,-0.9682358438
\H,4.0355572386,-4.1522254288,1.0219438025\H,4.6928296677,-2.621175440
2,0.3718763566\H,3.9322788111,-2.6653285008,1.9871275531\H,3.286551605
6,-2.9272967118,-1.6087946095\H,2.5830147491,-4.4224045311,-0.92491871
81\H,1.515400617,-3.0683482865,-1.3855049195\\Version=EM64L-G09RevB.01
\State=1-A\HF=-595.4619249\RMSD=5.244e-09\RMSF=9.046e-06\Dipole=-0.191
2932,0.0465925,0.5986685\Quadrupole=4.0218665,-0.1399428,-3.8819237,-2
.0282209,-1.1490124,0.2619565\PG=C01 [X(C8H17N1O3)]\\@

TEMPOP

1\1\GINC-X113\FOpt\RB3LYP\Gen\C19H35N1O5\GXG501\12-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\mt.freq\\0,1\C,-3.1729953086,2.7317961299,0.1302159366\C,-2.5994184

8,1.2865464368,0.1118055522\C,-1.052083884,1.4235629881,0.0759351089\C
,-0.1015480184,0.1927312666,-0.0921252099\H,-4.2651395945,2.7122443775
,0.20981993\H,-2.9102865576,3.2493644375,-0.7993971107\H,-2.7753591868
,3.3089213956,0.9720063107\C,-3.1882403053,0.5352737037,-1.0942967182\
H,-0.7540355492,1.9211488934,1.0040504382\H,-0.803092623,2.1022016386,
-0.746796958\C,1.333579492,0.6832848416,0.1314320054\C,-0.5231290753,-
0.8749519666,0.9444366791\C,-3.0393821419,0.6773372668,1.4505028405\O,
-2.4288050258,0.7967106095,2.4964451772\O,-4.2368104871,0.0666826118,1
.3704340638\C,-4.7252911983,-0.5066552099,2.5923852448\O,-1.4451044885
,-1.6507470769,0.7869345684\O,0.2101850498,-0.8174503021,2.0685623161\
C,-0.2302343642,-1.6610630971,3.1474064721\H,-5.718281021,-0.891600169
5,2.3577651981\H,-4.7787531834,0.2479854671,3.3813205792\H,-4.06840581
34,-1.3192475098,2.9138837239\H,0.5164257209,-1.5398522981,3.932818356
5\H,-0.2851240654,-2.7032602307,2.8235265563\H,-1.2105375485,-1.326742
4252,3.493200114\O,-0.3461082947,-0.3626395942,-1.410721314\H,-2.85444
78767,1.0140270861,-2.020625455\H,-4.2809456638,0.5653037593,-1.068290
0777\H,-2.8662285546,-0.5063826829,-1.1084840798\H,1.4350245354,1.0429
588571,1.1567177008\H,1.5590874932,1.5039021229,-0.5514868159\H,2.0630
941099,-0.1079751256,-0.0355376478\N,0.8098015007,-0.7644103991,-2.200
2454374\C,0.8697729341,-2.2714689034,-2.2545169099\C,0.6969079052,-0.0
148755313,-3.5037362707\C,1.9938599421,-2.6617170195,-3.2468833466\C,1
.3162226267,-2.8024307956,-0.8771213347\C,-0.4621646404,-2.9671706873,
-2.6108258354\C,1.8419986513,-0.4902386295,-4.4281545765\C,-0.66729565
72,-0.1456291638,-4.2232682436\C,0.9394847133,1.4793398762,-3.22411856
88\H,1.995304085,-3.755330103,-3.3330560633\C,1.8799406114,-2.00351716
67,-4.6179304972\H,2.9582676886,-2.3784805567,-2.8030548875\H,1.735734
3956,0.0277825428,-5.3895547749\H,2.7978238833,-0.1649406555,-3.995197
943\H,2.7364413854,-2.2850589783,-5.2435041605\H,0.9849742058,-2.35416
87913,-5.146424856\H,1.6051570613,-3.8553884877,-0.9766835791\H,2.1845
046115,-2.2518302735,-0.5025918898\H,0.5120212684,-2.7614612242,-0.142
8597666\H,-0.3675689901,-4.0439924979,-2.4267400201\H,-1.2647194526,-2
.5861968984,-1.9755449412\H,-0.7506813259,-2.8400134176,-3.6561557422\
H,0.9926908969,2.0243661423,-4.1735453849\H,0.1297804237,1.9176692564,
-2.6362506202\H,1.8846236227,1.6288739883,-2.6941711463\H,-0.746228153
7,0.6277769591,-4.9964298748\H,-0.8011715264,-1.1098146672,-4.71759407
63\H,-1.4883587576,-0.0070681185,-3.5180117381\\Version=EM64L-G09RevB.
01\State=1-A\HF=-1175.9337831\RMSD=7.716e-09\RMSF=3.016e-06\Dipole=0.1
064618,0.0222285,-0.0164409\Quadrupole=0.5424458,-2.1259937,1.5835478,
-1.8539864,-4.1608272,-3.8131673\PG=C01 [X(C19H35N1O5)]\\@

TS3a (c)

Single Point\\0,1\N,0,-2.168929,0.051613,0.305689\O,0,-2.595456,1.0204
68,-0.736314\C,0,-3.819477,0.76498,-1.618003\C,0,-3.908923,2.297401,-1
.803251\H,0,-2.956051,2.200243,-1.111619\C,0,-0.940107,-0.700036,-0.14
1946\C,0,-2.083688,0.888324,1.555993\H,0,-0.148813,-0.098616,-0.584543
\H,0,-1.243591,-1.439079,-0.880496\H,0,-0.560201,-1.260334,0.709807\H,
0,-1.681038,0.261517,2.348917\H,0,-1.511564,1.808302,1.455701\H,0,-3.0
91758,1.160499,1.861707\C,0,-4.970533,0.129471,-0.860524\H,0,-5.813083
,0.016402,-1.546622\H,0,-4.699897,-0.852175,-0.464813\H,0,-5.279693,0.
768456,-0.032548\C,0,-3.401679,-0.018545,-2.860958\O,0,-2.483015,0.283
573,-3.597615\O,0,-4.171605,-1.099403,-3.063114\C,0,-3.92224,-1.816423
,-4.283555\H,0,-2.897735,-2.189469,-4.311331\H,0,-4.634923,-2.64375,-4
.282327\H,0,-4.094721,-1.16115,-5.14091\H,0,-4.768984,2.645971,-1.2244
39\C,0,-3.794323,3.097967,-3.116467\H,0,-2.76079,3.288234,-3.398164\H,
0,-4.276272,4.058969,-2.949297\H,0,-4.349467,2.624383,-3.923484\\Versi
on=EM64L-G09RevB.01\State=1-A\HF=-591.8959646\PG=C01 [X(C8H17N1O3)]\\@

TS3a

1\1\GINC-X123\Freq\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\24-Aug-2012\0\\#B
3LYP/6-31G(d) 6D INT(grid=ultrafine) SCF=tight Freq=noraman maxdisk=13
42177280\\ts2_mt.freq\\0,1\N,-2.1610096,0.0673302,0.3227234\C,-2.60804
01,1.1693509,-0.6052166\C,-2.9752789,-1.1993354,0.378717\O,-0.8020474,

-0.4053264,-0.0463166\C,0.4292043,-0.0386614,0.7846193\C,0.1584317,-0.
0490374,2.2776539\C,1.0944521,-1.3146957,0.2190991\C,1.0141022,1.27941
34,0.2806567\H,1.1341029,-2.048068,1.0295454\C,2.367516,-1.4116041,-0.
6460563\H,0.0408219,-1.3436085,-0.3145536\C,-4.4502222,-0.8029599,0.62
38939\C,-4.9853981,0.1936712,-0.3964614\C,-4.1087405,1.4398297,-0.3380
277\C,-1.8611965,2.4621373,-0.2141778\C,-2.3631659,0.9258759,-2.113139
4\C,-2.8433574,-2.1216494,-0.8671332\C,-2.5346846,-2.0129572,1.6067587
\O,1.2761685,1.5253592,-0.8806845\O,1.2159476,2.1589189,1.2744555\C,1.
8829254,3.3750305,0.8976379\C,3.4721376,-0.4835078,-0.1291929\O,3.4639
719,0.1071994,0.9368971\C,2.9198863,-2.8562341,-0.4883\C,2.0805064,-1.
1757208,-2.1477765\O,4.527561,-0.4331835,-0.9724935\C,5.6319105,0.3733
639,-0.5385285\H,3.7942088,-3.0141542,-1.1265776\H,2.1451982,-3.575375
4,-0.7742872\H,3.2064373,-3.0622736,0.550293\H,6.3865339,0.2792788,-1.
3201064\H,6.0180825,0.017593,0.4204812\H,5.3257186,1.4177196,-0.431542
5\H,1.967668,3.9545421,1.8192518\H,1.3033664,3.9194908,0.1511661\H,2.8
725407,3.146084,0.4946066\H,1.3437151,-1.9137888,-2.4846363\H,2.989215
8,-1.3002995,-2.7435953\H,1.6770274,-0.177947,-2.3182272\H,1.0904727,0
.1834278,2.7979077\H,-0.1805933,-1.0356009,2.595743\H,-0.5976341,0.688
908,2.5556149\H,-4.4415124,2.1947273,-1.0597257\H,-4.209895,1.891054,0
.6594488\H,-5.0480512,-1.7249136,0.6407238\H,-4.5291404,-0.3588772,1.6
234163\H,-6.0283248,0.449708,-0.1675305\H,-4.9840838,-0.2443991,-1.402
3571\H,-2.4103146,3.3317594,-0.6028003\H,-1.7950971,2.5579333,0.874770
7\H,-0.8621383,2.4997777,-0.644008\H,-2.4749099,1.8742395,-2.6532616\H
,-1.3486798,0.5631497,-2.2785051\H,-3.074517,0.2166994,-2.5612728\H,-3
.1909225,-2.8867033,1.7184993\H,-1.5143806,-2.3829431,1.4946834\H,-2.5
99755,-1.4172159,2.5187877\H,-2.007441,-2.8429196,-0.743139\H,-3.77268
43,-2.6907555,-0.9638544\H,-2.647304,-1.5827698,-1.813172\\Version=EM6
4L-G09RevB.01\State=1-A\HF=-1175.854555\RMSD=6.688e-09\RMSF=9.915e-03\
ZeroPoint=0.5284346\Thermal=0.5566611\Dipole=-0.1095044,0.2113546,0.12
64433\ PG=C01 [X(C19H35N1O5)]\NImag=1\\@

TS3a M (c)

Single Point\\0,1\N,0,-2.018725,-0.129409,-0.116771\C,0,-2.664552,-1.4
85225,-0.003964\C,0,-2.8496,1.08255,0.232837\O,0,-1.568108,-0.019894,-
1.517533\C,0,-0.061985,0.132652,-2.031205\C,0,-0.617274,-0.125258,-3.4
10725\H,0,-1.629889,-0.153292,-2.796054\H,0,-3.395744,-1.706448,-0.778
666\H,0,-1.888124,-2.245939,-0.051053\H,0,-3.106969,-1.566508,0.986694
\H,0,-3.615429,1.355816,-0.490057\H,0,-3.301973,0.914836,1.208016\H,0,
-2.189216,1.939031,0.351484\C,0,0.793952,-0.922093,-1.344439\C,0,0.438
412,1.54995,-1.756475\H,0,-0.506989,0.702612,-4.110088\H,0,-0.347514,-
1.084609,-3.847043\O,0,1.261549,-0.783392,-0.233553\O,0,0.992213,-2.02
2626,-2.098163\C,0,1.821057,-3.032483,-1.499805\H,0,1.366363,-3.408442
,-0.579863\H,0,2.808496,-2.624946,-1.269658\H,0,1.894793,-3.826297,-2.
243502\H,0,-0.32029,2.215066,-2.178286\H,0,0.468715,1.711563,-0.67722\
C,0,1.833705,2.017283,-2.318388\H,0,1.790304,3.101357,-2.399899\H,0,2.
653226,1.751264,-1.654036\H,0,2.000874,1.614287,-3.315079\\Version=EM6
4L-G09RevB.01\State=1-A\HF=-591.8930322\ PG=C01 [X(C8H17N1O3)]\\@

TS3a M

1\1\GINC-X115\Freq\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\27-Aug-2012\0\\#B
3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17=4
) maxdisk=1342177280\\ts2_mt1.freq\\0,1\N,-2.0113769,-0.2076559,-0.132
0934\C,-2.6265702,-1.5813528,-0.0059275\C,-2.8755811,0.9850596,0.18197
36\O,-0.8541929,-0.1098565,0.7781505\C,0.6789819,0.0725998,0.3638799\C
,0.9343465,0.3354772,1.8279922\C,0.7773273,1.2095386,-0.6433244\C,1.22
51338,-1.2408944,-0.1938482\H,1.5785119,-0.3937161,2.3178596\H,1.19490
77,1.3621708,2.075998\H,-0.229101,0.1171066,1.8799567\C,2.7599301,-1.3
833715,-0.5180235\C,3.6056179,-0.6638818,0.5395197\O,3.7618521,0.64900
98,0.2524727\C,4.4874629,1.4137379,1.2278644\O,0.5740278,1.0692215,-1.
8311512\O,1.1253405,2.3875076,-0.0866773\C,1.2595787,3.4828606,-1.0070
078\C,-4.183133,0.8583565,-0.6357593\C,-4.9111104,-0.4593048,-0.416045
5\C,-3.9599541,-1.5887006,-0.7936933\C,-1.7134454,-2.6009633,-0.707506

6\C,-2.8632255,-2.0822541,1.4376605\C,-3.1794058,1.1888402,1.6986795\C
,-2.1711561,2.2534636,-0.3329132\C,3.0902231,-2.8882448,-0.4439496\C,3
.1057336,-0.8715983,-1.9332263\O,4.0807463,-1.1795804,1.5295129\H,4.12
81947,-3.074399,-0.7402708\H,2.4370845,-3.4473211,-1.1231477\H,2.95799
59,-3.2716068,0.5707448\H,0.9796498,-2.0006772,0.5534127\H,0.6898703,-
1.4845844,-1.1135967\H,4.5177663,2.4315511,0.8375936\H,5.4986521,1.016
8201,1.3500915\H,3.9739054,1.3879734,2.1921285\H,2.0165623,3.2537246,-
1.7610387\H,1.5644422,4.3362303,-0.4008043\H,0.3084338,3.6855721,-1.50
56227\H,2.5347825,-1.4404748,-2.6754593\H,4.1717477,-1.0224889,-2.1398
737\H,2.876841,0.1834783,-2.0729891\H,-4.4281238,-2.5726603,-0.6428674
\H,-3.7315408,-1.5092628,-1.8672491\H,-4.8200233,1.7169936,-0.3864671\
H,-3.9359755,0.9492077,-1.7019564\H,-5.8194345,-0.5069269,-1.0312292\H
,-5.2387472,-0.554808,0.6294432\H,-2.2702192,-3.5322316,-0.8705884\H,-
1.3874504,-2.223075,-1.6813377\H,-0.8372033,-2.8508354,-0.1077005\H,-3
.0679589,-3.1576462,1.4167538\H,-1.9745172,-1.9226244,2.0563747\H,-3.7
175752,-1.6021568,1.9263804\H,-2.8528314,3.10778,-0.231414\H,-1.279722
9,2.4776115,0.2529466\H,-1.8941228,2.1462764,-1.3857001\H,-4.2078472,1
.5547875,1.8482196\H,-3.0637294,0.2741016,2.2867095\H,-2.4982102,1.934
4571,2.1319621\\Version=EM64L-G09RevB.01\State=1-A\HF=-1175.8471578\RM
SD=3.768e-09\RMSF=9.295e-03\ZeroPoint=0.5280644\Thermal=0.5567607\Dipo
le=-0.3705925,0.7588083,-0.2398577\ PG=C01 [X(C19H35N1O5)]\NImag=1\\@

TS3b (c)

1\1\GINC-X87\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\30-Aug-2012\0\\#B3LY
P/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest
,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts2c_mtcore.freq\\0,1\N,-
1.6232228148,-0.0425053779,0.2472310296\C,-2.0751264328,-0.0383283507,
-1.1635481584\C,-2.4488855663,-0.8741611414,1.1470424372\O,-1.42547620
23,1.1822779677,0.7256564993\C,0.7528065791,1.0735504813,0.9400399002\
C,0.9566748974,-0.270764188,0.5707383264\H,-0.3929604531,-0.4928581485
,0.3047952344\H,-3.0782158839,0.3979328538,-1.2212142847\H,-2.08639487
,-1.0609014604,-1.5538922282\H,-1.369903572,0.576075574,-1.7222450957\
H,-3.4601828391,-0.4580412356,1.2037615961\H,-2.4842634472,-1.90346773
42,0.7761992976\H,-1.9901623568,-0.8449202084,2.1360547433\C,0.8047262
603,2.1567445351,-0.0824708028\C,0.7535158274,1.4731117047,2.393627091
6\O,0.7866705816,2.0161649365,-1.2945184894\O,0.8801448976,3.380156946
7,0.4958585532\C,0.8680315665,4.4868515188,-0.4138748641\H,1.715078356
3,4.4322733391,-1.1034456517\H,-0.0589259272,4.49643457,-0.9939643502\
H,0.9382483191,5.3790885971,0.2098614386\H,0.0282220422,2.2622952403,2
.5967721718\H,1.7454937948,1.8434497229,2.6887649018\H,0.5207915652,0.
6087739519,3.0240097006\C,1.6630719376,-0.760515873,-0.6907374003\H,1.
3896180546,-0.1735388151,-1.5667626218\H,1.4202303237,-1.8136776741,-0
.8768045779\H,2.7536472749,-0.698706882,-0.5742119475\H,1.1314030872,-
0.9228358505,1.4322525511\\Version=EM64L-G09RevB.01\State=1-A\HF=-595.
3994831\RMSD=5.902e-09\RMSF=6.524e-07\Dipole=-0.5476195,-0.7224332,0.1
792785\Quadrupole=-0.1096658,4.5325613,-4.4228955,4.8279997,2.0754884,
-1.2820636\PG=C01 [X(C8H17N1O3)]\\@

TS3b

1\1\GINC-X141\FTS\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\28-Aug-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigente
st,maxcyc=200,MaxStep=10) IOP(2/17=4) maxdisk=1342177280\\ts2c_mt.freq
\\0,1\N,-1.6726171641,0.3788365159,0.0718930811\C,-2.2930194909,0.2617
19309,-1.3520891844\C,-2.611271653,-0.0304594104,1.2480946647\O,-1.107
7607855,1.5641357531,0.279450596\C,1.0276535343,0.9942825359,0.6145277
369\C,1.1225202964,1.6123299906,1.9897438437\C,1.4308832194,1.89467863
91,-0.5050149592\C,0.8646110005,-0.4048205579,0.4947508158\C,1.6739046
238,-1.4754058262,-0.2841843176\C,2.9049439786,-1.780584991,0.60848249
5\O,3.5034301068,-2.944959594,0.2561266692\C,4.6939554635,-3.270483287
1,0.9897413105\O,1.5215232272,1.6157237008,-1.6875609757\O,1.701779744
1,3.1455794237,-0.0521122666\C,2.0550369158,4.0963235192,-1.0619663438
\C,-2.9765341072,-1.1111809542,-1.5141484568\C,-3.9643778722,-1.464970

3427,-0.4048130628\C,-3.2509984724,-1.3984250882,0.9439311167\C,-1.790
871398,-0.1495486694,2.5375939535\C,-3.6638620662,1.0681152074,1.49415
49676\C,-3.2610962688,1.4306730385,-1.618174181\C,-1.1622072692,0.3639
375455,-2.3758172182\C,0.8091722549,-2.7522207342,-0.4096010764\C,2.26
92572428,-1.139708968,-1.6717446948\O,3.3356538392,-1.0746135723,1.494
8588838\H,1.3943875401,-3.5902723014,-0.7950592566\H,-0.0226047471,-2.
569430605,-1.0976773453\H,0.3876327134,-3.0488088971,0.5586312982\H,0.
7376435186,-0.8252379114,1.4934006568\H,-0.569303115,-0.3522737072,0.1
301762279\H,5.0375664821,-4.2222125254,0.5825434984\H,4.4754210005,-3.
365079536,2.0568396478\H,5.4543213563,-2.4968130061,0.8528314652\H,2.2
50385186,5.028556503,-0.5300720382\H,1.234732147,4.2265809447,-1.77369
01853\H,2.9454824811,3.7716670854,-1.6078421775\H,1.4939086533,-0.8640
096213,-2.3856009166\H,2.7965808629,-2.0222571866,-2.0482104185\H,2.97
0694819,-0.3060040947,-1.6236946728\H,2.1746888704,1.8481619117,2.1959
328323\H,0.7982868617,0.909959672,2.7585254975\H,0.548425028,2.5375077
686,2.0700239352\H,-3.9416344876,-1.6331110961,1.7639041511\H,-2.46658
59053,-2.1682110426,0.9700910549\H,-3.4698490534,-1.1196737272,-2.4943
319181\H,-2.2010677238,-1.8884353856,-1.5545611066\H,-4.3630324541,-2.
4738167041,-0.5677981336\H,-4.8276892175,-0.7887959342,-0.4208961925\H
,-2.4668260522,-0.4356071058,3.3506102637\H,-1.0180618193,-0.917816023
5,2.4704191574\H,-1.3308350071,0.803915618,2.7961192116\H,-4.105804234
9,0.9209728303,2.4856754233\H,-3.1791812036,2.0468262637,1.4735191078\
H,-4.4812592312,1.0640627558,0.7729437541\H,-1.5874039867,0.2436440936
,-3.378735631\H,-0.6503560955,1.3228078299,-2.3230816998\H,-0.42202199
39,-0.4235900113,-2.2316711207\H,-3.4016370176,1.5319152808,-2.6997860
008\H,-4.2494860486,1.295583863,-1.1760993571\H,-2.8252610012,2.358129
3215,-1.2402091152\\Version=EM64L-G09RevB.01\State=1-A\HF=-1175.862936
3\RMSD=4.922e-09\RMSF=2.009e-06\Dipole=-0.7457759,-0.8284471,0.005294\
Quadrupole=4.268893,1.8753064,-6.1441994,-0.8684264,-0.6112724,-2.6601
955\PG=C01 [X(C19H35N1O5)]\\@

TS3b M (c)

1\1\GINC-X121\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\25-Aug-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts2c_mt1core.freq\\0,1\N
,1.7159424497,-0.1954235583,-0.0051845417\C,2.6166999825,0.93162179,0.
3188214698\C,2.4006585576,-1.501691067,-0.1270291187\O,0.9289571922,0.
0685517399,-1.0488146483\C,-0.993316307,0.0497527133,-0.0098614788\C,-
0.532907249,-0.2626921649,1.2767364721\H,0.8388060916,-0.2826771268,0.
921787458\H,-0.5982557163,0.5144574195,2.0384119564\H,-0.6528797574,-1
.2794612373,1.644349688\C,-1.4453203473,-1.046326779,-0.9131356544\O,-
2.2090247451,-0.9044940529,-1.8486044092\O,-0.9501233091,-2.2660062749
,-0.5639432483\C,-1.3810892818,-3.3494711063,-1.3979020748\H,-1.052574
4005,-3.1964218319,-2.4297057082\H,-0.919383278,-4.2446826327,-0.97819
28596\H,-2.4707387903,-3.4398859841,-1.3855537506\C,-1.4978840589,1.44
30564403,-0.3324139929\H,-1.1130197019,2.1204687437,0.4406377862\H,-2.
5900538352,1.4184908992,-0.1950655139\C,-1.1920032713,2.0205203412,-1.
720513955\H,-0.1141321879,2.0935791663,-1.877300978\H,-1.6336933495,3.
0204718426,-1.808065246\H,-1.6122984111,1.3885597857,-2.5052867848\H,3
.1701398881,0.7153393642,1.2381957156\H,3.3099853,1.0935352428,-0.5123
80564\H,1.9972972419,1.8194097657,0.451959248\H,3.0923233547,-1.470656
5572,-0.9749210551\H,2.943915836,-1.7249116851,0.7968333993\H,1.628550
1034,-2.2492141963,-0.3044476112\\Version=EM64L-G09RevB.01\State=1-A\H
F=-595.4002459\RMSD=9.395e-09\RMSF=9.413e-06\Dipole=1.3845932,-0.46423
54,1.1046196\Quadrupole=1.1774524,3.1437974,-4.3212498,0.9973273,0.339
6367,2.6770336\PG=C01 [X(C8H17N1O3)]\\@

TS3b M

1\1\GINC-X144\FTS\RB3LYP\6-31G(d)\C19H35N1O5\GXG501\23-Aug-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(MaxStep=10,TS,calcf
c,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts2c_mt1.fre
q\\0,1\N,-1.8524045357,0.0610068868,-0.0454918029\C,-2.5719489034,1.24

0319271,-0.7442236017\C,-2.6124083273,-1.2867165352,-0.0030314391\O,-0
.5889822355,-0.0627112673,-0.4300087591\C,0.475217719,0.4825186999,1.5
002637786\C,1.1609800821,1.6518296251,0.8676281594\C,1.2927854431,-0.7
760113118,1.7666006043\C,-0.7003730481,0.6881161566,2.2366931445\C,2.4
726436847,-1.2425954203,0.8731980171\C,3.6388122059,-0.2578760448,1.02
94930866\O,4.4698365817,-0.2648425055,-0.0327285903\C,5.5837972685,0.6
330839146,0.0586427951\O,2.0016510788,1.5990024645,-0.0104480663\O,0.7
71344414,2.8356906704,1.407709062\C,1.4224815888,3.99280922,0.86679743
39\C,-4.037742771,-1.0363201934,0.5293186777\C,-4.7979859316,0.0636975
592,-0.2128831857\C,-3.9967130408,1.3657512496,-0.1716184964\C,-1.7890
494245,2.5233472884,-0.4408340567\C,-2.5617064146,1.058187075,-2.27402
25568\C,-2.605860782,-1.9652341444,-1.3860487469\C,-1.8796952996,-2.22
76530841,0.962065874\C,2.99383986,-2.5721672705,1.4884264286\C,2.08829
62364,-1.496089328,-0.5934680032\O,3.8604515956,0.3890523903,2.0346496
476\H,3.8672583913,-2.9348142987,0.9361043979\H,2.2157310615,-3.342560
3787,1.4333084031\H,3.2794921876,-2.4430889874,2.5381293915\H,1.714814
335,-0.6302616134,2.7702537029\H,0.5935326161,-1.6113674979,1.85412668
15\H,6.1467563737,0.4972196203,-0.8658749032\H,6.205369109,0.396171610
1,0.9266769843\H,5.2292574133,1.6636236379,0.1436982118\H,1.0170526375
,4.8412063184,1.4198434801\H,1.2118004037,4.0951991185,-0.2015462238\H
,2.5040403436,3.9224080987,1.0087413683\H,1.2671628681,-2.2193617458,-
0.6382737097\H,2.9394193365,-1.9080975315,-1.1435235103\H,1.7600956365
,-0.5800617573,-1.0820473842\H,-0.9455437348,-0.0479249961,3.002294160
5\H,-0.9683482351,1.7066596405,2.5022763244\H,-1.6387810376,0.40824652
52,1.2019039963\H,-4.5150078993,2.1592799393,-0.7246089067\H,-3.927611
6651,1.7084621617,0.8705806959\H,-4.5858907511,-1.98595164,0.484924191
5\H,-3.9719882059,-0.7660374681,1.5928485592\H,-5.7792860373,0.2153195
279,0.2530726696\H,-4.9956125054,-0.2354204821,-1.2493932018\H,-2.3205
687686,3.3685052947,-0.8920104812\H,-1.7019439614,2.7155122672,0.62939
45033\H,-0.7886212923,2.4736018239,-0.8741136021\H,-2.7658902499,2.024
7797146,-2.747562192\H,-1.5722016046,0.7222777141,-2.5935508979\H,-3.3
110230978,0.3551347516,-2.6400304216\H,-2.4485110477,-3.1604828418,1.0
40066808\H,-0.882374317,-2.4638766634,0.5890775858\H,-1.7962631006,-1.
8053276008,1.9659261742\H,-2.8349838241,-3.0294763808,-1.2626080052\H,
-3.3409463818,-1.5554042571,-2.0798544757\H,-1.6114630404,-1.877252989
5,-1.830550779\\Version=EM64L-G09RevB.01\State=1-A\HF=-1175.8769738\RM
SD=4.524e-09\RMSF=3.413e-06\Dipole=-1.6278827,0.1109196,-0.1962405\Qua
drupole=4.5990934,4.0123442,-8.6114376,1.6015013,-2.1806684,-2.2433421
\PG=C01 [X(C19H35N1O5)]\\@

TS4 (c)

1\1\GINC-V1491\FTS\RB3LYP\Gen\C2H7N1O1\GXG501\02-Jun-2011\0\\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/
17=4) Freq=noraman maxdisk=268435456\\tsc2_core.freq\\0,1\O,-0.0739546
76,-0.7661327464,-0.1035088876\N,-1.3899406717,-0.0532392252,0.1446949
069\C,-1.297421104,1.2981251856,-0.3888755332\H,-1.0525961443,1.231936
2299,-1.4497072779\H,-0.4879591687,1.8271716584,0.1298008629\H,-2.2477
300926,1.8273142885,-0.2550151394\C,-1.7253983156,-0.1692528887,1.5565
91523\H,-0.9318319906,0.3052933221,2.1475250056\H,-2.691003626,0.30749
06948,1.7599848015\H,-1.770235706,-1.2285886059,1.8124853997\H,-1.2984
63128,-0.9532690898,-0.5140331766\\Version=EM64L-G09RevB.01\State=1-A'
\HF=-210.2574016\RMSD=5.106e-09\RMSF=3.280e-05\Dipole=-1.1560549,0.656
137,0.2405776\Quadrupole=-2.1000029,0.5171219,1.5828811,1.8820969,0.51
74447,-0.7050804\PG=CS [SG(H1N1O1),X(C2H6)]\\@

TS4

1\1\GINC-V1260\FTS\RB3LYP\Gen\C9H19N1O1\GXG501\01-Jun-2011\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2
/17=4) Freq=noraman maxdisk=268435456\\tsc2.freq\\0,1\N,-0.0066952641,
-0.7413657,-0.0700178834\C,-1.2933908552,-0.0146365011,0.1950530293\C,
-1.2096728841,1.3691794932,-0.4863983184\C,0.0766714319,2.1334022626,-
0.1590618768\C,1.2961974237,1.2944778396,-0.5524758629\C,1.3331624541,

-0.0929469807,0.1257713124\C,1.6954576492,-0.0092054327,1.6192723636\O
,-0.0302879607,-2.1168873418,0.5904272171\C,2.3626338531,-0.9878425736
,-0.5850214657\C,-2.4103414904,-0.8455382423,-0.4590912154\C,-1.570869
7999,0.0882136183,1.7054272179\H,0.090733453,3.085949266,-0.7027028252
\H,0.112420129,2.3893307144,0.9069401306\H,2.2285195827,1.819013364,-0
.3095731888\H,-2.0950336358,1.9479063313,-0.1955801755\H,1.2892755377,
1.1522842218,-1.6422659071\H,-1.2686158953,1.2285158621,-1.574814108\H
,2.0983932738,-1.1216492853,-1.6411188697\H,-2.2105312252,-0.993235979
4,-1.5274211458\H,3.3535962559,-0.5235114906,-0.5401507544\H,-3.368145
1441,-0.3230699131,-0.362845989\H,2.4068035501,-1.9694252376,-0.108575
8047\H,-2.4877609758,-1.8234719515,0.0206042786\H,2.7700876613,0.17413
41533,1.725565722\H,-2.6255126852,0.3353593891,1.8678746006\H,1.170650
2629,0.7940217235,2.1419534395\H,-0.9721396362,0.8577433429,2.19851419
04\H,1.4519949149,-0.9614699465,2.096894997\H,-1.3600094096,-0.8776834
121,2.1710298077\H,-0.0508812254,-1.736398286,-0.6204092998\\Version=E
M64L-G09RevB.01\State=1-A\HF=-484.2576102\RMSD=6.347e-09\RMSF=4.009e-0
6\Dipole=0.0201357,1.1230744,-0.498233\Quadrupole=2.8584066,-3.696936,
0.8385294,-0.1442862,0.0039538,1.9308673\PG=C01 [X(C9H19N1O1)]\\@

TS5 (c)

1\1\GINC-X113\FTS\UB3LYP\6-31G(d)\C8H18N1O3(2)\GXG501\10-Aug-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(Cartesian,TS,calc
fc,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_mtcore.
freq\\0,2\N,2.1012722094,-0.1988052846,-0.1186257958\O,1.0760639591,-1
.0790622758,-0.3631073344\C,3.0708824815,-0.2411540212,-1.2052706667\C
,2.6378511554,-0.395694547,1.2233984456\H,0.1199823203,-0.4716320776,-
0.3958486738\H,3.4157310682,0.3523144705,1.4056748885\H,3.0658057217,-
1.4024155315,1.3545386416\H,1.829811756,-0.2451989053,1.9416907598\H,3
.8317429514,0.5267313052,-1.0331165648\H,3.5634506487,-1.2238566709,-1
.2858355252\H,2.5528795715,-0.0271886669,-2.1427768948\C,-1.1038015237
,0.2986708917,-0.3410406669\C,-0.4693758665,1.5323137527,0.1766850604\
O,-0.2462844279,1.7573921044,1.3574633353\O,-0.0954576208,2.3876002744
,-0.8115138621\C,0.6152603971,3.5507783144,-0.3700466064\H,1.538623936
4,3.2639536588,0.1407815824\H,0.837581123,4.1200156807,-1.2738703133\H
,0.0030157279,4.1439497705,0.3149499284\C,-1.6038271291,0.2809488676,-
1.7687934963\C,-1.8858495879,-0.4958113577,0.6887041817\H,-0.865955905
6,0.6941067615,-2.4604077154\H,-2.5220721683,0.8771506517,-1.880963242
3\H,-1.8407405392,-0.7435061546,-2.0777689577\H,-2.0252806216,-1.51799
15894,0.3134880387\H,-1.2953831705,-0.5624240698,1.6074523482\C,-3.259
8015824,0.1165250317,1.0246885745\H,-3.9002443291,0.1871385933,0.13822
23384\H,-3.7819757006,-0.4994455857,1.7657696476\H,-3.1403348546,1.120
8786098,1.444329549\\Version=EM64L-G09RevB.01\State=2-A\HF=-596.005262
1\S2=0.7568\S2-1=0.\S2A=0.750033\RMSD=9.625e-09\RMSF=1.800e-05\Dipole=
0.5311407,0.2340533,-0.5156603\Quadrupole=4.6235572,-0.8980801,-3.7254
771,1.5940767,0.4646754,-2.1428968\PG=C01 [X(C8H18N1O3)]\\@

TS5

1\1\GINC-X154\FTS\UB3LYP\6-31G(d)\C19H36N1O5(2)\GXG501\05-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_mt.a2.freq\\0,2\
N,2.3265441733,-0.3750477408,0.0670158063\O,1.3968034484,0.2588589548,
0.8437191604\C,2.4264177188,-1.8267115093,0.4034203821\C,3.4149987025,
-2.4781136681,-0.5878623155\C,4.7379085945,-1.7204819933,-0.7186218889
\C,4.4635965535,-0.2754209922,-1.1401918224\C,3.5259712851,0.482989896
9,-0.1756020463\C,1.0350426082,-2.4522544512,0.1977462798\C,2.85097618
69,-2.0682025796,1.8709070593\C,3.0516160694,1.7759147385,-0.862612173
5\C,4.2501758147,0.8689509741,1.1355741274\C,-0.8059172606,1.020040760
1,-0.3573673837\C,-0.5409996295,0.687057367,-1.7680765005\O,-0.9957295
703,-0.550470495,-2.1182052987\C,-0.7299158581,-0.9335185661,-3.473795
6241\C,-0.6679521163,2.4859614793,0.006314278\C,-1.9329853921,3.398709
6067,-0.166677677\C,-3.014370531,3.0576417824,0.8645202464\O,-2.533186
5439,3.0908345266,2.1323218185\C,-3.4955068337,2.8221155311,3.16354512

79\C,-1.4901379668,4.8596238363,0.093260692\C,-2.5332467215,3.28426127
92,-1.5754567833\C,-1.7841106861,0.1750787441,0.4284359425\O,0.0591571
593,1.3993374752,-2.5640585278\O,-4.1769026979,2.8146327369,0.61611001
17\H,5.3759357461,-2.2115788163,-1.4637503771\H,5.2946128452,-1.749026
8832,0.2265629566\H,3.5855917123,-3.5143398837,-0.2705013306\H,5.39851
66337,0.2921213239,-1.2247719079\H,2.9357460192,-2.5229404689,-1.57535
19906\H,4.0031782357,-0.2791372017,-2.1373462754\H,0.6298747446,-2.194
4806052,-0.7850763655\H,2.4152858191,1.5577612962,-1.7246035961\H,1.11
06657837,-3.5431038907,0.2701250682\H,3.9239603277,2.3451272091,-1.203
5734923\H,0.3316475864,-2.1096846812,0.9606920227\H,2.4882613857,2.406
3635813,-0.1697694325\H,2.6997644654,-3.1225985921,2.1299295532\H,4.98
06051535,1.660623158,0.9327419525\H,3.901519441,-1.8308288284,2.054960
6784\H,4.7876907878,0.0327375646,1.5895529129\H,2.2365766537,-1.460030
8555,2.5408899338\H,3.5266087807,1.2500955737,1.8618623879\H,0.5133315
685,0.5307707799,0.2289927074\H,-2.3447602905,5.5441006612,0.038219974
5\H,-0.7642624557,5.1656999439,-0.6682218088\H,-1.0267315857,4.9676736
014,1.0782823183\H,-0.3417429262,2.5672971321,1.049503104\H,0.11608503
77,2.9186644886,-0.6214929672\H,-2.9475849564,2.9005427237,4.103279519
\H,-3.915551573,1.819421659,3.0462706806\H,-4.3093252048,3.551392972,3
.1303446852\H,-1.1626091494,-1.9285664138,-3.5869085465\H,0.3464127565
,-0.9583668209,-3.6665164658\H,-1.1948494716,-0.2320601089,-4.17197866
51\H,-1.7654023126,3.4925456501,-2.3261450018\H,-3.3579358278,3.992235
501,-1.7013876455\H,-2.9341219788,2.2842790318,-1.7642758368\H,-1.6584
381719,0.3506635292,1.5028317643\H,-1.650323916,-0.8897052972,0.228767
5455\H,-2.8255445329,0.4239076444,0.1768439356\\Version=EM64L-G09RevB.
01\State=2-A\HF=-1176.4991587\S2=0.756758\S2-1=0.\S2A=0.750033\RMSD=4.
666e-09\RMSF=4.129e-06\Dipole=0.9087844,-0.7229244,0.4663212\Quadrupol
e=-5.081034,2.987658,2.0933759,-1.1419081,-3.7175181,5.4328313\PG=C01
[X(C19H36N1O5)]\\@

EtCH(Me)COOMe (c)

1\1\GINC-X92\FOpt\RB3LYP\6-31G(d)\C6H12O2\GXG501\01-Jul-2012\0\\#B3LYP
/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134
2177280\\pmma_core.freq\\0,1\C,-3.845086886,2.5359755113,0.3774156392\
C,-2.8704295394,1.3910503573,0.1358190562\O,-1.6608013489,1.4723839914
,0.1812861324\O,-3.5234593121,0.2508505494,-0.1913255543\C,-2.68298016
34,-0.8714487723,-0.5050761811\H,-2.0534268565,-1.1308989936,0.3503238
193\H,-2.0403465669,-0.644906425,-1.3602319545\H,-3.363235134,-1.69001
46573,-0.7426739426\H,-4.7728236505,2.099987784,0.7685440373\C,-4.1593
338814,3.2018355959,-0.9792622098\H,-4.8873877311,4.0089294993,-0.8434
523406\H,-3.2519034804,3.6315189336,-1.4184505734\H,-4.5772156076,2.48
02800515,-1.688780544\C,-3.2777520633,3.5425701819,1.3909691003\H,-3.9
525429039,4.4081060238,1.4230690118\H,-2.3120401774,3.9041174035,1.018
6637538\C,-3.104902021,2.9729031194,2.8026146543\H,-2.7288153804,3.738
9333587,3.4897825818\H,-4.0572324822,2.6044647231,3.2043393589\H,-2.38
93968137,2.1437407643,2.807991155\\Version=EM64L-G09RevB.01\State=1-A\
HF=-386.3305476\RMSD=3.102e-09\RMSF=8.823e-06\Dipole=-0.5659762,-0.227
0887,-0.1440859\Quadrupole=-3.781932,3.7004499,0.0814821,-1.436349,-0.
1401946,1.17021\PG=C01 [X(C6H12O2)]\\@

PH

1\1\GINC-X148\FOpt\RB3LYP\6-31G(d)\C10H18O4\GXG501\01-Jul-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1
342177280\\pmma.freq\\0,1\C,-3.904713994,2.2524332534,0.1882516175\C,-
2.7708449244,1.2077439752,0.0689929588\C,-1.4109285871,1.9697406469,0.
1159422005\C,-0.1233917743,1.1845834765,-0.2237459439\H,-4.8855123399,
1.7650589782,0.2302638011\H,-3.8951178789,2.9111070078,-0.6879319226\H
,-3.7913164738,2.866689234,1.0854062841\C,-2.9362848708,0.4102163871,-
1.2347573123\H,-1.2954921225,2.4170956659,1.1090860405\H,-1.4793693354
,2.7980504322,-0.6018865809\C,1.0982853171,2.121884913,-0.1641437853\C
,0.0963034073,0.0312244781,0.7459302809\C,-2.8587768812,0.241083794,1.
2599208381\O,-2.8769850221,-0.9711807837,1.1793875157\O,-2.9057749965,

0.9021409311,2.4341919493\C,-2.8446133945,0.0830730697,3.6139733176\O,
0.1861668711,0.1552399441,1.9517939845\O,0.1901555038,-1.1501974288,0.
1055438569\C,0.3020571106,-2.3091507514,0.9521868219\H,-2.9623340625,0
.7708379028,4.4520755548\H,-1.8746503185,-0.4174112081,3.6621873664\H,
-3.6451244295,-0.6608452109,3.6090942216\H,0.4425716406,-3.1515640174,
0.2743566922\H,-0.6180334791,-2.4290380888,1.5287138403\H,1.1539987473
,-2.2102412451,1.6293351451\H,-0.200415684,0.7664617685,-1.2313670489\
H,-2.8067802335,1.0732179936,-2.0984009309\H,-3.9361588346,-0.03197026
36,-1.2919845206\H,-2.215207982,-0.4070724169,-1.3048403727\H,1.235395
1648,2.5069710142,0.8513105126\H,0.961660329,2.9705865991,-0.843324769
6\H,2.0145127957,1.5977814683,-0.4575376427\\Version=EM64L-G09RevB.01\
State=1-A\HF=-692.8290298\RMSD=5.576e-09\RMSF=1.167e-05\Dipole=0.03672
34,0.289359,-0.2000246\Quadrupole=-1.058278,0.4325819,0.6256961,-2.849
081,-2.6361052,-2.680937\PG=C01 [X(C10H18O4)]\\@

SG1-PMMA

TS2 (c)

1\1\GINC-X127\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\16-Oct-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_mscore.freq\\0,1\N,-
1.9012591902,0.8916491576,1.012304634\O,-1.0848766665,1.0747424302,2.0
340363277\C,-2.9052746917,-0.1401114016,1.2206391434\C,-1.241525327,0.
9274045287,-0.2855121194\H,-3.6527811201,-0.099117039,0.4221438024\H,-
3.3888805229,0.040917378,2.1829309999\H,-2.4513862831,-1.1466688187,1.
2350628322\H,-0.6448257664,0.0136964681,-0.4557848188\H,-1.9866959525,
1.0195008244,-1.0820746514\H,-0.5721858755,1.7887379676,-0.2982604652\
H,0.1565211173,0.4717383908,2.5839345813\C,1.0111775076,0.8454364937,3
.3710180435\C,0.4552086305,2.1266871813,3.6709569147\C,1.1507040002,-0
.2114440983,4.4624496846\H,1.4700117729,-1.1651307189,4.0297587108\H,1
.90021902,0.0824030302,5.2081413728\H,0.207745548,-0.387605859,4.99023
43427\C,-0.4106196392,2.3679909057,4.8677057649\H,0.2008297559,2.48064
94719,5.7774110781\H,-1.0792389536,1.5175736825,5.0403139351\H,-1.0097
100895,3.2718575018,4.7559021402\C,0.757204591,3.2092018703,2.71789579
17\O,1.4641638911,3.0968434055,1.7268748086\O,0.1757503153,4.391344064
3,3.065839106\C,0.4252320859,5.4742068483,2.1647213312\H,1.4985949191,
5.6616972539,2.0690243534\H,0.0195355142,5.2534133969,1.1727685093\H,-
0.0783177538,6.339913382,2.5977548109\H,1.8766561629,0.9188363019,2.70
57590357\\Version=EM64L-G09RevB.01\State=1-A\HF=-595.3768516\RMSD=6.57
9e-09\RMSF=3.280e-06\Dipole=-0.6660309,-0.3312551,0.0149853\Quadrupole
=-3.5573558,3.0333357,0.5240201,1.3097357,3.9616505,0.8977516\PG=C01 [
X(C8H17N1O3)]\\@

TS2

1\1\GINC-X108\FTS\RB3LYP\6-31G(d)\C21H42N1O8P1\GXG501\27-Aug-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200,MaxStep=10) IOP(2/17=4) maxdisk=1342177280\\ts1_ms.fre
q\\0,1\C,2.05761592,0.0171186416,0.5222658934\H,1.5067046364,-0.466350
5192,1.3320990694\C,3.125225081,0.9582922896,1.1393432192\C,2.34196866
67,-0.9008802962,-0.525121615\H,1.0936629016,0.666997574,0.0110473402\
O,0.0984987759,0.607755072,-0.9903873662\N,-0.9683686691,1.3488753438,
-1.2221345984\C,-0.723310332,2.7067991868,-1.814513813\C,-2.214280853,
0.9410398937,-0.5817222369\H,-2.9306446208,1.7475391207,-0.7477722225\
C,-2.8725154326,-0.3474413715,-1.2182952651\P,-2.0430553007,1.00104782
5,1.2888297999\O,-0.8714841931,1.7651462879,1.7997085217\O,-3.49934017
28,1.6520912816,1.6112116954\O,-2.2002279175,-0.4728177293,1.944303455
6\C,-3.8712043931,1.8725864561,2.9819733762\C,-1.1331652106,-1.0891018
405,2.7031684118\H,-3.1240828105,2.4910877951,3.4889693991\H,-3.980922
1854,0.9175268865,3.5054713758\H,-4.8300171712,2.3938446589,2.96280169
65\H,-1.6198209982,-1.752447739,3.4218248955\H,-0.553175292,-0.3277502
055,3.2296043611\H,-0.4882309421,-1.6633757165,2.0348909641\C,1.585633

4594,-2.16106385,-0.4980048881\O,1.7829433046,-2.9270961178,-1.6066431
014\C,1.1073469745,-4.1887516869,-1.6061453129\C,3.3015220765,-0.61811
37918,-1.6451450798\C,3.9307361943,1.7818980688,0.1296086335\O,3.14462
99351,2.5404236435,-0.6717343242\C,3.8487195924,3.4006844656,-1.583187
9529\C,2.4397616935,1.9525617104,2.1089527677\C,4.1175382518,0.0847441
162,1.9374037228\C,0.2275433501,2.5061176999,-3.0096990421\C,-2.028406
3181,3.3465476329,-2.3182799461\C,-0.0758701282,3.6388319556,-0.770768
386\C,-1.9649186105,-1.5865893991,-1.1503602588\C,-4.2168547633,-0.643
4839373,-0.5188151839\C,-3.1694050662,-0.0433859727,-2.7016982527\O,0.
8661933146,-2.5406820358,0.421283371\O,5.1417125324,1.8173691276,0.064
9000249\H,3.1827633618,2.6209364303,2.5596490153\H,1.9488435409,1.3977
049019,2.9148937214\H,1.6718119069,2.5484086334,1.6146626932\H,3.07616
54606,3.9431851027,-2.1279945981\H,4.4630248664,2.8119205921,-2.269572
9298\H,4.4938777496,4.0921687387,-1.0353318509\H,1.419437097,-4.688169
6556,-2.5247083638\H,0.0226786407,-4.0477012608,-1.5986885978\H,1.3906
400959,-4.7811401197,-0.731462274\H,3.573503577,-0.4955856421,2.689899
7392\H,4.860171251,0.707665481,2.4442845979\H,4.6520527537,-0.61231077
23,1.2859353601\H,3.0208445539,0.301169737,-2.1740818487\H,3.321598319
3,-1.434124279,-2.366544585\H,4.3222448615,-0.4651811278,-1.2699326055
\H,-1.7727169137,4.2641189365,-2.858409764\H,-2.6988502725,3.636821828
5,-1.5023747024\H,-0.7168336727,3.7588053723,0.1063022344\H,0.09424842
9,4.6259169285,-1.2183442618\H,0.8843871028,3.2410923463,-0.4403642555
\H,0.4683618654,3.4773678557,-3.4559963097\H,-0.2380221614,1.880363754
9,-3.7792495032\H,1.1516369006,2.0253931646,-2.686446445\H,-2.56950946
86,2.6940211192,-3.008916701\H,-4.7349830713,-1.4429488078,-1.06140953
05\H,-4.0800613586,-0.9757548401,0.5125560614\H,-4.872299176,0.2352376
892,-0.5122334886\H,-3.6063498302,-0.9283295446,-3.1789016081\H,-3.887
7356309,0.778287674,-2.8123707213\H,-2.2573900758,0.2149827837,-3.2489
362188\H,-2.5071647801,-2.4500389008,-1.5575387891\H,-1.055330147,-1.4
437949793,-1.7377932951\H,-1.6691250551,-1.8287896651,-0.128612324\\Ve
rsion=EM64L-G09RevB.01\State=1-A\HF=-1823.3627629\RMSD=4.711e-09\RMSF=
1.791e-06\Dipole=-1.1481086,0.3277065,-0.4401111\Quadrupole=-8.346192,
3.7901222,4.5560698,-1.4881565,-5.4111159,-1.9049747\PG=C01 [X(C21H42N
1O8P1)]\\@

TS2 M (c)

1\1\GINC-X140\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\19-Aug-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,MaxStep=10
,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_ms1core.f
req\\0,1\N,-2.5776201211,-1.2872772215,-0.0051198784\C,-2.0590854806,-
0.130961992,0.7334192213\C,-2.0443544557,-2.5724663962,0.4680727468\O,
-2.4896859744,-1.1573403282,-1.3186166798\H,-3.8358992274,-1.240405032
7,-1.6238741864\C,-5.0381952075,-1.3780434099,-1.3218870652\H,-5.53850
41476,-0.5789935111,-1.8695478628\H,-5.2870516771,-2.3722866305,-1.690
5840833\C,-4.9831498692,-1.2326626062,0.0920019612\C,-5.0149476704,-2.
4005707804,0.9999001501\O,-5.0442667187,-2.3252509556,2.2185098874\O,-
5.0217417263,-3.5942726834,0.3463760419\C,-5.0856717689,-4.7503575872,
1.1916684196\H,-5.1120498735,-5.6058373614,0.5154612449\H,-4.209920839
1,-4.8060258364,1.8448106994\H,-5.9845946291,-4.7240750822,1.813505481
7\C,-5.2886672492,0.0802306328,0.7847151692\H,-6.267837853,-0.03343649
8,1.2751337996\H,-4.5941415066,0.2244959158,1.6183936503\C,-5.32002839
86,1.3243719214,-0.1087870969\H,-6.1571422857,1.2964139855,-0.81476906
39\H,-4.4013601267,1.436191546,-0.6946590057\H,-5.4415942031,2.2231095
272,0.5053654293\H,-0.966207863,-0.0792670351,0.6316412757\H,-2.319210
9883,-0.2221853269,1.7916109276\H,-2.4956708608,0.7757662185,0.3166343
068\H,-2.2774730336,-2.6999512237,1.5290443116\H,-0.9562736812,-2.6029
328194,0.3212783541\H,-2.510273727,-3.3658204057,-0.1156775977\\Versio
n=EM64L-G09RevB.01\State=1-A\HF=-595.4014902\RMSD=5.995e-09\RMSF=4.732
e-06\Dipole=0.1043848,-0.1703661,0.3127073\Quadrupole=0.9270152,6.3786
956,-7.3057108,-0.16679,5.036977,0.2613352\PG=C01 [X(C8H17N1O3)]\\@

TS2 M

1\1\GINC-X138\FTS\RB3LYP\6-31G(d)\C21H42N1O8P1\GXG501\31-Jul-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,MaxStep
=10,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts1_ms1.fr
eq\\0,1\N,1.2961990053,1.4112813071,-0.1161145157\O,0.6053112995,0.651
7705698,-0.928679562\H,-0.8645202289,0.3833598502,-0.7535248471\C,-1.8
955897257,0.0720394062,-1.3352718483\C,-2.8032652307,-0.7509227976,-0.
6105323724\C,-2.5438582053,-2.1826126329,-0.4324954663\O,-1.3758310677
,-2.5952456084,-1.0070551862\C,-1.0993389827,-3.9942808787,-0.86752335
05\C,1.3733244647,2.8608719901,-0.518419972\C,1.7905480691,2.954091816
5,-2.0006657722\C,2.2243041667,0.7169165968,0.7838359267\P,3.442278593
,-0.2073039119,-0.3067169643\O,3.9107307561,0.6118109252,-1.458405516\
C,2.3757902726,3.6327170273,0.3497101755\C,-0.0349993784,3.459145388,-
0.336992342\C,1.5413989602,-0.0129567961,2.005756574\C,0.7426810271,-1
.2681841072,1.6113178045\C,0.5998131826,1.0022903002,2.6855578721\C,2.
6186393826,-0.4151985713,3.0363604606\O,2.8888449119,-1.6739999334,-0.
7131259312\C,2.2153095295,-1.8959137081,-1.970096038\O,4.5877082205,-0
.6017469037,0.7668926312\C,5.8149841782,-1.1769850609,0.2787743853\C,-
4.1024352716,-0.2503959473,-0.0426355476\C,-4.0894457816,0.4580478125,
1.36148746\C,-3.5201148191,1.8736189806,1.2303700931\O,-4.2605512281,2
.6321830221,0.3860340696\C,-3.8625263191,4.0061402926,0.2573267223\C,-
5.5557851828,0.5747595948,1.8410892959\C,-3.2698174572,-0.3378919025,2
.3846359175\O,-3.2841047906,-2.9633875943,0.1552841298\O,-2.5486173914
,2.3083026006,1.8151110479\H,2.8606893088,1.4858756282,1.2255415006\H,
2.129024496,3.5827708742,1.4157909594\H,2.34360423,4.6869524385,0.0561
017668\H,3.401523312,3.2827483482,0.1956745421\H,-0.3697249265,3.40938
01685,0.702686545\H,-0.7569027644,2.9189348308,-0.9555035454\H,-0.0301
958393,4.5075584611,-0.6565938664\H,2.7806271963,2.5188437838,-2.15048
73826\H,1.8016389559,4.0057623129,-2.3092821642\H,1.0774345355,2.41453
72569,-2.6285145004\H,1.1421205074,1.9037863132,2.9988897347\H,0.16744
50169,0.5536772239,3.5873740651\H,-0.228184562,1.3089228366,2.04289507
36\H,3.2291204911,0.4443580141,3.3401400366\H,3.2920597789,-1.18541545
56,2.6564742232\H,2.1249175406,-0.8054112399,3.9339216038\H,-0.0301391
916,-1.0470897178,0.8736242373\H,0.2558760935,-1.6810430788,2.50333104
36\H,1.3917966985,-2.0411500782,1.1915567294\H,1.1376820846,-1.8037124
46,-1.8228070624\H,2.4747873376,-2.9104756069,-2.2823416332\H,2.555364
482,-1.1772290952,-2.7191900173\H,6.4861182638,-1.2407305711,1.1369457
958\H,6.2538839873,-0.5408370416,-0.4948568612\H,5.6300328247,-2.17819
74066,-0.1223709327\H,-5.6170858541,1.1320609904,2.7832229573\H,-5.964
165014,-0.4266089289,2.0155497129\H,-6.1818413331,1.0825230271,1.10220
82343\H,-4.5657435005,0.4424359188,-0.7541837252\H,-4.7622866042,-1.11
62003587,0.0650359288\H,-4.6262090459,4.4736840093,-0.3653565591\H,-2.
8827865574,4.0817757347,-0.220564176\H,-3.817874513,4.4864717485,1.238
1468256\H,-0.1449958077,-4.1568657945,-1.3699568047\H,-1.886008431,-4.
593164772,-1.3353674731\H,-1.0276495425,-4.2713499569,0.18770843\H,-3.
6480994317,-1.3628746465,2.4421623992\H,-3.3345264906,0.1221023515,3.3
758774789\H,-2.2140883686,-0.3790750431,2.1071288648\H,-2.3116121819,1
.0364253768,-1.641491953\H,-1.3716261402,-0.427583536,-2.158296366\\Ve
rsion=EM64L-G09RevB.01\State=1-A\HF=-1823.3610857\RMSD=5.595e-09\RMSF=
3.416e-06\Dipole=0.1610786,0.5155104,-0.0098095\Quadrupole=0.6951095,5
.2834479,-5.9785574,-13.5472099,5.516321,2.9379115\PG=C01 [X(C21H42N1O
8P1)]\\@

$Me_2NOC(Me)(Et)COOMe$

1\1\GINC-X140\FOpt\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\11-Jul-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
1342177280\\ms_core.freq\\0,1\N,-1.9505522215,1.951459558,-0.991607151
\O,-0.7281967928,1.1715359813,-1.11344096\C,-2.9592292794,1.207829127,
-1.7505674869\C,-1.668035167,3.2386712625,-1.6264730154\H,-2.585644574
5,3.8364812395,-1.6066547154\H,-0.8958053218,3.7664432714,-1.063181083
8\H,-1.3358002999,3.1269393418,-2.671139621\H,-2.6728607378,1.07825726
67,-2.8068711724\H,-3.0952377907,0.2294532982,-1.2906916606\H,-3.89926
22601,1.7684639111,-1.7026102266\C,-0.1896452337,0.8334130529,0.172240

3704\C,0.3164744266,2.0812532581,0.9012693423\C,0.9467176717,-0.153425
1423,-0.1843293632\C,-1.2594921538,0.0567740417,0.9714298197\O,-1.9583
687753,-0.8168939942,0.5048951715\O,-1.2915242486,0.4069049874,2.27462
12324\C,-2.239231989,-0.3135030247,3.0805682823\H,-3.2554845639,-0.144
9937253,2.7151290024\H,-2.0273506545,-1.385702514,3.0571564647\H,-2.12
33849756,0.0807157389,4.0905514742\H,1.6301688035,0.3783013442,-0.8573
374401\H,0.4912528443,-0.9630568291,-0.7642768434\C,1.7210584804,-0.73
01563268,1.0051269105\H,2.478530139,-1.4367746282,0.6494615379\H,2.238
5384758,0.047324056,1.5770213469\H,1.0651780983,-1.2729492299,1.695340
406\H,0.7752472371,1.8299096958,1.8600427838\H,-0.5086774262,2.7702181
049,1.0966824961\H,1.0613962893,2.5830858769,0.2743060987\\Version=EM6
4L-G09RevB.01\State=1-A\HF=-595.4612189\RMSD=7.301e-09\RMSF=9.193e-06\
Dipole=0.0747613,0.4243761,0.5333758\Quadrupole=0.5115689,-1.9493326,1
.4377637,-1.8920946,-0.5846919,-3.4609783\PG=C01 [X(C8H17N1O3)]\\@

SG1P

1\1\GINC-X91\FOpt\RB3LYP\6-31G(d)\C21H42N1O8P1\GXG501\12-Jul-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdis
k=1342177280\\ms.freq\\0,1\C,-2.3044120234,-1.0213200469,-0.4816504975
\N,-1.5863312463,0.0457785766,0.3352105136\C,-0.3432504709,0.569495073
,-0.2928908939\O,-1.2222558837,-0.4843995369,1.6305370882\C,-2.9320454
153,-0.3134778515,-1.6989194855\C,-3.4484343984,-1.6185869984,0.351817
44\C,-1.4266643228,-2.1926368101,-0.9680854519\C,-0.2478845829,2.15481
44741,-0.3936687918\H,-0.3604854668,0.2360111201,-1.3332902407\P,1.258
4067078,-0.2020781026,0.3504236389\H,-3.5824726285,0.508506178,-1.3870
426057\H,-3.5344062003,-1.0362471262,-2.2597468285\H,-2.1828693969,0.0
84518235,-2.389858089\H,-4.1155041614,-0.8506039667,0.7510352919\H,-3.
0638280328,-2.2279811084,1.171320876\H,-4.0460392642,-2.2735207611,-0.
291191294\H,-0.600170789,-1.870886961,-1.6086665477\H,-2.046959873,-2.
8773113465,-1.5584326043\H,-1.0041536277,-2.7477940118,-0.1303818096\C
,-1.5824745339,2.697918809,-0.9445298523\C,0.8579613669,2.5295665689,-
1.4086135535\C,0.0691839638,2.8836605808,0.9269466465\O,2.0292613537,-
0.2637665984,-1.0847408136\O,1.0946271943,-1.7891111079,0.6207717573\O
,1.983328129,0.5110922055,1.4405565161\C,3.3835167085,-0.7415766832,-1
.1096376224\C,1.1745608376,-2.3537724754,1.9446581839\H,-1.7872458578,
2.3282829101,-1.9553235019\H,-1.5330646487,3.791841822,-0.9997591566\H
,-2.4239199387,2.4237109341,-0.3041012582\H,0.7278354339,2.0111105298,
-2.3658238166\H,1.8591808993,2.2998339911,-1.0362687805\H,0.8149945442
,3.6077750638,-1.6026950416\H,-0.7073553136,2.74465347,1.6798098632\H,
0.1356567292,3.9609707244,0.7279033606\H,1.0167171884,2.5516546785,1.3
537949472\H,4.0022209474,-0.1883138,-0.3963491711\H,3.7520599522,-0.57
75153273,-2.1241708421\H,3.4138481913,-1.8102933584,-0.87427189\H,1.64
32546876,-3.3345184394,1.8296718456\H,0.171409035,-2.4576605741,2.3613
23376\H,1.7895025148,-1.7226818705,2.5908385904\C,-1.926593468,0.03832
93748,2.82166397\C,-2.5997572317,-1.2259481815,3.4081486249\C,-2.92161
55944,1.1565992197,2.5368089431\C,-0.7546534159,0.4561756873,3.7548967
507\O,-2.0023411353,-2.2570161731,3.6385335749\O,-3.9174178078,-1.0739
331183,3.6448305869\C,-4.5821163189,-2.2208897956,4.2046817713\H,-5.62
10964692,-1.9186086527,4.3362231725\H,-4.1328695893,-2.4899972402,5.16
38836736\H,-4.5097128881,-3.0729537753,3.524054658\H,-0.1392158287,-0.
4385600278,3.8881691306\C,-1.0144166791,1.0389173863,5.1771459973\H,-0
.1457453861,1.1646382218,3.1915810269\C,-1.8417844738,0.1094280148,6.0
812183524\C,-1.7002210537,2.4102755688,5.1307479913\C,0.3804849564,1.2
521958721,5.8235123165\O,-2.7102171615,2.7129513129,5.7319144414\O,-1.
020754939,3.2907534586,4.3588000807\C,-1.5694019678,4.6173726892,4.303
1453739\H,-2.8776876641,0.0254503122,5.7445278056\H,-1.8700296837,0.49
97086289,7.1029196063\H,-1.3938082567,-0.889183327,6.1016174206\H,-1.6
002878306,5.0613601095,5.3016274505\H,-2.5829100929,4.5975715483,3.893
5159584\H,-0.9024109366,5.1814525098,3.6508807506\H,-3.6845734102,0.85
09779664,1.8224478735\H,-2.4145084215,2.0326021092,2.1368872996\H,-3.4
26989992,1.4359576886,3.463994582\H,1.0179881381,1.8842745994,5.199938
1761\H,0.8766860956,0.2845109775,5.9560693609\H,0.2843431983,1.7199009

527,6.8102237841\\Version=EM64L-G09RevB.01\State=1-A\HF=-1823.4204436\
RMSD=8.674e-09\RMSF=5.394e-06\Dipole=-0.5257101,-0.2670826,-0.5773201\
Quadrupole=0.7977563,2.0924434,-2.8901997,2.639245,0.2522759,-1.227152
1\PG=C01 [X(C21H42N1O8P1)]\\@

TS3b (c)

1\1\GINC-X127\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\30-Oct-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts2c_mscore.freq\\0,1\N,
-0.1219956825,-1.1871479687,2.0577781096\O,0.0680178201,-0.590386202,0
.8830056545\C,1.5755400242,-1.9482991612,0.0867755465\C,1.6077875909,-
2.9002470843,1.1203856774\H,0.6831137608,-2.2152966862,1.9060472496\C,
0.3608546591,-0.375649341,3.1987250026\C,-1.5010575322,-1.6927083181,2
.2153045264\H,2.466426063,-2.8038498014,1.7873220993\C,1.0806688661,-4
.3171435513,0.9535684154\H,0.9995176858,-4.8155862267,1.926077093\H,1.
7473714094,-4.9295027449,0.3311686948\H,0.0891747123,-4.3461648099,0.4
877186973\C,0.8967813342,-2.1669995132,-1.2369372544\C,2.5219709308,-0
.805263785,0.2317946493\H,0.0334001546,-2.8293471042,-1.1330742858\H,1
.5895934847,-2.6355069408,-1.9512452501\H,0.5602885297,-1.2228942608,-
1.6666214028\O,3.1893041545,-0.5648415992,1.2249532693\O,2.583063639,-
0.0447120402,-0.8853983807\C,3.4293673035,1.1074889397,-0.7931175966\H
,4.4577046035,0.8167941411,-0.5612016348\H,3.0697152391,1.7853872346,-
0.0138723868\H,3.3775679363,1.5884802642,-1.770902215\H,0.2929155372,-
0.9592548825,4.122426127\H,1.3982835208,-0.1161601422,2.9910869364\H,-
0.2466033167,0.5320533308,3.2813194779\H,-1.578701067,-2.2880889455,3.
1305187044\H,-2.1982467198,-0.8489526496,2.254430947\H,-1.7287956415,-
2.3082351514,1.3443835291\\Version=EM64L-G09RevB.01\State=1-A\HF=-595.
4029634\RMSD=8.619e-09\RMSF=4.993e-06\Dipole=-0.7339398,-0.2865278,0.4
735085\Quadrupole=-1.2715034,0.1102627,1.1612407,2.754044,-6.0990215,-
0.930706\PG=C01 [X(C8H17N1O3)]\\@

TS3b

1\1\GINC-X112\FTS\RB3LYP\6-31G(d)\C21H42N1O8P1\GXG501\30-Oct-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200,MaxStep=10) IOP(2/17=4) maxdisk=1342177280\\ts2c_ms.fr
eq\\0,1\C,-0.0150296054,-1.5037368575,1.9237677687\N,0.15850196,-0.529
3549892,0.7088135196\C,1.2827563756,-0.9546779329,-0.2443106488\O,0.36
86260838,0.7386500057,1.1240746826\C,-0.3782684593,-2.914350272,1.4412
922158\C,-1.1558698684,-0.9727741271,2.794203461\C,1.2660447238,-1.544
0798004,2.771336158\C,0.9375943093,-1.3993341784,-1.737005969\H,1.7384
683167,-1.8312402361,0.2177105238\P,2.6415321129,0.3542390767,-0.12007
75263\H,-1.3148842996,-2.9206851886,0.8799552867\H,-0.5227194049,-3.54
60623114,2.3246299122\H,0.4119312228,-3.3794345226,0.8437575285\H,-2.1
07521988,-1.0263361093,2.264556205\H,-0.9551870832,0.0492300802,3.1161
246573\H,-1.2389517183,-1.6050443241,3.6846291887\H,2.1349645062,-1.93
57401545,2.2362475559\H,1.0856141563,-2.2048879971,3.6264115376\H,1.51
74828305,-0.553426291,3.1503171048\C,-0.4338580896,-2.0988321955,-1.83
90376963\C,1.986528697,-2.4554670692,-2.166418075\C,0.9599920934,-0.24
3640434,-2.7592351609\O,3.8471165069,-0.6152193932,-0.6410905524\O,3.1
253285062,0.5154327645,1.4198248899\O,2.5278023598,1.6362881727,-0.864
8812133\C,5.1602651434,-0.0497073972,-0.7728356953\C,2.9096216704,1.74
19268354,2.1398347427\H,-0.5099911778,-2.9675041144,-1.1815284987\H,-0
.5545301015,-2.4577710088,-2.8677683595\H,-1.267662459,-1.427831733,-1
.6365834444\H,1.9573614669,-3.3372957099,-1.512662352\H,3.0007166064,-
2.0561564379,-2.1534812069\H,1.7607438126,-2.7920634625,-3.1847982004\
H,0.2965938791,0.5789194323,-2.486411234\H,0.6434763791,-0.6327763295,
-3.7347817832\H,1.9606091202,0.1782729203,-2.8772483661\H,5.1303547093
,0.8559032999,-1.3860830705\H,5.7778094667,-0.8070897753,-1.2598881075
\H,5.5733781342,0.1840469922,0.213669199\H,2.9183272268,2.5945596915,1
.4578854857\H,3.7304162696,1.8222195154,2.856973597\H,1.9487717519,1.7
01473164,2.6552025941\C,-1.3413916974,1.7823371678,0.4076700943\C,-0.4
900293791,2.6382308191,-0.5024964933\C,-1.688373302,2.4185191365,1.729

683561\C,-2.0186507791,0.7253329559,-0.2348736234\O,-0.472411094,2.541
655554,-1.7153656388\O,0.1858375828,3.5901757039,0.1654100623\C,1.0150
326798,4.4346314607,-0.6548429823\H,1.4451734143,5.1670294906,0.030521
1291\H,0.4124438758,4.9335380035,-1.4187641185\H,1.790686433,3.8288487
455,-1.1246796722\H,-1.7737525288,0.7185355446,-1.2980561884\C,-3.5292
731559,0.3587008878,-0.088271754\H,-1.0159677922,-0.3032359254,0.17116
51212\C,-4.2178406672,0.6404798251,1.2645662025\C,-3.6688171172,-1.150
9444162,-0.3415844848\C,-4.2882212584,1.1687163679,-1.1695584046\O,-3.
5656322068,-2.0077718633,0.5164849667\O,-3.9162327841,-1.4517132905,-1
.6338023238\C,-4.0689179822,-2.8496685257,-1.9329112085\H,-3.737181371
3,0.1408999996,2.1050484757\H,-5.2524376768,0.2813922512,1.2215842983\
H,-4.2519546469,1.7140477151,1.4618082026\H,-4.8686908649,-3.283913572
2,-1.3278135894\H,-3.1389410921,-3.388561099,-1.7361400274\H,-4.318957
3906,-2.8938973969,-2.9932325503\H,-0.7877468824,2.8219258344,2.193905
4445\H,-2.155479408,1.7172680005,2.4168727153\H,-2.3794055944,3.259716
0641,1.5771225912\H,-3.8851596968,0.9916788755,-2.1687547729\H,-4.1955
204336,2.2374018134,-0.9496230771\H,-5.3538313041,0.9104260118,-1.1811
522459\\Version=EM64L-G09RevB.01\State=1-A\HF=-1823.3540322\RMSD=6.407
e-09\RMSF=3.971e-06\Dipole=0.0186276,-0.7445645,0.5874966\Quadrupole=4
.8628524,0.3823836,-5.2452361,1.5109614,4.0647501,7.7963044\PG=C01 [X(
C21H42N1O8P1)]\\@

TS3b M (c)

1\1\GINC-X104\FTS\RB3LYP\6-31G(d)\C8H17N1O3\GXG501\30-Aug-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigentes
t,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts2c_ms1core.freq\\0,1\N
,1.5105007223,2.0682615188,1.4633451284\C,0.8360868196,0.9057712187,0.
8430486814\C,2.9445490642,1.8503928772,1.7516908478\O,0.8471836522,2.5
387625407,2.5216189922\H,1.4091921315,3.0657589937,0.6743015392\H,1.35
72714545,0.6190167705,-0.0759316186\H,-0.1851396311,1.2126706139,0.619
7882219\H,0.8286696351,0.0711540957,1.551083884\H,3.472455621,1.574422
5975,0.8332935453\H,3.3446038271,2.7827389996,2.1511872856\H,3.0483635
796,1.0598808527,2.5014249786\C,0.8863341836,4.3786321,0.4568934031\C,
0.3123019106,4.4764329924,1.7291782816\H,1.7731773734,4.9799011485,0.2
546905355\H,0.2407637316,4.2029252928,-0.4005335144\C,0.9488046737,5.2
860436553,2.8328128421\C,-1.1144373935,4.1079086744,1.9525104098\O,-1.
7587640288,4.4135697546,2.9368729334\O,-1.6526871223,3.3995792235,0.92
15460343\C,-3.0255937037,3.0284549406,1.1018943311\H,-3.6529498923,3.9
146294458,1.2316316807\H,-3.3067511504,2.4917391372,0.1943435227\H,-3.
1398665351,2.3856623086,1.9792644725\H,0.670008879,4.8560598799,3.7978
221601\H,2.038476362,5.205260464,2.7400117625\C,0.5358866098,6.7684667
764,2.7889426027\H,0.8189837513,7.2352052487,1.8382496716\H,-0.5463600
272,6.8699383488,2.9139749775\H,1.0234395024,7.3250345294,3.5978494074
\\Version=EM64L-G09RevB.01\State=1-A\HF=-595.4031534\RMSD=5.939e-09\RM
SF=4.941e-06\Dipole=0.8631092,-1.0043296,-1.2212867\Quadrupole=4.08949
78,1.2673744,-5.3568722,-0.2396769,2.2930177,1.7167379\PG=C01 [X(C8H17
N1O3)]\\@

TS3b M

1\1\GINC-X110\FTS\RB3LYP\6-31G(d)\C21H42N1O8P1\GXG501\29-Aug-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200,MaxStep=10) IOP(2/17=4) maxdisk=1342177280\\ts2c_ms1.f
req\\0,1\C,1.5668776998,2.1068129297,1.4929440957\N,1.0063642522,0.805
5342288,0.832054741\C,2.0414594679,-0.308623007,0.7027553094\O,0.41478
29068,1.0580264657,-0.3455251236\C,1.9374939676,1.8352865178,2.9562330
726\C,0.4679516772,3.172822661,1.4408742825\C,2.7831500403,2.632162477
1,0.7141995574\C,1.7667327734,-1.6897620885,1.4305608691\H,2.953492433
9,0.0706010204,1.1653060228\P,2.5071492593,-0.5082554288,-1.1205137669
\H,1.0899503889,1.4410740228,3.5249794777\H,2.2380836817,2.7807699467,
3.4200805409\H,2.7786058498,1.1448090727,3.060853606\H,-0.4261800448,2
.8735453713,1.9904692489\H,0.1919805156,3.3918705343,0.4087941776\H,0.
8538566632,4.0891302697,1.9001702991\H,3.6464702899,1.960991668,0.7508

903137\H,3.094145608,3.5837437824,1.1595724858\H,2.5303993631,2.802460
9903,-0.332595263\C,1.4758576657,-1.4567658826,2.9294210372\C,3.062185
1412,-2.5369894689,1.3556789622\C,0.6269490333,-2.5373404474,0.8347924
933\O,4.0926318926,-0.7713775105,-0.8436840547\O,2.6420013253,0.894771
1238,-1.9116825525\O,1.795361631,-1.5711245256,-1.8824317557\C,4.94038
68862,-1.0655125193,-1.9652211619\C,1.6856540352,1.2815301244,-2.92274
74269\H,2.3214689738,-0.9900367062,3.445191175\H,1.2971571171,-2.42640
01373,3.4082289064\H,0.5867426651,-0.8432721611,3.097182211\H,3.940589
301,-1.9813159972,1.7022949848\H,3.2643325808,-2.8913160715,0.34281747
97\H,2.9430628918,-3.4160763453,1.9992864841\H,-0.3525801616,-2.087673
7448,0.9877288098\H,0.6161270224,-3.5113648384,1.340162422\H,0.7694600
203,-2.7055173344,-0.2337268454\H,4.5309527087,-1.8928944355,-2.553135
092\H,5.9113995602,-1.3496141601,-1.5546749807\H,5.0511760269,-0.18067
28768,-2.5996221073\H,2.2329271819,1.9187579298,-3.6214871095\H,0.8632
009067,1.826897533,-2.4592859592\H,1.3048917508,0.3982325525,-3.440483
8582\C,-1.6589514356,0.6167956986,0.0764856844\C,-2.0429415664,1.99815
41814,-0.3725608472\C,-1.5197219267,0.3131528507,1.4356016784\C,-1.802
7884306,-0.4317739892,-1.0055322104\O,-1.9381864677,2.4105345366,-1.51
13479781\O,-2.5757256608,2.7475249967,0.6245009004\C,-2.9774068177,4.0
716421585,0.2440675913\H,-3.4129666402,4.5139966857,1.1407778122\H,-3.
71388016,4.0309459358,-0.5624734232\H,-2.1163706203,4.6557144103,-0.09
29479929\H,-1.5040123836,0.0186214296,-1.9553445713\C,-3.2451414216,-1
.0103106167,-1.2025933107\H,-1.1180821879,-1.2569556332,-0.8151590797\
C,-4.2753551533,0.0830570367,-1.5298618118\C,-3.7208456514,-1.75820951
99,0.0482508822\C,-3.1793975603,-2.0244383694,-2.3702400629\O,-4.74476
84611,-1.5369739994,0.6580984272\O,-2.8701468917,-2.7578077473,0.39902
22845\C,-3.2837699655,-3.5491525409,1.5232922141\H,-4.4251047252,0.761
5698162,-0.6854171877\H,-5.2478652589,-0.3639915731,-1.7575295035\H,-3
.9428359159,0.6668533797,-2.3931943385\H,-4.2440631961,-4.0310936774,1
.3208348603\H,-3.384247075,-2.9282799278,2.4178295393\H,-2.5007254728,
-4.2957978953,1.6596498004\H,-1.8546864841,1.0476639899,2.1631366056\H
,-1.6541416585,-0.7195322827,1.7459047909\H,-0.0669786702,0.4582941055
,1.4738969032\H,-2.4443349036,-2.8103624053,-2.176822849\H,-2.89519908
52,-1.5055644773,-3.2923704667\H,-4.1555981023,-2.495303092,-2.5354043
489\\Version=EM64L-G09RevB.01\State=1-A\HF=-1823.3682554\RMSD=7.674e-0
9\RMSF=2.340e-06\Dipole=1.2709905,0.49678,1.146806\Quadrupole=-5.35227
16,5.5613618,-0.2090902,0.2070974,0.9936883,0.0133626\PG=C01 [X(C21H42
N1O8P1)]\\@

TS4

1\1\GINC-X152\FTS\RB3LYP\6-31G(d)\C11H26N1O4P1\GXG501\01-Nov-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeigen
test,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\tsc3.freq\\0,1\C,-2.5
287251962,-0.719708302,-0.2599503247\N,-1.4101242495,0.0983987452,0.34
46668826\C,-0.1907318693,0.5055098785,-0.3795782361\O,-1.0020515255,-0
.4556559466,1.714712421\C,-2.9467987944,-0.1046165684,-1.6059416782\C,
-3.7017465631,-0.6163228236,0.7313965909\C,-2.1244973248,-2.1880680261
,-0.4365468124\C,0.090469786,2.0490332043,-0.1800291657\H,-0.363213504
9,0.3569084247,-1.4508609979\P,1.1882849253,-0.7184431902,0.0022586215
\H,-3.2214896673,0.9500345191,-1.5083261394\H,-3.823000671,-0.64691624
95,-1.9762550249\H,-2.1682067186,-0.1960743521,-2.3701624242\H,-4.0118
21249,0.4273399913,0.8683177083\H,-3.4170585044,-1.0294978496,1.700864
9973\H,-4.5603633227,-1.1755000474,0.3465394461\H,-1.3500422057,-2.314
2224864,-1.1956328279\H,-3.0068381205,-2.7640396622,-0.7387660139\H,-1
.7342877301,-2.5880591886,0.5000253112\C,-1.1185971268,2.8261710447,-0
.747515936\C,1.3388393972,2.495987355,-0.9690428952\C,0.2788265632,2.4
468759051,1.2984849242\O,2.0445150557,-0.2306693304,1.2882528736\O,2.1
894934449,-0.2810058428,-1.2021676355\O,0.8377201681,-2.1615555139,-0.
0130500825\C,1.8605192512,-0.8664094621,2.5705144107\C,3.3709211612,-1
.0703980991,-1.419957207\H,-1.265549801,2.6209376841,-1.8147043984\H,-
0.9484515857,3.9031801554,-0.6376580112\H,-2.0461310741,2.5822482337,-
0.2205829057\H,1.2863550414,2.1916959387,-2.0199318857\H,2.2599667103,

2.0875189015,-0.5501590101\H,1.4055457923,3.5897899714,-0.9369617346\H
,-0.603660298,2.2384256788,1.9128033245\H,0.459597001,3.5269132535,1.3
556827371\H,1.1308415718,1.9326012762,1.7461507512\H,1.0003448857,-0.4
256438069,3.0771776669\H,2.7800231098,-0.6836880264,3.1310815595\H,1.6
988858359,-1.9388877992,2.4432012334\H,3.8299802611,-0.6932348516,-2.3
358653119\H,3.1102189265,-2.125923432,-1.5385104559\H,4.0676014899,-0.
9528073094,-0.5835704052\H,-1.5917252757,0.5970120055,1.3587250603\\Ve
rsion=EM64L-G09RevB.01\State=1-A\HF=-1131.7476682\RMSD=6.517e-09\RMSF=
1.282e-06\Dipole=-0.1292959,0.9640174,-0.5096112\Quadrupole=6.0946033,
-5.9131311,-0.1814722,-1.5660844,1.6341951,0.8055785\PG=C01 [X(C11H26N
1O4P1)]\\@

TS5 (c)

1\1\GINC-X109\FTS\UB3LYP\6-31G(d)\C8H18N1O3(2)\GXG501\10-Aug-2012\0\\#
B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(MaxStep=5,TS,calc
fc,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_mscore.
freq\\0,2\N,-0.9661857381,-1.2800003051,-0.0117953574\O,-0.8447478697,
-0.0469705385,-0.6027691944\C,-0.0542787241,-1.3953256165,1.1208496969
\C,-2.3667213006,-1.5668543628,0.2735554254\H,-2.7915303216,-0.8651362
303,1.009335599\H,-2.9348178961,-1.4895192903,-0.6561252757\H,-2.44984
37423,-2.5868225273,0.6616591713\H,-0.1250565482,-2.4068604175,1.53302
9026\H,-0.283213868,-0.6642473992,1.9125293302\H,0.9622843652,-1.22737
32872,0.7591832894\C,0.2358935894,-0.4551483073,-2.9078192771\C,-0.142
0711794,-1.9105177676,-3.0786345086\C,-0.4526592948,0.5707699348,-3.78
82449599\C,1.6476173521,-0.1430839904,-2.5813497606\H,-0.0296330409,-2
.4629155972,-2.1383734819\H,0.4882451546,-2.413252543,-3.8258684189\H,
-1.1847147395,-1.9977501163,-3.4031618775\O,2.2064430265,0.9172059302,
-2.8073196779\O,2.2730327101,-1.1743332381,-1.9437498399\C,3.637772266
,-0.9229359051,-1.5826470699\H,4.2411210796,-0.7135595934,-2.470482148
5\H,3.7088125849,-0.0690838531,-0.902783928\H,3.9845272912,-1.83374982
75,-1.0921955515\H,-0.2078175701,1.574215329,-3.4258559278\H,-1.538552
3152,0.442334808,-3.6918226026\C,-0.0550464409,0.4673697513,-5.2737895
962\H,1.0196262897,0.6365967998,-5.3944739089\H,-0.5859498618,1.221677
5909,-5.8659241483\H,-0.2993701022,-0.5173824574,-5.6887966832\H,-0.34
95841557,-0.1991519727,-1.6171633436\\Version=EM64L-G09RevB.01\State=2
-A\HF=-596.0048939\S2=0.756463\S2-1=0.\S2A=0.750029\RMSD=6.710e-09\RMS
F=1.329e-06\Dipole=-0.3396287,-1.1405503,0.6199871\Quadrupole=2.777793
2,-5.1917307,2.4139375,-1.3289624,1.0763901,-1.3095499\PG=C01 [X(C8H18
N1O3)]\\@

TS5

1\1\GINC-X83\FTS\UB3LYP\6-31G(d)\C21H43N1O8P1(2)\GXG501\06-Aug-2012\0\
\#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_ms.a3.freq\\0,2
\N,1.5450580744,1.0164145886,-0.4915433197\O,0.5299957277,0.1365350474
,-0.7374010291\H,-0.4643451447,0.4791015813,-0.3844448787\C,-2.0066042
544,0.6439501881,-0.2006832486\C,-2.228207785,-0.6392054625,0.49661654
65\O,-2.3978649492,-0.4894737408,1.8383085592\C,-2.559173277,-1.709158
486,2.5760212042\C,1.863059778,1.9039116352,-1.672037649\C,1.654764093
3,1.1501913021,-3.0002702738\C,2.5399024455,0.4717923786,0.4395557629\
P,3.0780057768,-1.2128557955,-0.189919442\O,3.3752442129,-1.2045857613
,-1.6497984261\C,-2.3535302356,0.6239772879,-1.6778930232\C,-3.8494909
838,0.8930233575,-2.0698116138\C,-4.239946594,2.3496107463,-1.79547936
99\O,-3.380903547,3.223236148,-2.3794553264\C,-3.7074051288,4.61191185
39,-2.2119458211\C,-2.1777571847,1.9289097573,0.5769535735\C,3.3128780
522,2.4111796913,-1.6091522742\C,0.9102730668,3.1150932962,-1.60055220
59\C,2.1757361667,0.6726512929,1.9630341255\C,1.0566112533,-0.25663175
57,2.4644063335\C,1.7351563687,2.1404032037,2.1483550974\C,3.430818735
9,0.4522941382,2.8359035526\O,2.0669266897,-2.3809047161,0.2844470145\
C,1.0965842869,-2.9628169962,-0.6175555449\O,4.3567749729,-1.502910589
,0.7633051298\C,5.162876402,-2.6639543178,0.4884047169\C,-3.9792789192
,0.6568590391,-3.594680416\C,-4.8190284531,-0.0323151625,-1.3201354788

\O,-2.2296999079,-1.740890771,-0.0386303801\O,-5.2097199887,2.7147916192,-1.1649440265\H,3.4483170439,1.0579182166,0.2908587069\H,3.5244795804,2.9631685864,-0.686254157\H,3.4692091765,3.1039059173,-2.4423535625\H,4.029929007,1.5924552306,-1.7202425227\H,1.0636134055,3.6844523857,-0.6775259814\H,-0.1357082112,2.7992043003,-1.6427567644\H,1.0881263056,3.7829742978,-2.4511449605\H,2.2966568945,0.2681343262,-3.0431427202\H,1.9032905888,1.8198616114,-3.8315640516\H,0.6165520517,0.8325021332,-3.1167739775\H,2.5196616938,2.8392330017,1.8305923245\H,1.5313482292,2.3331897383,3.208066732\H,0.829712694,2.3689660265,1.5805920481\H,4.2699675378,1.0751994843,2.5014782813\H,3.7636966496,-0.5866042862,2.8285290047\H,3.2022681955,0.7315424258,3.8711100421\H,0.1177285828,-0.0893909618,1.9342743419\H,0.8725897601,-0.0618235981,3.5282266966\H,1.3264667534,-1.3099855245,2.3534590647\H,0.1168155526,-2.5191986052,-0.4342814285\H,1.0749981325,-4.0326138684,-0.3966175142\H,1.3970924735,-2.801076865,-1.6548237257\H,6.0212052882,-2.6080988565,1.1601807064\H,5.5002721054,-2.6574961393,-0.5518972903\H,4.5936608798,-3.576735682,0.6899393431\H,-4.9952783112,0.8804124143,-3.9404203284\H,-3.7687491867,-0.3935119671,-3.8240786425\H,-3.2797932408,1.2817777584,-4.1575967163\H,-1.7427084,1.3585601211,-2.2117523931\H,-2.0951191493,-0.3645761308,-2.069414368\H,-2.9331941324,5.1616728333,-2.7483697015\H,-3.7072417532,4.8825348894,-1.1525702336\H,-4.6936209464,4.8283080738,-2.6309911612\H,-2.7168315369,-1.4051370711,3.6115889725\H,-1.6643452177,-2.3321190272,2.4922395138\H,-3.4193243407,-2.272786245,2.2052502582\H,-4.5370675332,-1.077036413,-1.4802648746\H,-5.8438149857,0.1184891989,-1.6723630769\H,-4.8157306574,0.1633367823,-0.243931745\H,-1.7833663336,2.7805906644,0.0133274911\H,-1.6755203454,1.8865926976,1.5465702466\H,-3.239374051,2.137618527,0.7787202541\\Version=EM64L-G09RevB.01\State=2-A\HF=-1823.9857382\S2=0.757053\S2-1=0.\S2A=0.750034\RMSD=4.898e-09\RMSF=9.639e-07\Dipole=0.7112841,0.6042279,0.4603049\Quadrupole=-8.2197108,7.4595916,0.7601192,0.0295969,5.7341672,-7.7581949\PG=C01 [X(C21H43N1O8P1)]\\@

DPAIO_PMMA

•Iminopyrrol-*N*-oxyl (c)

1\1\GINC-X104\FOpt\UB3LYP\Gen\C4H5N2O1(2)\GXG501\11-Jun-2012\0\\#B3LYP/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\dpaio_rcore.freq\\0,2\O,-3.3104022109,2.5453399036,-0.8077170431\N,-4.3202832452,1.8662612565,-1.1611369289\C,-4.4257837195,0.498020431,-1.1538203747\C,-5.6540874247,0.0847450912,-1.5977521415\C,-6.4591419138,1.2531758743,-1.9377936939\C,-5.5812022667,2.4678054037,-1.6518358803\H,-3.5725020512,-0.0755675088,-0.8160793582\H,-5.9807759089,-0.9436692025,-1.6842991992\N,-7.6541048026,1.3742752162,-2.3875150438\H,-8.0781414459,0.4482796452,-2.5140585198\H,-5.9940219295,3.1209404818,-0.8778274329\H,-5.3726568522,3.0642346042,-2.5444436392\\Version=EM64L-G09RevB.01\State=2-A\HF=-340.0558865\S2=0.779502\S2-1=0.\S2A=0.750333\RMSD=2.128e-09\RMSF=4.551e-05\Dipole=-0.1511443,-1.0410843,-0.0208173\Quadrupole=-4.8595202,4.4546427,0.4048775,-0.5871922,-2.251992,-0.3289308\PG=C01 [X(C4H5N2O1)]\\@

DPAIO•

1\1\GINC-X98\FOpt\UB3LYP\Gen\C26H19N2O1(2)\GXG501\11-Jun-2012\0\\#B3LYP/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\dpaio_r.freq\\0,2\C,-3.2838933115,2.6178267893,-0.8266172098\C,-4.3916219258,1.8722053456,-1.2331472764\C,-4.3889573701,0.4681716799,-1.1508930736\C,-3.2874027798,-0.2235631334,-0.6583689173\C,-2.1874060531,0.538298078,-0.2542329141\C,-2.160644898,1.9444358217,-0.3325437152\H,-3.2960067534,3.6984962427,-0.8944642341\H,-5.2679229876,2.3844654809,-1.6187161273\H,-5.2648085852,-0.0866766328,-1.4759945004\H,-3.2595679545,-1.3039579303,-0.5767241053\N,-1.0031599775,0.0494283638,0.2722719312\C,-0.8712543618,2.4116215641,0.2082565965\C,-0.0463273398,1.1592

304868,0.6220481816\O,-0.7490798771,-1.1811295213,0.4588948159\C,0.255
7452771,1.0607469284,2.1224018366\C,1.2180071644,1.0741245417,-0.24687
76865\N,-0.3786416856,3.5755116009,0.3774652213\C,-1.0035792644,4.7570
827465,-0.066407319\C,-1.5760085897,5.6397805572,0.8625019876\C,-2.127
0597008,6.8468060006,0.4338906707\C,-2.0936341603,7.2034182159,-0.9160
745838\C,-1.499426858,6.338383839,-1.8378102723\C,-0.9561966909,5.1234
23663,-1.4219577194\C,2.2661337076,1.9714250481,0.007587969\C,3.412930
7035,1.9604752848,-0.7831333065\C,3.533097433,1.0524330677,-1.83806213
31\C,2.4962529347,0.1570951039,-2.0932366706\C,1.3426920431,0.16643610
64,-1.3042032731\H,-1.5840059363,5.3693927646,1.9143817409\H,-2.578175
0741,7.5152869231,1.1627145088\H,-2.5161464368,8.148770534,-1.24428154
68\H,-1.4560261728,6.6091582862,-2.8897077586\H,-0.484665582,4.4527721
345,-2.1344061914\H,2.1726055692,2.6840690705,0.8194692804\H,4.2151704
741,2.6627370011,-0.5725911013\H,4.4297774955,1.0420394582,-2.45203520
65\H,2.5795554242,-0.5586989443,-2.9067642006\H,0.5562574017,-0.551366
8509,-1.5057587585\C,-0.3849875172,1.8667098113,3.0701876094\C,-0.1319
493024,1.6963166721,4.4327948047\C,0.7566364101,0.7129942421,4.8655218
696\C,1.3913576321,-0.1021615553,3.9262653181\C,1.1434865797,0.0695208
108,2.5657742333\H,-1.0748809132,2.6398150071,2.7525536\H,-0.632272656
6,2.336923886,5.1542069792\H,0.9543352602,0.5824243509,5.9261788934\H,
2.0829239275,-0.8746246814,4.251774846\H,1.6354682787,-0.5699722596,1.
8415929072\\Version=EM64L-G09RevB.01\State=2-A\HF=-1186.8596551\S2=0.7
65472\S2-1=0.\S2A=0.75018\RMSD=5.975e-09\RMSF=2.575e-06\Dipole=-0.7420
795,0.5221245,-0.3695587\Quadrupole=4.3305546,-6.9965085,2.6659538,-2.
8518093,1.9861801,1.7844218\PG=C01 [X(C26H19N2O1)]\\@

TS2 (c)

1\1\GINC-X126\FTS\RB3LYP\6-31G(d)\C10H16N2O3\GXG501\19-Aug-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(grid=ultrafine) OP
T=(MaxStep=10,TS,readfc,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=13
42177280\\ts1_mdcore.freq\\0,1\O,3.5924235388,-1.7679518534,-2.3992637
265\N,2.7069144047,-2.4603020386,-3.0388214397\C,1.2843224335,-2.48742
85993,-2.6692331466\C,0.6591013827,-3.3471508897,-3.7689376137\C,1.752
2875464,-3.71935157,-4.6597029078\C,2.9133745032,-3.170689606,-4.18605
43226\H,3.9199045224,-3.2211288544,-4.5821960184\H,1.6570178872,-4.328
4984622,-5.549073074\N,-0.5955161221,-3.6193214782,-3.7773793771\H,-0.
816371936,-4.2158234361,-4.5826535514\H,1.1656185938,-2.9260654409,-1.
6744584605\H,0.8953046753,-1.4642031041,-2.6331086917\H,3.732725388,-0
.2132698972,-2.2598097487\C,3.9991732258,0.6510715931,-1.4920807901\H,
3.0388207028,1.1769504511,-1.4511303756\C,4.2201713804,-0.1326149597,-
0.3073917279\C,5.1365930009,1.4943694907,-2.0620765152\H,6.0352967344,
0.8988337863,-2.2535725914\H,4.8333613078,1.9486547674,-3.0105976091\H
,5.4132432626,2.306008259,-1.3776048878\C,3.0129621536,-0.6192233141,0
.3711828887\C,5.5874827026,-0.5101695611,0.1606724845\H,6.2055678473,-
0.857472722,-0.677224151\H,6.108986068,0.3635315138,0.5834574512\H,5.5
560153876,-1.2877633555,0.9235065147\O,1.8671922402,-0.3785851819,0.00
9280647\O,3.2869826988,-1.3737698323,1.4713249344\C,2.1385047936,-1.88
0091533,2.159528192\H,2.527181006,-2.4132902644,3.0282135259\H,1.48036
53586,-1.0638364561,2.4701635428\H,1.5710453504,-2.5606710588,1.517068
731\\Version=EM64L-G09RevB.01\State=1-A\HF=-725.7144576\RMSD=6.501e-09
\RMSF=2.350e-06\Dipole=1.2807543,-0.1422749,-0.1767061\Quadrupole=-8.6
722344,0.7605646,7.9116698,1.3847857,-1.4357092,1.981625\PG=C01 [X(C10
H16N2O3)]\\@

TS2

1\1\GINC-X88\FTS\RB3LYP\6-31G(d)\C36H36N2O5\GXG501\14-Aug-2012\0\\#B3L
YP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(grid=ultrafine) OPT
=(MaxStep=10,TS,readfc,noeigentest,maxcyc=200) IOP(2/17=4) maxdisk=134
2177280\\ts1_md.freq\\0,1\C,2.710753649,-2.2241017769,-1.715778558\C,2
.0359955898,-3.2328194384,-2.4042245064\C,0.6313637029,-3.2378909292,-
2.4697802042\C,-0.1306590453,-2.2446783437,-1.8616868714\C,0.559542174
3,-1.2369257988,-1.1727258037\C,1.9710271373,-1.2160033437,-1.08760687

53\H,3.7930040903,-2.2216411068,-1.6697056421\H,2.6008302224,-4.018857
1901,-2.8959311349\H,0.1263217371,-4.0316485363,-3.0142641982\H,-1.213
2030195,-2.2323443234,-1.9149116319\N,0.0162585464,-0.1558708491,-0.52
74961321\C,2.3618567264,-0.0110211729,-0.3405538758\C,1.0563129775,0.7
458883461,0.051006093\O,-1.2639561649,0.0930232837,-0.4715199086\C,0.9
110774259,2.1358988763,-0.5857051624\C,0.9603888504,0.7724103065,1.583
2082705\N,3.4919433533,0.4685386921,0.0097207318\C,4.7132125141,-0.201
382373,-0.189039559\C,5.6321623907,0.277450243,-1.1363115546\C,6.87570
49438,-0.3364363142,-1.2807772549\C,7.2335759562,-1.4163578751,-0.4705
724565\C,6.3317242846,-1.8774039417,0.4913203221\C,5.0809940747,-1.278
6114562,0.6355377746\C,1.6212082659,1.7783730488,2.3006999626\C,1.6100
582589,1.7765723508,3.6947793972\C,0.941667795,0.7694036006,4.39373257
84\C,0.2893155537,-0.2393019084,3.6854482294\C,0.3005235499,-0.2407307
999,2.2884888589\H,5.3600619834,1.1292686196,-1.7528333749\H,7.5716277
93,0.0383412997,-2.0271079803\H,8.2069787759,-1.8859597331,-0.58029060
59\H,6.6020016827,-2.7093556,1.1369126269\H,4.3813893352,-1.6284074193
,1.3891839741\H,2.1500990803,2.5584451219,1.7644405203\H,2.1266898554,
2.5653838092,4.2351044256\H,0.9309318208,0.7712863513,5.4804635335\H,-
0.2309050342,-1.0326654641,4.2161316124\H,-0.2132859349,-1.0337899678,
1.7556765517\C,1.7844150632,2.6065106585,-1.5731876607\C,1.5852554724,
3.8582672226,-2.1600741562\C,0.5083512254,4.6543974349,-1.7721749931\C
,-0.3738373346,4.1868085526,-0.7955543462\C,-0.1759035186,2.9380357174
,-0.2083185852\H,2.6343186754,2.008403052,-1.8789857795\H,2.279467147,
4.2090801472,-2.9193059809\H,0.359030656,5.6315492232,-2.2245732879\H,
-1.2217586282,4.7885112696,-0.4805349779\H,-0.8794565869,2.5877370718,
0.5375591317\C,-3.7685702374,-1.1937400234,2.9243968548\C,-4.023023851
,-1.3494427067,1.4092854557\C,-3.4972260759,-0.047081509,0.7235179483\
C,-3.8910718402,0.4213567534,-0.5631285699\H,-4.0335228937,-2.10863472
11,3.4645928292\H,-4.3884092087,-0.3780077209,3.3125822371\H,-2.723260
8497,-0.9596918007,3.1390261378\C,-5.5361700452,-1.5410704704,1.175798
8706\H,-2.2908707787,-0.1862710335,0.5133726007\H,-3.4724111064,0.7812
396381,1.4377946926\C,-4.3007245341,-0.4333392704,-1.7206006061\C,-3.8
06893792,1.8875693974,-0.7577480665\C,-3.2858441875,-2.5837315019,0.85
95112449\O,-3.6252628457,-3.2231969464,-0.1166956545\O,-2.1955780724,-
2.9035243437,1.5885852656\C,-1.476514549,-4.0762744387,1.1602230344\O,
-3.5276634853,2.7022908239,0.1106834738\O,-4.113574186,2.2446514723,-2
.0295511469\C,-4.0441377007,3.6488698353,-2.3093778553\H,-0.70058828,-
4.2284399734,1.9108753383\H,-1.0303471022,-3.9133831824,0.1769024739\H
,-2.148119265,-4.9370446319,1.1168864309\H,-4.4024339319,3.7608139415,
-3.3335652088\H,-3.0125325624,4.0012055357,-2.2249301796\H,-4.67357198
55,4.2133883831,-1.6160388959\H,-6.0733774754,-0.6377463922,1.48307798
92\H,-5.9104045364,-2.3800055384,1.7739797072\H,-5.7670930339,-1.74989
56361,0.1306465194\H,-3.7423729038,-0.1541229466,-2.6196211353\H,-5.36
08188327,-0.2631186941,-1.9626537163\H,-4.1603220472,-1.4944772905,-1.
5163414381\\Version=EM64L-G09RevB.01\State=1-A\HF=-1879.0147137\RMSD=3
.826e-09\RMSF=3.181e-06\Dipole=-0.2530795,-0.7536932,-0.213522\Quadrup
ole=-3.2172739,2.6045383,0.6127357,-5.7122044,-3.664952,-8.0314415\PG=
C01 [X(C36H36N2O5)]\\@

Iminopyrrol-NOH (c)

1\1\GINC-X57\FOpt\RB3LYP\Gen\C4H6N2O1\GXG501\18-Jun-2012\0\\#B3LYP/gen
 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\\
dpaioh_core.freq\\0,1\N,-3.3888814689,2.6286149419,-0.3427269507\C,-4.
524448427,1.8300455428,-0.4981973189\C,-4.2408111686,0.5104458156,-0.5
482611541\C,-2.7842549952,0.3487801461,-0.5489179417\C,-2.2218596452,1
.7681191242,-0.6397852268\O,-3.4424380068,3.7954433677,-1.1722901944\H
,-3.2343590613,4.5118373234,-0.5499209391\H,-5.4884586464,2.3245584363
,-0.5135261921\H,-4.9596283645,-0.2994766542,-0.5340178809\N,-2.024524
6801,-0.6777776067,-0.4735089292\H,-2.5912065144,-1.5296062939,-0.3979
956533\H,-1.875934976,1.9866738754,-1.6566764554\H,-1.4029920459,1.938
2369812,0.0632858367\\Version=EM64L-G09RevB.01\State=1-A\HF=-340.66254
01\RMSD=4.898e-09\RMSF=3.176e-05\Dipole=-0.7606475,0.6845247,0.2491979

\Quadrupole=-0.8281226,3.1549871,-2.3268646,4.6877623,-0.491052,1.7700
271\PG=C01 [X(C4H6N2O1)]\\@

DPAIOH

1\1\GINC-X114\FOpt\RB3LYP\Gen\C26H20N2O1\GXG501\20-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\dpaioh.freq\\0,1\C,-3.3727921718,2.6157374094,-0.4868791672\C,-4.54
13751878,1.877561812,-0.6655272257\C,-4.508826478,0.4748697352,-0.6257
385652\C,-3.3183828564,-0.2210275382,-0.4220828303\C,-2.1524021999,0.5
276973257,-0.2573822199\C,-2.167653629,1.9352483601,-0.2689074342\H,-3
.3987326955,3.6988951467,-0.4980663411\H,-5.4842843605,2.3911855118,-0
.8271275278\H,-5.4321854523,-0.0840523361,-0.7543256701\H,-3.288086749
9,-1.3035255007,-0.3771775964\N,-0.8515328335,0.0454250388,-0.12650430
86\C,-0.8084654737,2.3984799669,0.049910297\C,0.0297370328,1.134744918
1,0.4225213181\O,-0.7712346277,-1.2058432471,0.5318092843\C,0.18097490
61,0.9886818458,1.9474176329\C,1.3762348599,1.1455936515,-0.3079454683
\N,-0.2677115103,3.551627508,0.1075415148\C,-0.9191868279,4.7339421569
,-0.2877407092\C,-1.2243358982,5.7105336801,0.6740063621\C,-1.80340946
,6.9186210253,0.2884317397\C,-2.0608209247,7.1848318614,-1.0585171622\
C,-1.7319215556,6.2265637301,-2.0200342948\C,-1.1663309643,5.009103421
6,-1.6435380093\C,2.4212431441,1.9537802223,0.164208123\C,3.6388239157
,2.0058540236,-0.5115461699\C,3.8367356959,1.2512504326,-1.670407647\C
,2.8011072239,0.4522408898,-2.1518970244\C,1.5780506694,0.4047556927,-
1.4779328655\H,-1.0037583071,5.5068710317,1.7178423169\H,-2.045922623,
7.6597924737,1.0458499618\H,-2.5023915275,8.1317320437,-1.3560893494\H
,-1.9158640656,6.4259988888,-3.0728155097\H,-0.9023062378,4.2657949011
,-2.3902032515\H,2.2745743396,2.5464660055,1.0600192656\H,4.4358880592
,2.6389075816,-0.1305683412\H,4.7888080188,1.2894485124,-2.1931913684\
H,2.9383995383,-0.1345662303,-3.0566490876\H,0.7662961357,-0.198302114
8,-1.8722953522\C,-0.6377675311,1.6860149159,2.8448835664\C,-0.5166352
562,1.4914444795,4.2224590978\C,0.4241522066,0.5952821716,4.7269198192
\C,1.2436550035,-0.107875354,3.8419716984\C,1.1213301902,0.0872001255,
2.4678765539\H,-1.372960491,2.3936394663,2.4785949313\H,-1.1593109457,
2.0481721138,4.899387913\H,0.5211382166,0.4474190563,5.7992416712\H,1.
9816294303,-0.8100918672,4.2209612338\H,1.7679265151,-0.4610850289,1.7
908449525\H,-0.2260742603,-1.7376099164,-0.0728087565\\Version=EM64L-G
09RevB.01\State=1-A\HF=-1187.4642378\RMSD=6.977e-09\RMSF=8.360e-06\Dip
ole=-0.2743481,-0.6257116,-0.1944659\Quadrupole=0.5355404,0.3063127,-0
.8418531,-4.7646316,0.9700993,3.8025235\PG=C01 [X(C26H20N2O1)]\\@

Iminopyrrol-NOC(Me)(Et)COOMe (c)

1\1\GINC-X129\FOpt\RB3LYP\6-31G(d)\C10H16N2O3\GXG501\09-Aug-2012\0\\#B
3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk
=1342177280\\md_core.freq\\0,1\N,2.7029736556,2.885301281,-0.042403186
7\C,1.8565412891,3.9667135745,0.2382918848\C,0.5487662963,3.6712518525
,0.0889350507\C,0.4390493793,2.314861962,-0.4562461633\C,1.8721632383,
1.8750327509,-0.7453838744\O,3.8296754801,3.2972078308,-0.8318512324\H
,2.3107179183,4.8876373139,0.583549099\H,-0.2853567284,4.3031522059,0.
3690322488\N,-0.5650364749,1.5514164508,-0.67249311\H,-1.4316289242,2.
0251172916,-0.3938010375\H,2.0933888937,1.92799802,-1.8165172471\H,2.0
885349771,0.8657512828,-0.3952182361\C,5.0796530005,2.9981561144,-0.17
9578235\C,5.2465312258,3.8499955066,1.0803542593\C,6.1122025666,3.3375
530037,-1.2802302074\C,5.1436270114,1.4815498824,0.0932298941\H,4.4528
236178,3.6294617184,1.7990125927\H,5.1946308429,4.9094094564,0.8061316
405\H,6.2034609525,3.6596457893,1.5699976081\O,4.6797385946,0.63814122
71,-0.6416636005\O,5.8337006903,1.1913785778,1.2155269578\H,5.94036009
22,4.3834560999,-1.5620938207\H,5.8597869572,2.7266286613,-2.153742531
2\C,7.5813603552,3.1314064466,-0.8980022187\H,8.2232170282,3.372183067
4,-1.7519094034\H,7.8838929486,3.7757517348,-0.0659326788\H,7.78932608
55,2.0951124474,-0.6105164955\C,5.9790176537,-0.2118401051,1.502145869
1\H,6.563464627,-0.2624587944,2.4209479041\H,4.9988235517,-0.674366940
7,1.6418973256\H,6.497950198,-0.7181247098,0.6842529443\\Version=EM64L

-G09RevB.01\State=1-A\HF=-725.7911219\RMSD=9.387e-09\RMSF=5.650e-06\Di
pole=1.1596708,0.8596128,0.9334469\Quadrupole=0.2297732,1.3702475,-1.6
000207,-8.3623414,-2.3981737,-3.325054\PG=C01 [X(C10H16N2O3)]\\@

DPAIOP

1\1\GINC-X82\FOpt\RB3LYP\6-31G(d)\C36H36N2O5\GXG501\11-Aug-2012\0\\#B3
LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
1342177280\\md.freq\\0,1\C,2.5334791766,1.3017189586,0.0959905602\C,2.
9904565066,2.563428391,-0.2799805342\C,2.1106858728,3.4856044408,-0.86
2959184\C,0.7751570243,3.1661236161,-1.109148256\C,0.3328052039,1.8886
446236,-0.7633712456\C,1.1923721886,0.9709919799,-0.1322978681\H,3.197
8844726,0.5961167775,0.5804634928\H,4.0255147923,2.8393099898,-0.10225
60343\H,2.4716809783,4.4769483667,-1.12469742\H,0.0955153828,3.8962912
839,-1.5290946302\N,-0.932318395,1.3170169861,-0.9933455218\C,0.384522
0543,-0.1876633733,0.2703076973\C,-1.1091038878,0.185534086,0.01379331
94\O,-1.9655667393,2.2907554423,-1.0007283866\C,-1.7687827418,0.701668
0732,1.3076244636\C,-1.8019071905,-1.0218749334,-0.6225734844\N,0.6702
844196,-1.3149144895,0.7919672533\C,1.9871929551,-1.7667966766,0.98620
22397\C,2.4621591673,-1.9714211719,2.2920212093\C,3.740065436,-2.48740
79061,2.5015251251\C,4.551929496,-2.8354217776,1.4192048076\C,4.070548
0403,-2.6612905859,0.1196333499\C,2.8003470222,-2.1306642155,-0.100992
987\C,-2.5429077641,-1.9254232366,0.1479964872\C,-3.0561551872,-3.0930
181379,-0.4188662178\C,-2.8225466999,-3.3873682279,-1.7620375029\C,-2.
0689538652,-2.5012252144,-2.5348645345\C,-1.5640452776,-1.3304796171,-
1.9691506698\H,1.8186548044,-1.720126896,3.1301192586\H,4.098633413,-2
.6278038553,3.5181720295\H,5.5428619451,-3.2479212364,1.5867568352\H,4
.6869922759,-2.9403260859,-0.7313492888\H,2.4205525073,-2.0028818283,-
1.1105306001\H,-2.7149403539,-1.7217654887,1.1984383563\H,-3.632033964
3,-3.7779384322,0.1978793387\H,-3.2153061629,-4.3011524657,-2.20049884
02\H,-1.8673437516,-2.7224133767,-3.5801312619\H,-0.9710728197,-0.6520
238452,-2.5733290874\C,-1.019953352,0.9657960557,2.4632498795\C,-1.628
1672962,1.4714208367,3.6143036753\C,-2.998914486,1.7200146704,3.633664
151\C,-3.7553376979,1.4596355437,2.4897395758\C,-3.1492097464,0.958333
3913,1.3387075668\H,0.0457384637,0.7710938938,2.4842720267\H,-1.023487
411,1.6641727343,4.4967144798\H,-3.4740683333,2.1092135449,4.530542641
6\H,-4.8260146188,1.6476585238,2.4880516397\H,-3.7535007363,0.77442992
72,0.4591766076\C,-2.6572546357,2.467694894,-2.2814230209\C,-1.6877333
252,2.579887968,-3.4543983408\C,-3.4236512502,3.7815993889,-1.96210628
46\C,-3.6835562735,1.3200485336,-2.4464768222\O,-4.5185844657,1.041825
0785,-1.6120909341\O,-3.5938748967,0.6998935501,-3.6353894835\H,-1.045
8928891,3.4542011895,-3.3292017212\H,-2.231673141,2.6811971193,-4.3955
035893\H,-1.0608366335,1.6890593915,-3.5243843915\H,-4.0928870891,3.54
90558656,-1.1275696927\C,-4.2609363966,4.5101214631,-3.0517513579\H,-2
.6720440205,4.4794886056,-1.5831446039\C,-4.5810858,-0.3227235583,-3.8
754324801\C,-5.342620422,3.6236643826,-3.6909216788\C,-3.3785543827,5.
0912371663,-4.1649418145\C,-4.949128696,5.71178461,-2.350963393\H,-4.3
765311459,-0.6889197526,-4.8816344537\H,-5.5853449906,0.1044504577,-3.
8163504825\H,-4.477760529,-1.1244560442,-3.1426256962\H,-4.9109172154,
2.8270287459,-4.3010391436\H,-5.9820753554,4.2195892979,-4.3485200561\
H,-5.9651852021,3.1732015791,-2.9114402087\H,-5.6498297721,5.345097319
4,-1.5929090467\H,-5.5160550027,6.3093955626,-3.0737643649\H,-4.218869
5155,6.3630529092,-1.8626952489\O,-3.5508715279,4.9309705765,-5.354529
4212\O,-2.381230327,5.8646531855,-3.66964627\C,-1.544219081,6.49430248
85,-4.6538802881\H,-0.8238846439,7.0871433266,-4.0891958799\H,-2.13892
99949,7.1341520588,-5.3108215701\H,-1.0326234991,5.7424765776,-5.26087
27726\\Version=EM64L-G09RevB.01\State=1-A\HF=-1879.0785172\RMSD=3.094e
-09\RMSF=2.941e-06\Dipole=0.2969449,0.9333881,-0.556366\Quadrupole=2.8
051402,2.2830981,-5.0882383,5.7035022,-0.6449941,3.8427223\PG=C01 [X(C
36H36N2O5)]\\@

Iminopyrrol-NH→O (c)

1\1\GINC-X134\FOpt\RB3LYP\Gen\C4H6N2O1\GXG501\14-Jun-2012\0\\#B3LYP/ge

n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\
\dpaio_xcore.freq\\0,1\N,-3.3271394972,2.5437869315,-0.3408914263\C,-4
.5121706004,1.665103941,-0.350351194\C,-4.2110337152,0.3839366582,-0.5
756253964\C,-2.7512736324,0.2094746097,-0.6606379443\C,-2.1486176477,1
.6044482575,-0.6225598301\N,-2.0294151495,-0.8375030645,-0.7532635331\
H,-2.6161689428,-1.6789759371,-0.769066315\H,-4.9256309625,-0.42168984
22,-0.7024371227\H,-5.4564439854,2.1824890404,-0.2578436895\O,-3.51282
4226,3.5170107158,-1.2632224001\H,-3.1976753808,2.9325898288,0.6136154
437\H,-1.7828790305,1.9272175005,-1.5971631839\H,-1.3701182296,1.71523
03604,0.1353105917\\Version=EM64L-G09RevB.01\State=1-A\HF=-340.6167594
\RMSD=5.648e-09\RMSF=7.276e-05\Dipole=-0.6012067,-0.9392379,1.1921713\
Quadrupole=2.187847,-3.8228333,1.6349863,5.0574866,-0.5011832,4.64407\
PG=C01 [X(C4H6N2O1)]\\@

DPAIH→O

1\1\GINC-X123\FOpt\RB3LYP\Gen\C26H20N2O1\GXG501\14-Jun-2012\0\\#B3LYP/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\\dpaio_x.freq\\0,1\C,-3.3290038167,2.5700463858,-0.3168559803\C,-4.4
74764471,1.7982721119,-0.5131349285\C,-4.4009064651,0.4032750767,-0.63
99015876\C,-3.1704169787,-0.2542843318,-0.5725529003\C,-2.0532141155,0
.5381048319,-0.3906476171\C,-2.0862363883,1.9213980525,-0.2565645031\H
,-3.40398851,3.6436196018,-0.1967782654\H,-5.4435605887,2.287732442,-0
.5548767507\H,-5.3113436912,-0.171937187,-0.7828486534\H,-3.0599000482
,-1.3311921181,-0.6314558982\N,-0.6779980308,-0.0013729662,-0.32476456
89\C,-0.7155060973,2.4182563573,0.0109743484\C,0.1719792803,1.19551447
31,0.3407290504\O,-0.5706704317,-1.2369409571,0.1757954385\C,0.2197746
927,1.071456776,1.8671427683\C,1.5486502565,1.1073315522,-0.3052855505
\N,-0.244142817,3.6004793164,0.0760197583\C,-0.9955481075,4.7587334907
,-0.2083250831\C,-1.3134044572,5.6418423262,0.835373071\C,-1.992959407
9,6.8282579004,0.5637906232\C,-2.3380576489,7.1655623728,-0.7475032244
\C,-1.9973553431,6.3008553164,-1.7894925434\C,-1.3316659975,5.10359019
01,-1.5273664089\C,2.293261871,-0.0604403029,-0.0549680278\C,3.5331214
828,-0.2497932654,-0.6608316146\C,4.0557313537,0.7230870825,-1.5163414
584\C,3.3227674815,1.8814862832,-1.7693545947\C,2.0728644199,2.0728172
675,-1.1743930351\H,-1.0272265706,5.3811430727,1.8499042304\H,-2.24572
3379,7.4971013957,1.3824169795\H,-2.8578368086,8.0964123332,-0.9554068
768\H,-2.250836247,6.5565576574,-2.8151341475\H,-1.0636421315,4.431834
2739,-2.3381218419\H,1.8722944955,-0.8231952019,0.5907352648\H,4.09322
27086,-1.1594023252,-0.461139931\H,5.0278218927,0.5785532035,-1.980595
8633\H,3.7206948393,2.6461405594,-2.4313547226\H,1.5235723028,2.985779
0881,-1.3658443991\C,-0.6360209153,0.2516406744,2.6148043585\C,-0.5751
525458,0.2668919809,4.0104660415\C,0.3247361768,1.0976555048,4.6761270
78\C,1.1769250029,1.9187100441,3.9349310515\C,1.1250035988,1.905300624
6,2.5427539434\H,-1.300252407,-0.4326934858,2.1048343661\H,-1.23676160
92,-0.384156384,4.5760420158\H,0.3664241456,1.1033069607,5.7622946914\
H,1.8862257974,2.5701362525,4.4387391509\H,1.7848446051,2.5517900517,1
.9731798376\H,-0.3127333776,0.0174246405,-1.2962080905\\Version=EM64L-
G09RevB.01\State=1-A\HF=-1187.4273711\RMSD=2.948e-09\RMSF=3.823e-06\Di
pole=-0.9696294,0.9736855,-0.6848715\Quadrupole=7.4092658,-9.5886656,2
.1793997,-0.9743659,0.6161388,1.2778064\PG=C01 [X(C26H20N2O1)]\\@

TS5 (c)

1\1\GINC-X104\Freq\UB3LYP\6-31G(d)\C10H17N2O3(2)\GXG501\12-Aug-2012\0\
\#B3LYP/6-31G(d) 6D SCF=Tight guess=read geom=check INT(Grid=Ultrafine
) Freq=noraman maxdisk=1342177280\\ts4_mdcore.freq\\0,2\N,-0.114769762
4,-0.2732195304,0.2218837244\C,-1.1916708052,0.5235541954,-0.065540986
5\C,-2.3664487476,-0.0716045062,0.2780477287\C,-2.0792586784,-1.410272
2726,0.7935117793\C,-0.5623366969,-1.5971581155,0.670879072\O,1.078142
8027,-0.1041536873,-0.3866223402\H,-1.0102494386,1.4960242856,-0.50661
74504\H,-3.3492859031,0.3749077426,0.2035777144\N,-2.8277778095,-2.330
0522385,1.2789986654\H,-3.8049134545,-2.0176597872,1.2865276836\H,-0.3
047331546,-2.3445934514,-0.088472239\H,-0.0895941991,-1.8678890023,1.6

185270539\H,1.806433628,0.220589936,0.3752802562\C,2.8129139769,0.6694
173065,1.4280546719\C,3.923244588,1.2556720363,0.5892029493\C,2.995636
5699,-0.6639840885,2.0364604736\C,1.9307329587,1.6158194511,2.21408329
35\H,3.5638391357,2.1259290456,0.0284626269\H,4.7625009902,1.594775279
5,1.2163268547\H,4.3280479589,0.5252203283,-0.115652712\O,2.244318634,
-1.1578707859,2.8674120733\O,4.0679079253,-1.3313060323,1.5368377118\C
,4.2484829019,-2.6623385826,2.0400135685\H,3.3844796213,-3.2877663307,
1.7977259594\H,5.1449928568,-3.041867154,1.5482690515\H,4.3806395841,-
2.6512260069,3.1253139648\H,1.0371076865,1.0792068901,2.5500435615\H,1
.603076339,2.4292113849,1.5534011771\C,2.6320833288,2.2181314718,3.450
2284542\H,2.9358042215,1.4259638205,4.1421224548\H,3.5218473,2.7919919
934,3.1680316631\H,1.9519986418,2.8915444048,3.9839435404\\Version=EM6
4L-G09RevB.01\State=2-A\HF=-726.3374581\S2=0.757972\S2-1=0.\S2A=0.7500
53\RMSD=6.554e-09\RMSF=1.236e-04\ZeroPoint=0.2618504\Thermal=0.2792729
\Dipole=0.4580737,1.0319436,-0.4894932\PG=C01 [X(C10H17N2O3)]\NImag=1\
\@

TS5

1\1\GINC-X111\FTS\UB3LYP\6-31G(d)\C36H37N2O5(2)\GXG501\04-Aug-2012\0\\
#B3LYP/6-31G(d) 6D SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=1342177280\\ts4_md.a3.freq\\0,2\
N,0.3056201245,0.4104960711,-0.73695269\C,1.3397404711,0.7620893438,0.
2920527313\C,0.8636542478,-0.2496719192,-1.8174416798\O,-0.7618236488,
1.2068830522,-0.9272634819\H,-1.7168406827,0.7596278558,-0.5180503968\
C,-3.1882045852,0.5377894912,-0.3356236055\C,-3.2620910589,0.297038441
1,1.1248155982\C,-3.5997311539,1.8973905385,-0.8612872299\C,-3.4308423
571,-0.6811122266,-1.2048666145\C,-4.9133626119,-1.0057696879,-1.60836
93829\C,-5.4567044816,0.0295837258,-2.6003445179\O,-4.6422908531,0.177
9100329,-3.675671794\C,-5.1052553321,1.1003224689,-4.6751203908\C,2.19
68347667,-0.6173878971,-1.5430443002\C,2.928512049,-1.3251979983,-2.50
45124854\C,2.3209978278,-1.6433911629,-3.7183910854\C,0.9979017163,-1.
2509657298,-3.9777744223\C,0.2503321188,-0.5467567856,-3.0374293832\C,
2.5649300842,-0.0487434414,-0.2372482542\N,3.6326812781,-0.0843309593,
0.4588022169\C,4.7524380876,-0.8698245908,0.1308256989\C,5.9566901596,
-0.2460553345,-0.2324022838\C,7.0940525816,-1.011092707,-0.4865748507\
C,7.0588428087,-2.4013030309,-0.3552450807\C,5.8698202241,-3.021716420
1,0.0350456416\C,4.7224878288,-2.2673560867,0.2768368073\C,1.563607071
4,2.2818287498,0.2746202401\C,2.6344298094,2.8699613023,-0.4079005746\
C,2.7728068614,4.2591211291,-0.4526668181\C,1.8402964601,5.0794196614,
0.1799306227\C,0.7643143437,4.5015228315,0.8570971537\C,0.626835569,3.
1158295027,0.9039430915\C,0.9604810497,0.2290020488,1.6779322614\C,1.6
709534549,0.6679950148,2.8055297595\C,1.3918836993,0.1415094655,4.0647
501801\C,0.3980216478,-0.8290973124,4.2200962616\C,-0.3095727406,-1.27
20945376,3.103537186\C,-0.0221523254,-0.7509987193,1.8387835364\O,-3.3
083820265,-0.806186273,1.650969062\O,-3.2360241978,1.4471109101,1.8455
471229\C,-3.283011858,1.281883743,3.2717332516\C,-4.9064208292,-2.3765
569699,-2.3291198868\C,-5.8473080896,-1.069479135,-0.3913584496\O,-6.5
010693478,0.6356824541,-2.4867346693\H,3.9556885147,-1.6107015827,-2.3
130897282\H,2.8783316626,-2.1914989277,-4.4718422729\H,0.5459267888,-1
.497726896,-4.9348400654\H,-0.7642562255,-0.2234326793,-3.2382365876\H
,5.9858808604,0.8367080597,-0.3126003248\H,8.0158479393,-0.5151272411,
-0.7798329394\H,7.9501755509,-2.9929266379,-0.5437910056\H,5.832357580
7,-4.1016722214,0.1538561298\H,3.7991999296,-2.7462932522,0.5897343952
\H,2.4475651481,1.4158343542,2.6914743987\H,1.9526669179,0.4913746506,
4.927532812\H,0.1787039957,-1.234828355,5.2043450426\H,-1.0971145948,-
2.0126687177,3.2039428008\H,-0.5766300725,-1.1115047364,0.9795063506\H
,3.3749397309,2.2498265246,-0.8999309607\H,3.615268046,4.6960837143,-0
.9822808619\H,1.9501100567,6.1601835165,0.1475019715\H,0.0287194511,5.
1306141582,1.3513718434\H,-0.2163740708,2.6768008507,1.4267431101\H,-5
.9096864917,-2.6344803219,-2.6876886266\H,-4.587173955,-3.1584757341,-
1.6312987444\H,-4.2257983999,-2.3759658968,-3.1856093497\H,-2.86184089
89,-0.5776025155,-2.134513432\H,-3.0504905926,-1.5601564474,-0.6756665

693\H,-4.347698803,1.0871972136,-5.4595678744\H,-5.2053263347,2.104571
404,-4.2547099791\H,-6.0743219233,0.7845120016,-5.0702969666\H,-3.3044
531543,2.2931819032,3.6800104233\H,-2.4006382851,0.7427858809,3.625206
4333\H,-4.1810366574,0.7312840645,3.564766682\H,-5.4583416218,-1.78151
08542,0.3414532648\H,-6.8514609669,-1.3793568867,-0.6958313616\H,-5.94
43015528,-0.0959128317,0.0972937648\H,-3.2706421007,2.0186939368,-1.89
86437092\H,-3.1677367204,2.7022939532,-0.2630945915\H,-4.6920829123,2.
02169964,-0.8434575675\\Version=EM64L-G09RevB.01\State=2-A\HF=-1879.63
61899\S2=0.757858\S2-1=0.\S2A=0.750048\RMSD=8.153e-09\RMSF=1.280e-06\D
ipole=0.5028327,0.0355351,-0.8805947\Quadrupole=-12.8206661,2.4705649,
10.3501012,-0.1930626,-3.5809726,4.8835546\PG=C01 [X(C36H37N2O5)]\\@