

Revising the Mechanism of Polymer Autooxidation

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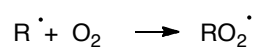
Electronic Supporting Information

Additional references

- A1** L. Reich, S. Stivala, *Autooxidation of Hydrocarbons and Polyolefins*, Marcel Dekker, New York, 1969, pp. 32,38,70,430-431; A. Davis, D. Sims, *Weathering of Polymers*, Applied Science Publishers LTD, London, 1983, p. 111; P. P. Klemchuk, *Polymer Stabilization and Degradation*, ACS Symposium Series, American Chemical Society: Washington, DC, 1985, pp. 37, 72, 218, 245, 249, 367; J. Pospisil, P. P. Klemchuk, *Oxidation Inhibition in Organic Materials*, CRC Press, Boca Raton, 1990, vol. 2, p. 220; N. S. Allen, M. Edge, *Fundamentals of Polymer Degradation and Stabilisation*, Elsevier, London, 1992, pp. 13-19; J. F. Rabek, *Polymer Photodegradation*, Chapman and Hall, London, 1995, pp. 24-26, 30-31; Yu. A. Shlyapnikov, S. G. Kiryushkin, A. P. Mar'in, *Antioxidative Stabilization of Polymers*, Taylor & Francis, London, 1996, pp. 46-48; C. Maier, T. Calafut, *Polypropylene: The Definitive User's Guide and Databook*, Plastics Design Library, New-York, 1998, p. 6; G. A. George, M. Celina, in *Handbook of Polymer Degradation*, ed. Hamid, S. H., Marcel Dekker, New York, 2nd edn., 2000, pp. 277-313.
- A2** P. I. Levin, V. V. Mikhailov *Russ. Chem. Rev.*, 1970, **39** (9), 799; H. Naarmann, *Pure Appl. Chem.*, 1973, **36**, 253; Yu. A. Shlyapnikov, I. A. Serenkova, *Polym. Degrad. Stab.*, 1992, **35**, 67; X. Colin, B. Fayolle, L. Audouin, J. Verdu, *Int. J. Chem. Kinet.*, 2006, **38**, 666; M. M. Silaev, *Theor. Found. Chem. Eng.*, 2007, **41**, 831.
- A3** M. B. Neiman, *Russ. Chem. Rev.*, 1964, **33**, 13; C. E. H. Bawn, S. A. Chaundhri, *Polymer*, 1968, **9**, 123; Ye. T. Denisov, A. I. Vol'pert, V. P. Filipenko, *Polym. Sci. U.S.S.R.*, 1986, **28**, 2314; S. Verdu, J. Verdu, *Macromolecules*, 1997, **30**, 2262; L. Matisova-Rychla, J. Rychly, *Polym. Degrad. Stab.*, 2000, **67**, 515; J. L. Philippart, J. L. Gardette, *Polym. Degrad. Stab.*, 2001, **71**, 189; J. Rychly, L. Matisova-Rychla, P. Tiemblo, J. Gomez-Elvira, *Polym. Degrad. Stab.*, 2001, **71**, 253; J. L. Philippart, J. L. Gardette, *Polym. Degrad. Stab.*, 2001, **73**, 185; L. M. Rincon-Rubio, B. Fayolle, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2001, **74**, 177; P. Gijsmana, F. Verdun, *Polym. Degrad. Stab.*, 2001, **74**, 533; I. I. Eyenga, W. W. Focke, L. C. Prinsloo, A. T. Tolmay, *Macromol. Symp.*, 2002, **178**, 139; P. Eriksson, T. Reitberger, B. Stenberg, *Polym. Degrad. Stab.*, 2002, **78**, 183; S. M. Lomakin, E. V. Koverzanova, S. V. Usachev, N. G. Shilkina, G. E. Zaikov, *J. Appl. Polym. Sci.*, 2002, **86**, 3300; S. de Goede, R. Brull, H. Pasch, N. Marshall, *Macromol. Symp.*, 2003, **193**, 35; L. Matisova-Rychla, J. Rychly, P. Tiemblo, J. M. Gomez-Elvira, M. Elvira, *Macromol. Symp.*, 2004, **214**, 261; I. Yakimets, D. Lai, M. Guigon, *Polym. Degrad. Stab.*, 2004, **86**, 59; A. Astruc, P. Bartolomeo, B. Fayolle, L. Audouin, J. Verdu, *Polym. Test.*, 2004, **23**, 919; E. Richaud, F. Farcas, P. Bartolomeo, B. Fayolle, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2006, **91**, 398; I. Blakey, B. Goss, G. George, *Aust. J. Chem.*, 2006, **59**, 485; A. A. Calhoun, P. D. Nicholson, A. B. Barnes, *Polym. Degrad. Stab.*, 2006, **91**, 1964; S. M. Thornberg, R. Bernstein, A. N. Irwin, D. K. Derzon, S. B. Klamo, R. L. Clough, *Polym. Degrad. Stab.*, 2007, **92**, 94; E. Richaud, F. Farcas, B. Fayolle, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2007, **92**, 118; X. Y. Wang, R. H. Gong, *J. Appl. Polym. Sci.*, 2007, **104**, 391; D. M. Mowery, R. A. Assink, D. K. Derzon, S. B. Klamo, R. Bernstein, R. L. Clough, *Radiat. Phys. Chem.*, 2007, **76**, 864; H. Nakatani, N. Manabe, Y. Yokota, H. Minami, S. Suzuki, F. Yamaguchi, M. Terano, *Polym. Int.*, 2007, **56**, 1152; C. Stroud, M. C. Branch, *Combust. Sci. Technol.*, 2007, **179**, 2091; R. Bernstein, S. M. Thornberg, R. A. Assink, D. M. Mowery, M. K. Alam, A. N. Irwin, J. M. Hochrein, D. K. Derzon, S. B. Klamo, R. L. Clough, *Nucl. Instrum. Methods Phys. Res., Sect. B*, 2007, **265**, 8; E. Richaud, F. Farcas, L. Divet, J. P. Benneton, *Geotext. Geomembr.*, 2008, **26**, 71; R. Bernstein, S. M. Thornberg, A. N. Irwin, J. M. Hochrein, D. K. Derzon, S. B. Klamo, R. L. Clough, *Polym. Degrad. Stab.*, 2008, **93**, 854; M. Malikova, J. Rychly, L. Matisova-Rychla, *Polym. Degrad. Stab.*, 2008, **93**, 2113; S. Sarrabi, X. Colin, A. Tcharkhtchi, *J. Appl. Polym. Sci.*, 2008, **110**, 2030; S. S. Fernando, P. A. Christensen, T. A. Egerton, J. R. White, *Polym. Degrad. Stab.*, 2009, **94**, 83; M. Gryta, J. Grzechulska-Damszel, A. Markowska, K. Karakulski, *J. Membr. Sci.*, 2009, **326**, 493; K. Rajakumar, V. Sarasvathy, A. Thamarai Chelvan, R. Chitra, C. T. Vijayakumar, *J. Polym. Environ.*, 2009, **17**, 191; E. Stromberg, S. Karlsson, *J. Appl. Polym. Sci.*, 2009, **112**, 1835.
- A4** N. T. Notley, *Trans. Farad. Soc.*, 1962, **58**, 66; T. Kelen, M. Iring, F. Tudos, *Eur. Polym. J.*, 1976, **12**, 35; M. Iring, T. Kelen, F. Tudos, *Polym. Degrad. Stab.*, 1979, **1**, 297; Xiao, C. Zhang, Y. An, S. Jia, G. J. *J. Appl. Polym. Sci.* 2000, **77**, 2877-2881; F. Gugumus, *Polym. Degrad. Stab.*, 2002, **76**,

- 329; X. Colin, B. Fayolle, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2003, **80**, 67; X. Colin, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2004, **86**, 309; N. Khelidj, X. Colin, L. Audouin, J. Verdu, C. Monchy-Leroy, V. Prunier, *Polym. Degrad. Stab.*, 2006, **91**, 1593; N. Khelidj, X. Colin, L. Audouin, J. Verdu, C. Monchy-Leroy, V. Prunier, *Polym. Degrad. Stab.*, 2006, **91**, 1598; E. Richaud, X. Colin, B. Fayolle, L. Audouin, J. Verdu, *Inter. J. Chem. Kinet.*, 2008, **40**, 769; E. Richaud, X. Colin, C. Monchy-Leroy, L. Audouin, J. Verdu, *Polym. Degrad. Stab.*, 2009, **94**, 410; W. W. Focke, I. van der Westhuizen, *J. Therm. Anal. Calorim.*, 2010, **99**, 285.
- A5** M. Iring, F. Tudos, *Prog. Polym. Sci.*, 1990, **15**, 217; T. J. Zaharescu, *Mater. Sci. Lett.*, 1995, **14**, 923; X. Colin, E. Richaud, J. Verdu, C. Monchy-Leroy, *Radiat. Phys. Chem.*, 2010, **79**, 365.
- A6** T. A. Skowronski, J. F. Rabek, B. Ranby, *Polym. Photochem.*, 1983, **3**, 341; J. R. White, A. Turnbull, *J. Mater. Sci.*, 1994, **29**, 584; H. Kaczmarek, *Eur. Polym. J.*, 1995, **31**, 1175; N. S. Allen, M. Edge, M. Rodriguez, C. M. Liauw, E. Fontan, *Polym. Degrad. Stab.*, 2001, **71**, 1.
- A7** R. L. Gray, R. E. Lee, B. M. Sanders, *J. Vinyl Addit. Technol.*, 1996, **2**, 265; C. Wilhelm, J.-L. Gardette, *Polymer*, 1997, **38**, 4019; C. Wilhelm, J.-L. Gardette, *Polymer*, 1998, **39**, 5973; C. Peinado, N. S. Allen, E. F. Salvador, T. Corrales, F. Catalina, *Polym. Degrad. Stab.*, 2002, **77**, 523; K. Sathiyalekshmi, S. Gopalakrishnan, *Adv. Polym. Tech.*, 2004, **23**, 91.
- A8** G. Botelho, A. Queiros, P. Gijsman, *Polym. Degrad. Stab.*, 2000, **68**, 35; D. J. Kim, H. J. Kang, K. H. Seo, *J. Appl. Polym. Sci.*, 2001, **81**, 637; C. A. Lukey, *Prog. Org. Coat.*, 2001, **41**, 129; G. J. M. Fechine, M. S. Rabello, R. M. Souto Maior, L. H. Catalani, *Polymer*, 2004, **45**, 2303; M. Schmid, A. Ritter, A. Grubelnik, M. Zinn, *Biomacromolecules*, 2007, **8**, 579; G. J. M. Fechine, R. M. Souto-Maior, M. S. Rabello, *J. Appl. Polym. Sci.*, 2007, **104**, 51; M. A. Sabino, *Polym. Degrad. Stab.*, 2007, **92**, 986.
- A9** G. G. Cameron, G. P. Kerr, *Eur. Polym. J.*, 1970, **6**, 423; V. A. Ponomarenko, V. N. Shelgayev, A. G. Kechina, A. A. Yarosh, S. P. Krukowskii, *Vysokomol. Soedin., Ser. A*, 1974, **16**, 553; J. B. Adeniyi, G. Scott, *Polym. Degrad. Stab.*, 1987, **17**, 117; N. Bensemra, T. Van Hoang, A. Guyot, *Polym. Degrad. Stab.*, 1990, **28**, 173; A. Jonas, R. Legras, *Polymer*, 1991, **32**, 2691-2706; S. Mayeda, N. Tanimoto, H. Niwa, M. Nagata, *J. Anal. Appl. Pyrolysis*, 1995, **33**, 243; H. Becker, H. Spreitzer, K. Ibrom, W. Kreuder, *Macromolecules*, 1999, **32**, 4925; H. Becker, H. Spreitzer, W. Kreuder, E. Kluge, H. Schenk, I. Parker, Y. Cao, *Adv. Mater.*, 2000, **12**, 42.

Fig. S1. A set of radicals and the corresponding values of Gibbs free energy (kJ/mol) of their reaction with oxygen, calculated at the G3MP2-RAD//B3LYP/6-31G(d) level of theory.



$R^{\bullet} =$

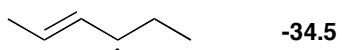
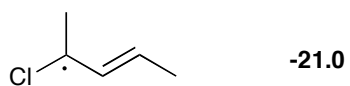
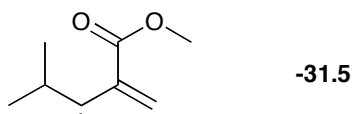
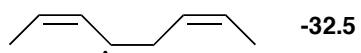
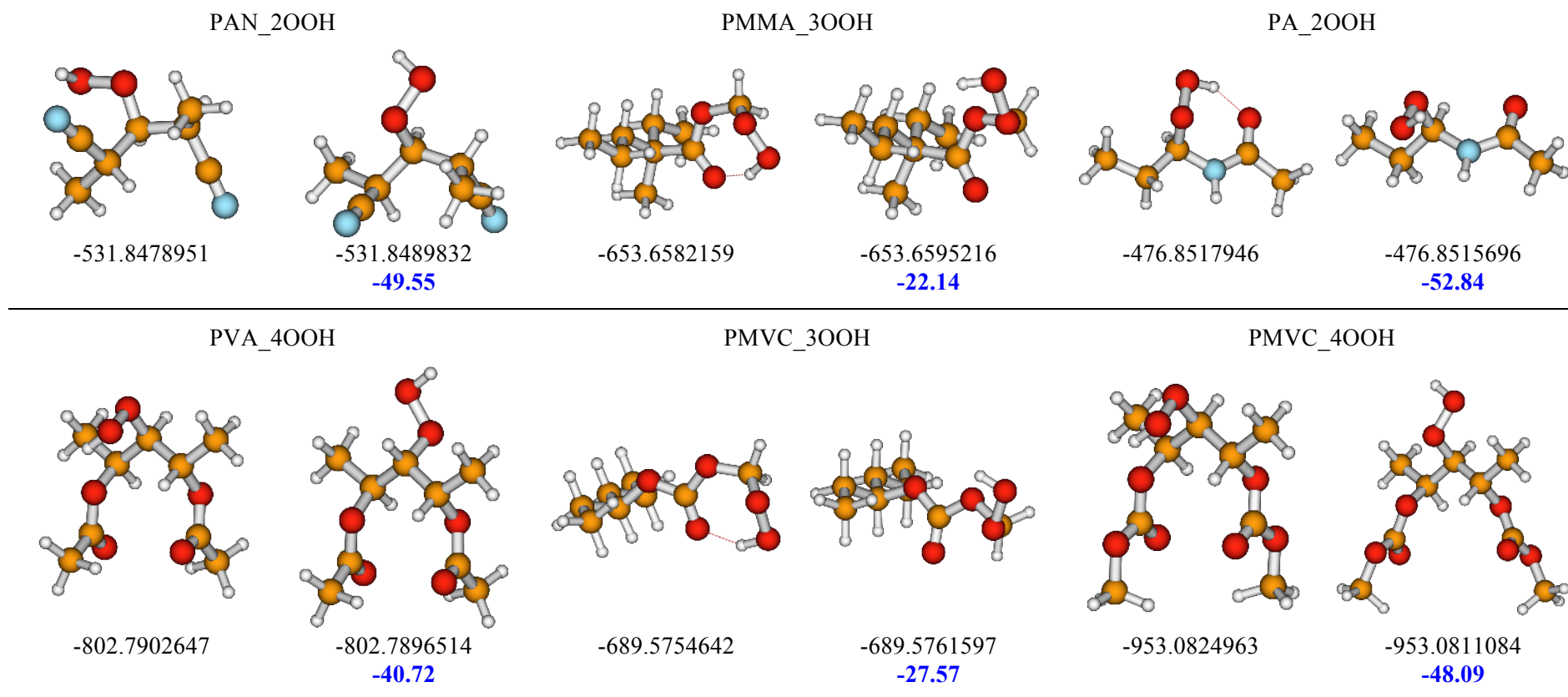
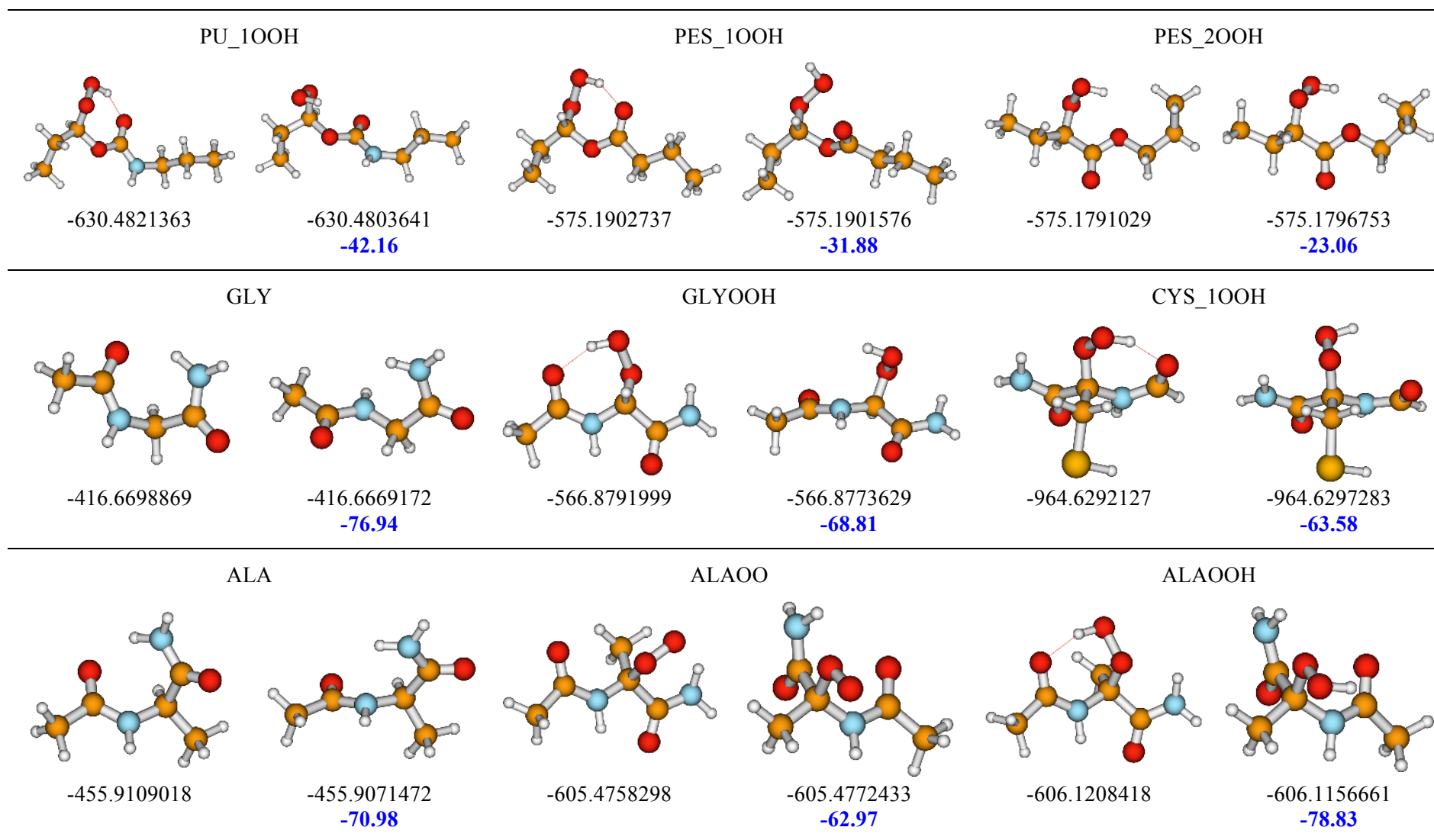
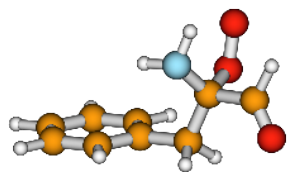


Fig. S2. Structures and G3MP2-RAD//B3LYP/6-31G(d) energies (Hartrees) of gas-phase (left) and corresponding solution conformers (right), as well as COSMO-RS/BP/TZVP solvation energies (blue, kJ/mol) of solution conformers.

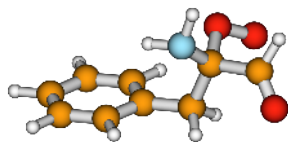




PHE_100



-628.3749260



-628.3740698
-32.39

PHE_200



-628.3631160



-628.3632350
-33.71

Fig. S3. Gas-phase G3MP2-RAD//B3LYP/6-31G(d) reaction Gibbs' free energies of propagation and subsequent chain branching reactions (4-6) in BAS for R = C₂H₅.

Reaction scheme	Reaction number in Scheme 1	ΔG_{gas} , kJ/mol
$\text{C}_2\text{H}_5\text{OO}\cdot + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_5\text{OOH} + \text{C}_2\text{H}_5\cdot$	4	55.43
$\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{O}\cdot + \text{HO}\cdot$	5	134.93
$2 \text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{OO}\cdot + \text{C}_2\text{H}_5\text{O}\cdot + \text{H}_2\text{O}$	6	-4.09

Table S1. Contributions to the gas and solution-phase free energies of reaction species according to the following scheme $X + XOO \rightarrow XOOH + XR$, where X is the name of the specie in Fig. 4-13.

Species	E_{gas}^0 (Hartrees)	T_c (Hartrees)	$ZPVE$ (Hartrees)	S_{gas} (Jmol/K)	G_{gas} (Hartrees)	ΔG_{solv} (water) (kJ/mol)
PBD	-312.82710	0.01118	0.19574	416.54	-312.66748	4.26
PBDOO	-462.38826	0.01312	0.19158	479.57	-462.23802	-9.18
PBDOOH	-463.03715	0.01350	0.20319	469.50	-462.87378	-18.79
PBDR	-312.18049	0.01132	0.18197	432.23	-312.03629	3.18
PS	-428.24481	0.01229	0.23822	437.80	-428.04401	-1.05
PSOO	-577.80872	0.01423	0.23380	482.15	-577.61544	-10.38
PSOOH	-578.45523	0.01474	0.24518	484.14	-578.25029	-22.29
PSR	-427.59142	0.01222	0.22541	435.70	-427.40326	-3.29
PAN1	-289.64108	0.00954	0.15738	373.94	-289.51663	-13.78
PAN1OO	-439.19540	0.01151	0.15244	420.33	-439.07919	-9.80
PAN1OOH	-439.84419	0.01202	0.16400	422.68	-439.71618	-28.01
PAN1R	-288.98341	0.00994	0.14341	410.39	-288.87667	-14.73
PAN1	-381.76873	0.01114	0.15625	413.34	-381.64829	-33.08
PAN1OO	-531.32168	0.01306	0.15198	460.56	-531.20894	-30.99
PAN1OOH	-531.97337	0.01331	0.16383	455.03	-531.84790	N/A
PAN1R	-381.09324	0.01151	0.14166	434.42	-380.98941	-29.95
PAN1OOH ^a	-531.97318	0.01368	0.16332	464.97	-531.84898	-49.55
PE_1	-197.50843	0.00800	0.15842	331.21	-197.37963	8.89
PE_1OO	-347.07155	0.00976	0.15459	385.76	-346.95100	-4.93

PE_1OOH	-347.71814	0.01032	0.16585	389.32	-347.58618	-17.41
PE_1R	-196.83686	0.00842	0.14356	355.78	-196.72529	7.87
PE_2OO	-425.59540	0.01249	0.21064	449.21	-425.42328	-3.59
PE_2OOH	-425.57125	0.01322	0.20729	463.00	-425.40331	-12.49
PP_1	-315.29731	0.01192	0.24192	422.42	-315.09145	9.72
PP_1OO	-464.86430	0.01369	0.23775	460.38	-464.66515	-4.26
PP_1OOH	-465.50528	0.01422	0.24908	467.29	-465.29505	-14.79
PP_1R	-314.62924	0.01242	0.22757	449.71	-314.44032	9.37
PP_2 ^c	-315.29731	0.01192	0.24192	422.42	-315.09145	9.72
PP_2OO	-464.85920	0.01386	0.23812	471.54	-464.66077	-5.79
PP_2OOH	-465.50432	0.01431	0.24947	470.10	-465.29393	-14.91
PP_2R	-314.62552	0.01239	0.22733	442.99	-314.43611	8.89
PP_3 ^c	-315.29731	0.01192	0.24192	422.42	-315.09145	9.72
PP_3OO	-464.85390	0.01356	0.23894	470.27	-464.65480	-4.25
PP_3OOH	-465.50143	0.01438	0.24991	483.18	-465.29201	-16.85
PP_3R	-314.62255	0.01234	0.22700	436.08	-314.43273	8.89
PVC_1	-695.92916	0.01023	0.17774	393.89	-695.78591	0.38
PVC_1OO	-845.48920	0.01220	0.17288	440.78	-845.35417	-2.88
PVC_1OOH	-846.13914	0.01258	0.18472	439.24	-845.99172	-11.92
PVC_1R	-695.26115	0.01055	0.16409	416.02	-695.13376	3.32
PVC_2 ^c	-695.92916	0.01023	0.17774	393.89	-695.78591	0.38
PVC_2OO	-845.48804	0.01212	0.17375	443.25	-845.35251	-4.68
PVC_2OOH	-846.13672	0.01263	0.18511	444.76	-845.98949	-18.42
PVC_2R	-695.25875	0.01066	0.16332	412.66	-695.13163	-2.75
PVC_3	-1115.82563	0.00980	0.14082	391.47	-1115.71947	-7.35

PVC_3OO	-1265.37874	0.01177	0.13657	442.12	-1265.28061	-11.11
PVC_3OOH	-1266.02737	0.01235	0.14788	443.32	-1265.91748	-26.67
PVC_3R	-1115.15394	0.01027	0.12657	410.41	-1115.06371	-9.04
PVC_4	-656.66149	0.00890	0.15028	368.75	-656.54418	-0.77
PVC_4OO	-806.22286	0.01074	0.14620	418.92	-806.11349	-12.29
PVC_4OOH	-806.87098	0.01129	0.15751	422.04	-806.75010	-24.01
PVC_4R	-655.98964	0.00938	0.13543	402.32	-655.89052	-1.32
PMMA_1	-503.66664	0.01510	0.25642	497.45	-503.45161	-9.64
PMMA_1OO	-653.22260	0.01683	0.25333	540.14	-653.01377	-14.30
PMMA_1OOH	-653.86995	0.01736	0.26459	542.92	-653.64966	-27.28
PMMA_1R	-502.99083	0.01532	0.24157	502.59	-502.79102	-8.24
PMMA_2 ^c	-503.66664	0.01510	0.25642	497.45	-503.45161	-9.64
PMMA_2OO	-653.22718	0.01710	0.25229	545.01	-653.01968	-17.00
PMMA_2OOH	-653.87375	0.01753	0.26367	540.66	-653.65395	-29.81
PMMA_2R	-502.99426	0.01539	0.24195	509.31	-502.79476	-8.96
PMMA_3 ^c	-503.66664	0.01510	0.25642	497.45	-503.45161	-9.64
PMMA_3OO	-653.22530	0.01670	0.25291	543.99	-653.01746	-10.80
PMMA_3OOH	-653.88021	0.01657	0.26533	527.56	-653.65822	N/A
PMMA_3R	-502.99433	0.01517	0.24182	498.99	-502.79401	-5.04
PMMA_3OOH ^a	-653.87925	0.01715	0.26437	544.18	-653.65952	-22.14
PVA_1	-464.40921	0.01385	0.22810	484.12	-464.22224	-11.43
PVA_1OO	-613.97170	0.01564	0.22349	515.19	-613.79108	-11.04
PVA_1OOH	-614.61811	0.01618	0.23495	520.65	-614.42611	-28.83
PVA_1R	-463.73672	0.01400	0.21454	491.37	-463.56398	-10.63
PVA_2 ^c	-464.40921	0.01385	0.22810	484.12	-464.22224	-11.43

PVA_2OO	-613.96932	0.01554	0.22438	515.06	-613.78789	-19.72
PVA_2OOH	-614.61741	0.01584	0.23611	512.30	-614.42363	-26.20
PVA_2R	-463.73701	0.01396	0.21409	486.66	-463.56423	-9.71
PVA_3 ^c	-464.40921	0.01385	0.22810	484.12	-464.22224	-11.43
PVA_3OO	-613.95652	0.01539	0.22494	526.48	-613.77599	-15.85
PVA_3OOH	-614.60970	0.01547	0.23695	514.45	-614.41571	-23.34
PVA_3R	-463.73916	0.01345	0.21479	474.50	-463.56481	-12.08
PVA_4	-652.78969	0.01640	0.24238	524.01	-652.59041	-23.88
PVA_4OO	-802.34524	0.01846	0.23799	576.85	-802.15429	-24.15
PVA_4OOH	-802.99449	0.01863	0.24993	566.56	-802.79026	N/A
PVA_4R	-652.11453	0.01685	0.22771	541.37	-651.93145	-20.87
PVA_4OOH ^a	-802.99254	0.01901	0.24937	576.76	-802.78965	-40.72
PMVC_1	-539.55985	0.01458	0.23392	496.11	-539.36768	-11.58
PMVC_1OO	-689.11478	0.01656	0.22889	535.37	-688.93013	-15.06
PMVC_1OOH	-689.76281	0.01682	0.24085	529.45	-689.56526	-25.99
PMVC_1R	-538.88721	0.01480	0.22024	507.92	-538.70985	-10.34
PMVC_2 ^c	-539.55985	0.01458	0.23392	496.11	-539.36768	-11.58
PMVC_2OO	-689.11881	0.01646	0.22990	536.89	-688.93342	-21.55
PMVC_2OOH	-689.76888	0.01664	0.24183	529.75	-689.57057	-24.72
PMVC_2R	-538.88754	0.01473	0.21978	501.34	-538.70996	-10.21
PMVC_3 ^c	-539.55985	0.01458	0.23392	496.11	-539.36768	-11.58
PMVC_3OO	-689.11748	0.01622	0.23034	549.93	-688.93337	-13.11
PMVC_3OOH	-689.77313	0.01617	0.24252	537.35	-689.57546	N/A
PMVC_3R	-538.88689	0.01457	0.21951	496.72	-538.70921	-5.93
PMVC_3OOH ^a	-689.77224	0.01666	0.24183	549.58	-689.57616	-27.57

PMVC_4	-803.09002	0.01818	0.25342	566.65	-802.88276	-26.04
PMVC_4OO	-952.64446	0.02017	0.24922	615.08	-952.44491	-27.06
PMVC_4OOH	-953.29532	0.02031	0.26128	605.55	-953.08250	N/A
PMVC_4R	-802.41395	0.01853	0.23896	580.31	-802.22236	-24.85
PMVC_4OOH ^a	-953.28970	0.02107	0.26005	638.67	-953.08111	-48.09
PU_1	-480.44643	0.01338	0.21856	471.96	-480.26808	-22.00
PU_1OO	-630.01125	0.01526	0.21418	524.43	-629.84136	-27.17
PU_1OOH	-630.66618	0.01515	0.22660	508.21	-630.48214	N/A
PU_1R	-479.77647	0.01355	0.20447	483.66	-479.61337	-21.71
PU_1OOH ^a	-630.66210	0.01575	0.22560	524.91	-630.48036	-42.16
PU_2 ^c	-480.44643	0.01338	0.21856	471.96	-480.26808	-22.00
PU_2OO	-630.01234	0.01510	0.21458	514.74	-629.84112	-22.28
PU_2OOH	-630.66154	0.01566	0.22597	519.95	-630.47896	-39.30
PU_2R	-479.78317	0.01347	0.20468	475.16	-479.61898	-22.39
PES_1	-425.14137	0.01222	0.20098	448.62	-424.97912	-11.19
PES_1OO	-574.70437	0.01408	0.19663	493.69	-574.54973	-13.32
PES_1OOH	-575.35883	0.01400	0.20899	479.41	-575.19027	N/A
PES_1R	-424.47097	0.01238	0.18687	453.32	-424.32320	-7.93
PES_1OOH ^a	-575.35639	0.01460	0.20808	497.15	-575.1901576	-31.88
PES_2 ^c	-425.14137	0.01222	0.20098	448.62	-424.97912	-11.19
PES_2OO	-574.69487	0.01395	0.19710	490.55	-574.53953	-14.42
PES_2OOH	-575.34667	0.01420	0.20889	489.00	-575.17910	N/A
PES_2 R	-424.47816	0.01212	0.18778	449.96	-424.32935	-13.39
PES_2OOH ^a	-575.34774	0.01420	0.20900	485.52	-575.17968	-23.06
PES_3	-495.71668	0.01113	0.13118	423.54	-495.62246	-25.17

PES_3OO	-645.26704	0.01315	0.12651	478.51	-645.18172	-23.42
PES_3OOH	-645.92458	0.01348	0.13830	473.02	-645.82652	-39.22
PES_3R	-495.05400	0.01116	0.11767	427.20	-494.97368	-25.01
PES_4	-534.98492	0.01261	0.15871	450.97	-534.86482	-25.34
PES_4OO	-684.53789	0.01456	0.15342	493.74	-684.42598	-21.03
PES_4OOH	-685.19359	0.01485	0.16531	487.85	-685.06882	-35.70
PES_4R	-534.32099	0.01277	0.14514	460.75	-534.21541	-23.90
PET	-534.98757	0.01222	0.15938	445.69	-534.86658	-25.85
PETOO	-684.54536	0.01432	0.15462	501.13	-684.43333	-23.81
PETOOH	-685.19980	0.01466	0.16630	496.18	-685.07518	-39.30
PETR	-534.31558	0.01279	0.14472	475.02	-534.21202	-25.17
PA_1	-326.76047	0.00988	0.15722	390.29	-326.63769	-32.12
PA_1OO	-476.31906	0.01185	0.15308	442.36	-476.20436	-26.65
PA_1OOH	-476.97063	0.01226	0.16466	436.88	-476.84333	-45.74
PA_1R	-326.09603	0.01013	0.14335	404.74	-325.98852	-36.11
PA_2	-326.76311	0.01003	0.15684	398.42	-326.64149	-37.23
PA_2OO	-476.32832	0.01173	0.15269	438.31	-476.21367	-32.22
PA_2OOH	-476.98033	0.01165	0.16515	425.06	-476.85179	N/A
PA_2R	-326.10045	0.01004	0.14295	397.63	-325.99262	-39.41
PA_2OOH ^a	-476.97710	0.01235	0.16410	448.46	-476.85157	-52.84
GLY	-416.76358	0.00992	0.12832	392.27	-416.66989	N/A
GLYOO	-566.32152	0.01182	0.12360	442.09	-566.23630	-50.66
GLYOOH	-566.97864	0.01164	0.13637	427.68	-566.87920	N/A
GLYR	-416.11382	0.01000	0.11496	403.35	-416.03467	-63.00
GLY ^a	-416.75885	0.01025	0.12760	404.27	-416.66692	-76.94

GLYOOH ^a	-566.97477	0.01224	0.13534	441.84	-566.87736	-68.81
ALA	-456.03079	0.01128	0.15593	416.71	-455.91090	N/A
ALAOO	-605.58770	0.01312	0.15094	459.52	-605.47583	N/A
ALAOOH	-606.24663	0.01295	0.16368	447.70	-606.12084	N/A
ALAR	-455.37894	0.01151	0.14290	433.60	-455.27377	-55.39
ALA ^a	-456.02507	0.01161	0.15530	431.43	-455.90715	-70.98
ALAOO ^a	-605.58763	0.01348	0.15033	470.50	-605.47724	-62.97
ALAOOH ^a	-606.23853	0.01388	0.16198	466.74	-606.11567	-78.83
PHE_1	-478.94296	0.01129	0.18070	424.35	-478.79916	-34.74
PHE_1OO	-628.51046 ^b	0.01326	0.17578	471.17	-628.37493	N/A
PHE_1OOH	-629.16294	0.01309	0.18858	456.77	-629.01314	-34.04
PHE_1R	-478.31376	0.01097	0.16878	427.19	-478.18253	-44.65
PHE_1OO ^a	-628.50977	0.01324	0.17578	469.58	-628.37407	-32.39
PHE_2 ^c	-478.94296	0.01129	0.18070	424.35	-478.79916	-34.74
PHE_2OO	-628.49877	0.01331	0.17624	474.58	-628.36312	N/A
PHE_2OOH	-629.14946	0.01306	0.18920	457.02	-628.99910	-38.47
PHE_2R	-478.28662	0.01148	0.16689	433.64	-478.15750	-36.86
PHE_2OO ^a	-628.49883	0.01340	0.17625	476.00	-628.36324	-33.71
CYS_1	-814.51567	0.01103	0.12826	415.43	-814.42356	-45.79
CYS_1OO	-964.07127	0.01292	0.12338	459.36	-963.98713	-42.63
CYS_1OOH	-964.72719	0.01281	0.13586	446.45	-964.62921	N/A
CYS_1R	-813.86630	0.01090	0.11597	418.56	-813.78697	-44.38
CYS_1OOH ^a	-964.72580	0.01346	0.13498	461.13	-964.62973	-63.58
CYS_2	-645.96549	0.00845	0.10042	356.08	-645.89706	-17.27
CYS_2OO	-795.52412	0.00997	0.09621	397.04	-795.46302	-17.33

CYS_2OOH	-796.17688	0.01033	0.10805	394.69	-796.10332	-25.76
CYS_2R	-645.30431	0.00832	0.08692	360.38	-645.25000	-10.84
DEF_1	-1155.08740	0.01109	0.16886	413.78	-1154.95444	
DEF_1OO	-1304.64422	0.01308	0.16404	459.38	-1304.51926	
DEF_1OOH	-1305.29533	0.01329	0.17595	450.65	-1305.15727	
DEF_1R	-1154.42194	0.01191	0.15445	448.84	-1154.30655	
DEF_2	-1155.08243	0.01100	0.16942	417.37	-1154.94941	
DEF_2OO	-1304.64046	0.01292	0.16475	456.72	-1304.51466	
DEF_2OOH	-1305.29117	0.01324	0.17653	454.41	-1305.15300	
DEF_2R	-1154.41734	0.01161	0.15541	441.56	-1154.30047	
DEF_3	-1574.97559	0.01084	0.13182	415.57	-1574.88011	
DEF_3OO	-1724.52611	0.01273	0.12663	454.34	-1724.43834	
DEF_3OOH	-1725.17942	0.01306	0.13857	452.32	-1725.07916	
DEF_3R	-1574.31157	0.01122	0.11839	434.02	-1574.23126	
DEF_4	-616.16460	0.00718	0.09826	328.87	-616.09650	
DEF_4OO	-765.72338	0.00912	0.09395	384.45	-765.66397	
DEF_4OOH	-766.37337	0.00954	0.10551	382.93	-766.30180	
DEF_4R	-615.51828	0.00725	0.08452	333.34	-615.46437	
DEF_5	-616.16645	0.00722	0.09829	330.73	-616.09849	
DEF_5OO	-765.72118	0.00915	0.09375	384.60	-765.66195	
DEF_5OOH	-766.37690	0.00952	0.10552	380.78	-766.30511	
DEF_5R	-615.51990	0.00710	0.08471	331.94	-615.46578	
DEF_6	-655.43229	0.00849	0.12619	355.69	-655.33800	
DEF_6OO	-804.99073	0.01045	0.12106	403.05	-804.90499	
DEF_6OOH	-805.64498	0.01083	0.13286	401.36	-805.54686	

DEF_6R	-654.78679	0.00881	0.11221	368.82	-654.70766
DEF_7	-1193.11493	0.01217	0.17345	448.88	-1192.98029
DEF_7OO	-1342.67073	0.01416	0.16911	499.07	-1342.54413
DEF_7OOH	-1343.32064	0.01467	0.18057	506.81	-1343.18295
DEF_7R	-1192.46660	0.01223	0.15995	455.66	-1192.34617
DEF_8	-1231.14171	0.01355	0.17693	473.57	-1231.00500
DEF_8OO	-1380.69439	0.01551	0.17190	517.76	-1380.56578
DEF_8OOH	-1381.34926	0.01590	0.18365	514.94	-1381.20818
DEF_8R	-1230.49552	0.01349	0.16394	478.32	-1230.37241
DEF_9	-196.27649	0.00765	0.13472	329.68	-196.17156
DEF_9OO	-345.83070	0.00937	0.13150	386.26	-345.73368
DEF_9OOH	-346.47962	0.00981	0.14291	386.91	-346.37084
DEF_9R	-195.62629	0.00742	0.12137	331.56	-195.53515
DEF_10	-196.27324	0.00749	0.13502	328.14	-196.16799
DEF_10OO	-345.83304	0.00928	0.13109	377.72	-345.73556
DEF_10OOH	-346.48025	0.00978	0.14249	380.80	-346.37122
DEF_10R	-195.62633	0.00742	0.12137	331.56	-195.53520
DEF_11	-235.53849	0.00899	0.16275	361.40	-235.40780
DEF_11OO	-385.09986	0.01087	0.15876	413.58	-384.97719
DEF_11OOH	-385.74855	0.01131	0.17025	413.01	-385.61389
DEF_11R	-234.89107	0.00899	0.14914	367.75	-234.77470
DEF_12	-274.80500	0.01007	0.19058	384.10	-274.64797
DEF_12OO	-424.35931	0.01175	0.18750	434.86	-424.20944
DEF_12OOH	-425.00774	0.01232	0.19866	440.23	-424.84675
DEF_12R	-274.15220	0.00981	0.17697	383.73	-274.00899

DEF_13 ^d	-274.80500	0.01007	0.19058	384.10	-274.64797
DEF_13OO	-424.36521	0.01213	0.18640	437.19	-424.21632
DEF_13OOH	-425.01413	0.01242	0.19812	429.39	-424.85235
DEF_13R	-274.15368	0.01022	0.17677	397.83	-274.01186
DEF_14	-274.80574	0.01042	0.19008	390.71	-274.64961
DEF_14OO	-424.36920	0.01222	0.18561	430.49	-424.22025
DEF_14OOH	-425.01539	0.01262	0.19716	429.53	-424.85439
DEF_14R	-274.15681	0.01061	0.17649	399.38	-274.01506
DEF_15 ^e	-274.80574	0.01042	0.19008	390.71	-274.64961
DEF_15OO	-424.36079	0.01217	0.18697	444.59	-424.21213
DEF_15OOH	-425.00974	0.01260	0.19839	444.39	-424.84921
DEF_15R	-274.15368	0.01022	0.17677	397.81	-274.01186
DEF_16	-235.54080	0.00896	0.16235	357.47	-235.41008
DEF_16OO	-385.09511	0.01075	0.15908	415.46	-384.97245
DEF_16OOH	-385.74404	0.01118	0.17052	415.56	-385.60953
DEF_16R	-234.89038	0.00872	0.14911	359.48	-234.77337
DEF_17	-235.53790	0.00874	0.16266	354.39	-235.40675
DEF_17OO	-385.09612	0.01069	0.15863	407.16	-384.97304
DEF_17OOH	-385.74503	0.01092	0.17041	398.95	-385.60900
DEF_17R	-234.89039	0.00872	0.14911	359.49	-234.77338
DEF_18	-235.53957	0.00863	0.16319	346.63	-235.40711
DEF_18OO	-385.09950	0.01050	0.15920	405.62	-384.97586
DEF_18OOH	-385.74640	0.01098	0.17062	407.18	-385.61104
DEF_18R	-234.88964	0.00903	0.14885	375.03	-234.77434
DEF_19	-463.17151	0.01292	0.20566	451.93	-463.00425

DEF_19OO	-612.72944	0.01494	0.20152	501.13	-612.56989
DEF_19OOH	-613.37889	0.01542	0.21291	500.25	-613.20737
DEF_19R	-462.52033	0.01302	0.19190	467.91	-462.36855
DEF_20	-384.64487	0.01055	0.14941	401.23	-384.53048
DEF_20OO	-534.19879	0.01238	0.14598	455.94	-534.09221
DEF_20OOH	-534.84828	0.01285	0.15739	455.49	-534.72976
DEF_20R	-383.99116	0.01038	0.13572	410.49	-383.89168
DEF_21	-690.80138	0.01788	0.24802	575.56	-690.60084
DEF_21OO	-840.35346	0.01970	0.24312	602.25	-840.15903
DEF_21OOH	-841.00409	0.01976	0.25539	596.38	-840.79666
DEF_21R	-690.15900	0.01726	0.23607	552.13	-689.96837
DEF_22	-427.01240	0.01167	0.21525	429.77	-426.83428
DEF_22OO	-576.57241	0.01360	0.21129	475.19	-576.40148
DEF_22OOH	-577.22226	0.01402	0.22284	473.28	-577.03915
DEF_22R	-426.36186	0.01176	0.20126	442.51	-426.19910
DEF_23	-462.92194	0.01146	0.19192	426.82	-462.76702
DEF_23OO	-612.75021	0.01336	0.18787	474.98	-612.60293
DEF_23OOH	-613.39999	0.01374	0.19945	473.29	-613.24054
DEF_23R	-462.26220	0.01144	0.17890	438.77	-462.12169
DEF_24	-345.37957	0.00907	0.12139	375.01	-345.29170
DEF_24OO	-494.93930	0.01100	0.11671	426.53	-494.86003
DEF_24OOH	-495.59342	0.01095	0.12906	414.00	-495.50043
DEF_24R	-344.73240	0.00905	0.10732	375.76	-344.65870

^a Solution conformer; ^b ROMP2 calculation were carried out with Gaussian 03 program package; ^c Identical to X_1; ^d Identical to DEF_12; ^e Identical to DEF_14.

Table S2. Reaction Gibbs free energies, kJ/mol.

Reaction	<i>Gas phase^a</i>		<i>Water solution^{a,b}</i>
	298.15 K	373.15 K	298.15 K
PBD	-12.0	-12.5	-22.7
PS	15.5	15.5	1.4
PA_1	7.8	4.8	-11.4
PA_2	52.2	54.0	34.0
PE_1	50.3	48.1	36.8
PE_2	52.4	51.3	43.5
PP_1	55.7	53.1	44.9
PP_2	58.2	56.7	48.3
PP_3	56.5	54.4	43.0
PVC_1	38.4	36.7	32.3
PVC_2	45.4	43.8	28.6
PVC_3	49.6	48.0	32.4
PVC_4	44.8	41.9	32.5
PMMA_1	64.9	64.2	53.3
PMMA_2	59.3	58.6	47.2
PMMA_3	44.2	45.3	34.1
PVA_1	61.0	60.0	44.0
PVA_2	58.5	58.4	53.7
PVA_3	46.5	48.1	38.4
PVA_4	60.3	59.7	48.4
PMVC_1	59.6	59.1	49.9
PMVC_2	54.0	54.1	52.2
PMVC_3	43.0	43.8	32.4
PMVC_4	59.9	59.5	43.7
PU_1	36.6	36.9	26.5
PU_2	29.6	28.8	12.2
PES_1	40.3	41.0	25.3
PES_2	26.8	26.7	14.4
PES_3	10.5	10.5	-5.2
PES_4	17.3	16.9	4.0
PET_1	33.4	31.4	18.6
PA_1	26.8	26.0	3.7
PA_2	28.2	29.2	6.0
GLY	-20.2	-20.0	-27.4
ALA	-20.7	-21.1	-13.5

PHE_1	-59.6	-55.8	-70.5
PHE_2	14.9	15.5	8.3
CYS_1	-14.4	-13.7	-35.3
CYS_2	17.7	17.5	15.7

^a Calculated at G3MP2-RAD//B3LYP/6-31G(d) level of theory; ^b Solvation Gibbs free energy calculated at COSMO-RS/BP/TZVP level of theory.

APPENDIX S1: Geometries of the species in this study

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

Gas-phase conformers

PBD

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1\1\GINC-V1292\FOpt\RB3LYP\Gen\C8H14\GXG501\26-Jun-2010\0\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\
\pbd1.freq\0,1\C,-0.3762521113,-0.8999952556,0.422451302\C,-0.2480899
14,0.1428039691,1.4979598994\C,0.8668082991,0.5717383496,2.1022796355\
C,2.2857693162,0.1360267992,1.8533209611\C,3.1881007479,1.3040836815,1
.3831219159\C,4.6302508811,0.8956668461,1.2464689739\C,5.3932575256,0.
9104077732,0.146565052\C,5.0133545642,1.3551896499,-1.238504382\H,-0.8
608222569,-0.4815352663,-0.4702032594\H,-1.0096029667,-1.7322782247,0.
7589269577\H,0.5867317497,-1.3171282887,0.1157194622\H,-1.1916950644,0
.5895533323,1.8143818953\H,0.7574169261,1.3446187517,2.8655801114\H,2.
7067266741,-0.2734743596,2.7846696842\H,2.3337686819,-0.6714686943,1.1
153175587\H,2.7936182284,1.7037516883,0.4430948104\H,3.1115268136,2.11
89408426,2.1196346312\H,5.0877027024,0.5324704829,2.1688379011\H,6.423
1370252,0.5652075059,0.2479728653\H,5.1639381216,0.543611238,-1.963359
0076\H,3.9719265868,1.679990151,-1.3116802496\H,5.6479883334,2.1889826
707,-1.5687668397\Version=EM64L-G09RevA.02\State=1-A\HF=-313.246093\R
MSD=2.259e-09\RMSF=1.224e-06\Dipole=-0.0237689,-0.0279772,-0.1151137\Q
uadrupole=0.6953617,-1.1411737,0.445812,-0.1296889,0.0020854,0.4384835
\PG=C02 [X(C8H14)]\@
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PBDOO

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1\1\GINC-V1288\FOpt\UB3LYP\Gen\C8H13O2(2)\GXG501\27-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pbd1oo.freq\0,2\C,-0.1803158317,0.3381797255,0.3716381376\C,0.1
210735639,0.3850224847,1.8428476329\C,1.304245671,0.2342683503,2.45016
43515\C,2.6419321618,-0.0286745987,1.8139958927\C,3.6524780471,1.09606
88227,2.0999518396\C,3.3854859315,2.3659603534,1.3543579044\C,3.209291
4096,3.584519317,1.8783251041\C,3.2401814417,3.9943602108,3.3225541293
\H,-0.6458203844,1.2767464362,0.0420297025\H,-0.8982210611,-0.46207883
63,0.1467249645\H,0.7083996585,0.1719262139,-0.2429271396\H,-0.7462446
014,0.5585657457,2.4809405555\H,1.3235373813,0.3020149897,3.5389108034
\H,3.0757805036,-0.9489927236,2.2269943295\H,2.5600259021,-0.164284637
4,0.7305423656\H,3.7531874198,1.2502804157,3.1765171323\H,3.324119061,
2.2505176939,0.2726073635\H,3.0065433392,4.3967473093,1.1794800587\H,2
.2688674855,4.4068270514,3.6264767052\H,3.4826314683,3.1725243336,4.00
09899408\H,3.9805953617,4.7898457813,3.4776608576\O,4.9929068971,0.642
1125235,1.6412155936\O,5.4554251088,-0.3369960037,2.3969205818\Versio
n=EM64L-G09RevA.02\State=2-A\HF=-462.9543785\S2=0.753183\S2-1=0.\S2A=0
.750007\RMSD=2.962e-09\RMSF=3.695e-06\Dipole=-1.1081165,0.7717431,0.01
82596\Quadrupole=-4.5388041,1.6590412,2.8797629,3.0934881,0.7508573,1.
3134096\PG=C01 [X(C8H13O2)]\@
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PBDOOH

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1\1\GINC-V1285\FOpt\RB3LYP\Gen\C8H14O2\GXG501\27-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pbd1ooh.freq\0,1\C,0.0219927274,-0.2607384024,-0.1368523958\C,-0.0
```

327768429,-0.1464622913,1.3606602919\C,0.9858850002,-0.0159458477,2.21
 87099602\C,2.4573041324,0.0441201269,1.9046336261\C,3.1198600564,1.315
 8322802,2.4632099919\C,2.6402105825,2.5741009541,1.7864905897\C,2.4057
 838174,3.7622850723,2.3599792989\C,2.5162078368,4.1279738417,3.8141982
 789\H,-0.5675163004,0.5367337336,-0.6090063584\H,-0.4158472089,-1.2112
 293676,-0.4707667107\H,1.0392596386,-0.2057823123,-0.533729491\H,-1.03
 72295192,-0.1827818722,1.7841809721\H,0.7440858692,0.0489976021,3.2805
 406335\H,2.9724079497,-0.8141015503,2.3577362232\H,2.6441122369,-0.007
 8706702,0.8269591982\H,2.9734808557,1.3616743735,3.5480666768\H,2.5120
 421059,2.4885057475,0.7069085716\H,2.0783187988,4.5737957482,1.7079799
 75\H,1.5280061822,4.3704640843,4.2283928299\H,2.9612442877,3.335764032
 3,4.4195493858\H,3.1327538554,5.0280446068,3.9363298749\O,4.5288579552
 ,1.1178850402,2.2129425438\O,5.2564594901,2.1367135131,2.9412208525\H,
 5.1988498633,2.8860735248,2.3173234327\\Version=EM64L-G09RevA.02\State
 =1-A\HF=-463.5860654\RMSD=5.718e-09\RMSF=3.708e-06\Dipole=-0.8077327,0
 .5932146,-0.2987928\Quadrupole=-4.217325,3.0385348,1.1787902,2.9784277
 ,-1.4867466,0.6139157\PG=C01 [X(C8H14O2)]\\@

PBDR

1\1\GINC-V1293\FOpt\UB3LYP\Gen\C8H13(2)\GXG501\26-Jun-2010\0\#B3LYP/g
 en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684354
 56\pbdIr.freq\0,2\C,-0.8089002475,-0.8932007854,0.8508010701\C,-0.23
 15466053,0.3095792376,1.5437359021\C,1.0470654235,0.5478881959,1.86105
 11738\C,2.2525412558,-0.3252868412,1.5859813297\C,3.239714538,0.351538
 9302,0.6724581053\C,4.5419220331,0.6667544775,1.0341390208\C,5.5122474
 224,1.3013376718,0.2642437058\C,5.3564026986,1.7943104148,-1.141189897
 6\H,-1.3343099707,-0.5985317002,-0.0678774629\H,-1.5520963005,-1.39148
 57067,1.4881416592\H,-0.0526585379,-1.6347629495,0.5789420965\H,-0.962
 560728,1.0713631057,1.8184358362\H,1.2802186812,1.4891022753,2.3593780
 82\H,2.7485324595,-0.568687503,2.536855523\H,1.9330015401,-1.281830997
 8,1.1498156711\H,2.8702009748,0.6168477982,-0.3161886662\H,4.844867917
 3,0.3796200031,2.0430124767\H,6.4885972972,1.4570049192,0.7198155646\H
 ,6.0596770916,1.2889693394,-1.8195004915\H,4.3480464308,1.6403523861,-
 1.5350359363\H,5.580969626,2.8684877289,-1.2105347625\\Version=EM64L-G
 09RevA.02\State=2-A\HF=-312.6061665\S2=0.778266\S2-1=0.\S2A=0.750172\R
 MSD=7.110e-09\RMSF=1.851e-06\Dipole=-0.0277793,-0.0256276,-0.1131603\Q
 uadrupole=1.5522257,-1.0985386,-0.4536871,1.2064946,0.2030262,-0.35274
 67\PG=C01 [X(C8H13)]\\@

PS

1\1\GINC-V1362\FOpt\RB3LYP\Gen\C11H16\GXG501\25-Jun-2010\0\#B3LYP/gen
 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456
 \ps1.freq\0,1\C,0.1043028574,0.0770867279,-0.2481892644\C,0.19896635
 7,0.0910254281,2.5741065466\C,1.2349028244,0.5427766367,0.4357036739\C
 ,-0.9811538814,-0.3827884849,0.5145588155\C,-0.9364777973,-0.376694332
 3,1.9085101589\C,1.2859927173,0.5513641522,1.8314494901\C,0.0579924837
 ,0.0714751368,-1.7714859166\C,-0.0757624156,-1.3577823842,-2.348158227
 6\C,1.0866638768,-2.2907960507,-1.9952361006\C,-1.0557430052,0.9905066
 012,-2.3267991721\C,-0.8990430077,2.4674177298,-1.9519822511\H,2.17617
 81661,0.9182699437,2.3362281688\H,0.2343426239,0.0959557367,3.66030822
 19\H,-1.7901772241,-0.7380933883,2.4764626648\H,-1.8739431734,-0.75088
 39754,0.0143776076\H,-0.9273968758,2.6107714137,-0.8666711087\H,0.0557
 347995,2.8680639667,-2.3151649144\H,-1.7010507779,3.0707648687,-2.3923
 552744\H,-1.0652794558,0.8929778871,-3.4211202776\H,1.0181182055,0.475
 3809462,-2.1273667848\H,-1.0204134176,-1.8008734696,-2.0034949014\H,-0
 .1588318185,-1.278985502,-3.4408750141\H,2.0881918578,0.903905429,-0.1
 344180217\H,1.1755720238,-2.428621131,-0.9124840326\H,2.0406621753,-1.
 8882277608,-2.3583348879\H,0.9486074347,-3.2783119183,-2.4501279622\H,
 -2.0328952706,0.6253184173,-1.9813875396\\Version=EM64L-G09RevA.02\Sta
 te=1-A\HF=-428.8198169\RMSD=7.880e-09\RMSF=1.113e-05\Dipole=-0.027631,
 -0.0112094,-0.0709557\Quadrupole=0.9548461,-2.6666648,1.7118188,1.8246
 755,-0.0965446,-0.0876503\PG=C01 [X(C11H16)]\\@

PSOO

1\1\GINC-X111\FOpt\UB3LYP\Gen\C11H15O2(2)\GXG501\25-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=13421
77280\psloo.freq\0,2\C,0.0453360983,-0.0257390409,-0.0144619804\C,0.
0153844516,0.0105867929,2.8037059369\C,1.2423882662,-0.0353188938,0.71
38486259\C,-1.1664372416,0.0023477372,0.6936657462\C,-1.1829213438,0.0
204635293,2.0874114003\C,1.2244120278,-0.0172644175,2.1106962246\C,0.0
060903566,-0.0445342691,-1.5403424611\C,-0.6692365583,-1.3131329996,-2
.1015908478\C,-0.057939476,-2.6376205814,-1.6349054011\C,-0.6292206574
,1.2298538917,-2.1340570848\C,0.0236493798,2.5459439639,-1.7011262765\
H,2.1649201099,-0.0251423618,2.6553172688\H,0.0047038938,0.0245772063,
3.8901438787\H,-2.1340822065,0.0421639493,2.6127378843\H,-2.1102590508
,0.0104531793,0.1547104247\H,-0.0377038001,2.6910585452,-0.6179052787\
H,1.0794513358,2.5759788383,-1.9880274361\H,-0.4786055942,3.3910085962
, -2.1842286343\H,-0.5866962241,1.1332643123,-3.2242314144\H,-1.7298184
375,-1.2721653993,-1.8251598325\H,-0.6240969647,-1.2458002828,-3.19385
95812\H,2.1914725154,-0.0568968525,0.1922531758\H,-0.123412824,-2.7530
189281,-0.5483574034\H,0.9962810309,-2.7081931221,-1.9205064028\H,-0.5
867373244,-3.4785170698,-2.0964764812\H,-1.6904490749,1.2293517437,-1.
857070507\O,1.4395130205,-0.0724846967,-1.963472932\O,1.5828757167,-0.
091421375,-3.2745026065\Version=EM64L-G09RevA.02\State=2-A\HF=-578.52
90153\S2=0.753328\S2-1=0.\S2A=0.750007\RMSD=6.325e-09\RMSF=8.453e-06\D
ipole=-0.8031405,0.0195563,0.6288942\Quadrupole=1.0248797,-1.0198645,-
0.0050152,0.0037692,3.5012899,-0.0442946\PG=C01 [X(C11H15O2)]\@

PSOOH

1\1\GINC-V1363\FOpt\RB3LYP\Gen\C11H16O2\GXG501\25-Jun-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684354
56\pslooh.freq\0,1\C,-0.0101690056,0.0041484505,-0.0092565102\C,0.01
01334649,0.0102613731,2.8110014451\C,1.19840548,-0.0336504173,0.699156
4322\C,-1.2080391405,0.0423735615,0.7213750571\C,-1.1998306748,0.04558
88452,2.1155418218\C,1.2061779405,-0.0299064758,2.0961073858\C,-0.0651
973594,-0.0025572949,-1.5419553336\C,-0.7500458164,-1.2842227345,-2.07
39007877\C,-0.0526422877,-2.5900623578,-1.6840337946\C,-0.7758175234,1
.257840858,-2.0904666765\C,-0.1384745452,2.5871744064,-1.6743613038\H,
2.1558886965,-0.0599764814,2.6241326402\H,0.0184582686,0.0128355443,3.
8976870148\H,-2.1415162006,0.0753855911,2.6576087471\H,-2.1615377433,0
.0684139573,0.2005957873\H,-0.1757850794,2.728114744,-0.5895448346\H,0
.9147855117,2.6368248195,-1.9728551654\H,-0.6613612416,3.4279931528,-2
.1433434859\H,-0.7924140729,1.1763726983,-3.1833616803\H,-1.7859289111
, -1.2888307248,-1.712148898\H,-0.7998464363,-1.2058378618,-3.165236848
8\H,2.1357283909,-0.0691457665,0.1573530948\H,-0.0284586706,-2.7262939
784,-0.5977433001\H,0.9782515796,-2.6044865088,-2.0496652564\H,-0.5798
886791,-3.4462621304,-2.1194340373\H,-1.8233682449,1.2329983692,-1.767
7046597\O,1.3298119915,0.0116740077,-1.9437020183\O,1.4061030941,-0.05
57781089,-3.3932117839\H,1.7284188703,0.8430799016,-3.5855546464\Vers
ion=EM64L-G09RevA.02\State=1-A\HF=-579.1583989\RMSD=2.965e-09\RMSF=3.8
43e-06\Dipole=-0.3239923,0.5503393,-0.0082482\Quadrupole=0.8427384,-3.
0129126,2.1701742,1.6953295,-0.0766301,-3.3013832\PG=C01 [X(C11H16O2)]
\@

PSR

1\1\GINC-V1287\FOpt\UB3LYP\Gen\C11H15(2)\GXG501\26-Jun-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\pslr.freq\0,2\C,-0.0412676081,-0.1095083846,0.172949603\C,0.1202
302021,-0.1456584316,3.0229051648\C,1.2038775763,0.0125495388,0.861162
5771\C,-1.200882409,-0.2507116289,0.9940932702\C,-1.1171568391,-0.2656
815502,2.3788673107\C,1.2771233,-0.0076173608,2.2464645561\C,-0.122110
4388,-0.0914123366,-1.2536856856\C,-1.4277835316,-0.2867049424,-1.9849
992839\C,-2.192223576,1.0329006906,-2.2305401861\C,1.0928814465,0.1241
785625,-2.1226254355\C,1.8228034103,-1.1877004627,-2.4862258929\H,2.24
66310266,0.0840324842,2.7302177953\H,0.1816820437,-0.1594139554,4.1073

472244\H,-2.0259491544,-0.3709220746,2.9665603276\H,-2.1778115765,-0.3
 389675991,0.5309487165\H,2.1974401238,-1.6907556318,-1.5884542011\H,1.
 1495416035,-1.8835707619,-2.9999143002\H,2.6734377799,-0.9902024645,-3
 .1493470969\H,0.7779545609,0.6148027774,-3.0539810972\H,-1.2207744473,
 -0.7531725846,-2.958071537\H,-2.0824321135,-0.9856546135,-1.4512125581
 \H,2.1223667742,0.1138868484,0.2930156461\H,-1.5802965764,1.7425003163
 ,-2.7992285296\H,-2.4623358949,1.5125588751,-1.2837674879\H,-3.1125976
 036,0.8510133803,-2.7981163279\H,1.8046338991,0.8103459699,-1.64869884
 57\Version=EM64L-G09RevA.02\HF=-428.1751108\S2=0.777658\S2-1=0.\S2A=0
 .750529\RMSD=2.972e-09\RMSF=1.890e-05\Dipole=-0.0139492,0.0031224,-0.2
 461615\Quadrupole=255.4729465,-258.0274921,2.5545456,142.6751093,-12.5
 544521,-11.3830801\PG=C02 [C2(C1C1C1H1),X(C8H14)]\@

PAN_1

1\1\GINC-X86\FOpt\RB3LYP\Gen\C6H11N1\GXG501\25-Jun-2010\0\#B3LYP/gen
 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1342177280
 \pan1.freq\0,1\C,-0.0186047131,-0.065051015,-0.022295247\C,-0.021625
 1386,0.03161833,1.5055064132\C,1.3901134256,0.0582016051,2.1400643126\
 C,1.3401204652,0.2562700478,3.6745498184\C,2.7158831984,0.3860665836,4
 .3333075577\C,2.1340488803,-1.1661618146,1.7998242381\N,2.7071637787,-
 2.1427893235,1.5411684434\H,0.4695504109,-0.9845739331,-0.3624997849\H
 ,0.5104279411,0.7832566702,-0.4732868069\H,-1.0424294774,-0.0641248777
 ,-0.4111729568\H,-0.535255486,0.9486512582,1.8209686343\H,-0.583983286
 6,-0.8073627833,1.9344346891\H,1.9488904232,0.8989045199,1.7021858119\
 H,0.7478579182,1.1603307596,3.8647634957\H,0.787611712,-0.581086178,4.
 1191666083\H,3.2726217045,1.2389449956,3.9264469978\H,2.6140155937,0.5
 39091071,5.412960454\H,3.3193091483,-0.5144397216,4.1767110476\Versio
 n=EM64L-G09RevA.02\HF=-290.0112534\RMSD=8.451e-09\RMSF=1.572e-06\Dipol
 e=-1.0129564,1.0851025,0.3058566\Quadrupole=-36.5781403,-234.0262897,2
 70.6044299,-179.4177152,368.5293644,191.4537348\PG=CS [SG(C2H1N1),X(C4
 H10)]\@

PAN_100

1\1\GINC-X103\FOpt\UB3LYP\Gen\C6H10N1O2(2)\GXG501\25-Jun-2010\0\#B3LY
 P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1342
 177280\pan100.freq\0,2\C,-0.0363977361,-0.0675425172,0.0048583491\C,
 -0.017977478,-0.0020096088,1.534356731\C,1.386090632,0.03462232,2.1663
 037861\C,1.346299061,0.1091544925,3.7041448016\C,2.7171603312,0.156697
 3244,4.3841981017\C,2.2118454275,-1.0944018756,1.7049168212\N,2.831682
 3833,-2.0133827144,1.3622130788\H,0.4564387495,-0.9724340886,-0.365658
 0104\H,0.4655568536,0.799390613,-0.4350837018\H,-1.070481103,-0.076305
 7503,-0.3540540941\H,-0.5333908987,0.8976606149,1.8865021848\H,-0.5428
 066401,-0.8651486573,1.9606130292\H,0.764258517,1.0034621491,3.9501449
 848\H,0.7745546824,-0.7577260856,4.0559595929\H,3.2911340827,1.0293693
 675,4.0584959074\H,2.5912190417,0.2220627759,5.4695965916\H,3.30611681
 99,-0.7404585728,4.1668506542\O,2.1268690525,1.2311844535,1.6393187334
 \O,1.517425518,2.3523441261,1.9659448234\Version=EM64L-G09RevA.02\Sta
 te=2-A\HF=-439.7119577\S2=0.753368\S2-1=0.\S2A=0.750008\RMSD=3.880e-09
 \RMSF=4.873e-06\Dipole=-1.072655,0.1302853,0.6674797\Quadrupole=1.5162
 203,-5.4858413,3.969621,2.9139501,2.2374319,-1.2804092\PG=C01 [X(C6H10
 N1O2)]\@

PAN_100H

1\1\GINC-X97\FOpt\RB3LYP\Gen\C6H11N1O2\GXG501\25-Jun-2010\0\#B3LYP/ge
 n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=13421772
 80\pan100h.freq\0,1\C,-0.046303295,0.0032703356,0.0301907305\C,-0.02
 91830587,-0.0478881818,1.5601321636\C,1.3805119345,0.0127449028,2.1908
 333671\C,1.3237227307,-0.0388418523,3.7347275914\C,2.688443189,0.05296
 62722,4.420942049\C,2.2097203013,-1.1008798628,1.6765117175\N,2.821329
 1058,-2.0077262785,1.2894319102\H,0.4777704358,-0.8538088906,-0.405316

886\H,0.4367277564,0.9113651486,-0.3459056735\H,-1.0772139489,-0.00855
33673,-0.3383868487\H,-0.5958877649,0.7903983932,1.978918191\H,-0.5138
777539,-0.9658800448,1.9127664974\H,0.6831557455,0.7899620476,4.053342
1984\H,0.8129625709,-0.967551422,4.0172161615\H,3.1987216726,0.9818925
58,4.1517405813\H,2.5637262853,0.0335037915,5.5086600488\H,3.335849002
9,-0.7853621113,4.1417154312\O,2.1216374468,1.1733400473,1.7314925088\
O,1.4168265373,2.3554427519,2.2047300515\H,1.1697022118,2.7505933082,1
.3491088895\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-440.3436787\\RMSD=6
.587e-09\\RMSF=4.681e-06\\Dipole=-1.2987928,0.8687077,0.1606319\\Quadrupo
le=-0.5271991,-1.7844929,2.311692,1.8754243,2.4205701,-4.5778413\\PG=CO
1 [X(C6H11N1O2)]\\@

PAN_1R

1\1\GINC-X86\FOpt\UB3LYP\Gen\C6H10N1(2)\GXG501\25-Jun-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=1342177
280\\pan1r.freq\\0,2\C,-0.0701564376,-0.3354095529,0.0444466511\C,-0.0
736764573,0.0704367365,1.5208840536\C,1.2374274323,-0.0856713681,2.250
7687097\C,1.3005433641,0.2988652482,3.7083382625\C,2.6587460868,0.1146
109382,4.3909406926\C,2.3633089488,-0.5732195265,1.594458727\N,3.31579
06235,-0.9857953024,1.0388063388\H,0.1989850418,-1.3895151186,-0.07843
69367\H,0.6471241945,0.2592311951,-0.5305319573\H,-1.0628953654,-0.185
2634448,-0.3920436981\H,-0.3948255702,1.1203105981,1.6188485161\H,-0.8
372825203,-0.5085643572,2.0655665548\H,0.9771175694,1.3488298603,3.797
6344562\H,0.5308480641,-0.2785179996,4.2460947898\H,3.433797968,0.7161
205805,3.9049737096\H,2.5998034493,0.420397019,5.4405215159\H,2.981965
1706,-0.9309597127,4.3594521691\\Version=EM64L-G09RevA.02\\State=2-A\\HF
=-289.3640775\\S2=0.765728\\S2-1=0.\\S2A=0.750114\\RMSD=2.121e-09\\RMSF=1.3
05e-05\\Dipole=-1.2684189,0.5499676,0.739494\\Quadrupole=-2.1513164,0.74
4388,1.4069284,1.8976322,3.2635115,-0.9181482\\PG=C01 [X(C6H10N1)]\\@

PAN_2

1\1\GINC-X103\FOpt\RB3LYP\Gen\C7H10N2\GXG501\25-Jun-2010\0\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=134217728
0\\pan2r.freq\\0,1\C,0.0158142205,0.2043604161,-0.1190855522\C,-0.01064
59634,-0.0433095503,1.4032727829\C,1.4145721137,-0.276499715,1.9589043
323\C,1.4900119018,-0.4874932503,3.49201408\C,0.7045395889,-1.71771253
19,3.9919081911\C,-0.6671952561,1.0756112262,2.0989944224\C,2.90321819
32,-0.5945110294,3.8881445829\N,-1.1695661965,1.9600889034,2.659286734
8\N,4.0205491257,-0.6939014875,4.1874805389\H,-0.9955167846,0.34252186
08,-0.5117852848\H,0.6026939051,1.096560481,-0.3587948425\H,0.46942482
42,-0.654456206,-0.6242872832\H,1.8323048151,-1.1546364744,1.452189912
7\H,2.0427138212,0.5790991595,1.6866120572\H,1.0432971156,-2.629603109
5,3.4886071472\H,0.8423564584,-1.8513790756,5.0684230994\H,-0.36592087
7,-1.5899554069,3.8054229808\H,1.08672194,0.4084447311,3.9831998824\H,
-0.6193601404,-0.9362288988,1.5952659478\\Version=EM64L-G09RevA.02\\Sta
te=1-A\\HF=-382.2462225\\RMSD=3.961e-09\\RMSF=1.209e-06\\Dipole=-0.7898229
,-1.0143346,-1.1722251\\Quadrupole=-8.4954589,1.4708754,7.0245835,6.810
2803,-3.3894841,-0.6759684\\PG=C01 [X(C7H10N2)]\\@

PAN_200

1\1\GINC-X100\FOpt\UB3LYP\Gen\C7H9N2O2(2)\GXG501\25-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=13421
77280\\pan200h.freq\\0,2\C,0.0147914159,-0.0929767469,0.0202385641\C,-
0.0608651732,0.1228771635,1.548669657\C,1.3467506579,0.2121538987,2.17
37791426\C,1.4695410214,0.1112516456,3.7178449991\C,0.7708680819,1.220
4292919,4.5307967716\C,-0.9002711447,1.2944338324,1.8474983463\C,1.020
0695954,-1.224694814,4.1324142067\N,-1.5892231708,2.2075380426,2.04328
07584\N,0.6382980097,-2.2795192069,4.4322548067\H,-0.9894847212,-0.176
0816066,-0.4030162362\H,0.5280647969,0.7416746288,-0.4643963248\H,0.55
98629847,-1.0172194448,-0.1965090247\H,1.9628744726,-0.5759426604,1.73

13910655\H,-0.3165650113,1.1658838184,4.4533017111\H,1.0460883478,1.12
46266268,5.5847925433\H,1.0951428619,2.2011082836,4.17386623\H,2.54898
36293,0.1680192496,3.9094005484\H,-0.5459149422,-0.7508795708,2.004352
307\O,1.9208311307,1.4817678019,1.7334274117\O,3.2311692472,1.50460522
52,1.9158822421\Version=EM64L-G09RevA.02\State=2-A\HF=-531.9461122\S2
=0.753103\S2-1=0.\S2A=0.750007\RMSD=4.966e-09\RMSF=3.499e-06\Dipole=0.
5503218,-0.3993832,-0.5118729\Quadrupole=-0.9613403,-6.5808438,7.54218
41,2.1527032,2.5523953,7.8547228\PG=C01 [X(C7H9N2O2)]\@

PAN_20OH

1\1\GINC-V1360\FOpt\RB3LYP\Gen\C7H10N2O2\GXG501\25-Jun-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\pan20oh.freq\0,1\C,-0.1373753439,-0.3471706215,0.1301028078\C,-0
.0041973884,0.1708751726,1.578782056\C,1.4863172433,0.1895890754,2.066
9004189\C,1.6873495369,-0.3198376444,3.5210615724\C,0.9583540349,0.516
5079386,4.5937006472\C,-0.6061712194,1.5043590171,1.7078704861\C,1.293
7146201,-1.7341460829,3.5898837728\N,-1.0608943685,2.5711896867,1.7723
245346\N,0.9540590358,-2.8437000075,3.6310804007\H,-1.1841312028,-0.35
16136487,-0.1868169782\H,0.4403700137,0.277832454,-0.5548456004\H,0.24
21014715,-1.3725333018,0.0772084805\H,2.0666216695,-0.4497200429,1.390
2644573\H,-0.1272089443,0.4834647314,4.4629627699\H,1.1904910168,0.131
8097228,5.5905771396\H,1.2844098204,1.5568716635,4.5314626023\H,2.7667
82103,-0.2693079926,3.712067216\H,-0.5708210602,-0.5064343785,2.230695
8559\O,2.0702824763,1.4839986978,2.0930470723\O,2.0908860805,1.9899838
735,0.730872642\H,1.4431931091,2.7166614743,0.8174499032\Version=EM64
L-G09RevA.02\State=1-A\HF=-532.5817474\RMSD=8.054e-09\RMSF=2.878e-06\D
ipole=0.3265805,0.0522482,-0.1354801\Quadrupole=1.342683,-8.8778884,7.
5352054,2.5882576,2.3006694,3.9478854\PG=C01 [X(C7H10N2O2)]\@

PAN_2R

1\1\GINC-X94\FOpt\UB3LYP\Gen\C7H9N2(2)\GXG501\25-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=13421772
80\pan2r.freq\0,2\C,0.1522882146,0.3876054559,-0.1254469038\C,-0.096
0273179,-0.1730745552,1.2978596329\C,1.1834830039,-0.6454418293,1.9423
309188\C,1.4607166717,-0.5481256412,3.4182310472\C,0.7105544826,-1.630
1441247,4.2496799498\C,-0.8032431442,0.8182268629,2.1267668174\C,2.910
1093124,-0.6348904319,3.6642738794\N,-1.3548414399,1.5980399963,2.7867
339559\N,4.0514911183,-0.7230973047,3.8562992385\H,-0.7916241485,0.666
6136774,-0.6023735069\H,0.8012715736,1.2665062185,-0.0854712994\H,0.63
96066114,-0.377456327,-0.7378139544\H,1.8194213522,-1.2819285748,1.333
5147566\H,1.0008162872,-2.6350115942,3.9297549626\H,0.9415448496,-1.52
01842596,5.3136668864\H,-0.3686878437,-1.5111690815,4.1157204238\H,1.1
260949801,0.4335445528,3.7826201035\H,-0.7862515632,-1.0303340398,1.19
44420915\Version=EM64L-G09RevA.02\State=2-A\HF=-381.5767462\S2=0.7541
74\S2-1=0.\S2A=0.750012\RMSD=9.298e-09\RMSF=5.896e-06\Dipole=-0.853284
3,-0.9234498,-1.0953255\Quadrupole=-10.1094702,2.1503057,7.9591646,5.8
3735,-1.6053575,-0.9846935\PG=C01 [X(C7H9N2)]\@

PE_1

1\1\GINC-V1281\FOpt\RB3LYP\6-31G(d)\C5H12\GXG501\30-May-2010\0\#B3LYP/
/6-31G* OPT Freq=noraman maxdisk=268435456\pe1.freq\0,1\C,-0.0166576
148,0,0.0117787124\C,0.0393079131,0,1.5446162444\C,1.468186129,0,2.
0973320658\C,-1.4431755233,0,-0.5519319373\C,-1.4879882585,0,-2.0833
298457\H,-0.5009718082,-0.8780853915,1.926340865\H,0.5245063781,-0.878
520551,-0.3708820167\H,0.5245063781,0.878520551,-0.3708820167\H,2.0228
55143,0.8846283165,1.7607977499\H,1.4744699646,0,3.193422487\H,2.0228
55143,-0.8846283165,1.7607977499\H,-1.9831621874,-0.8780853915,-0.1697
928713\H,-0.9858109913,-0.8846283165,-2.4940987019\H,-0.9858109913,0.8
846283165,-2.4940987019\H,-2.5192976061,0,-2.4546177765\H,-0.50097180
82,0.8780853915,1.926340865\H,-1.9831621874,0.8780853915,-0.1697928713

\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-197.771782\\RMSD=8.272e-09\\RM
SF=2.286e-05\\Dipole=-0.0175069,0,0.0123792\\Quadrupole=-0.1923596,0.50
6035,-0.3136755,0,-0.1715666,0.\\PG=C02V [C2(C1),SGV(C4H2),SGV'(H2),X(
H8)]\\@

PE_100

1\\1\\GINC-V1284\\FOpt\\UB3LYP\\6-31G(d)\\C5H11O2(2)\\GXG501\\30-May-2010\\0\\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pe100.freq\\0,2\\C,-0.
0386973174,0.0428154675,0.0275315231\\C,0.0285067966,-0.0033961485,1.55
30897982\\C,1.4548414543,-0.0338061272,2.110903131\\C,-1.4545989731,-0.0
031305015,-0.5443943577\\C,-1.505013485,-0.0335172171,-2.0750945114\\H,-
0.5215337914,-0.895294161,1.8805271991\\H,0.581025263,-0.7494450238,-0.
4107578217\\H,2.0133869027,0.8598696973,1.815790005\\H,1.4415757275,-0.0
766465842,3.2051455617\\H,2.0066029239,-0.9100316147,1.7490885716\\H,-1.
9468650044,-0.8949216423,-0.1349766516\\H,-0.980202942,-0.9098894436,-2
.474678465\\H,-1.0403233907,0.8600298006,-2.5033009848\\H,-2.5410931262,
-0.0760611416,-2.4273826928\\H,-0.5143976443,0.865472137,1.9425934342\\H
,-2.0026143335,0.8658564262,-0.1623813623\\O,0.6636350204,1.2509018629,
-0.4689603685\\O,0.0818418073,2.3654243138,-0.0573234746\\Version=EM64L
-G09RevA.02\\State=2-A\\HF=-347.4820501\\S2=0.753278\\S2-1=0.\\S2A=0.750007
\\RMSD=4.087e-09\\RMSF=3.895e-05\\Dipole=-0.3081799,-0.9717697,0.217773\\Q
uadrupole=0.576149,-1.7062271,1.1300781,-0.687064,0.7831663,0.485292\\P
G=C01 [X(C5H11O2)]\\@

PE_100H

1\\1\\GINC-V1284\\FOpt\\RB3LYP\\6-31G(d)\\C5H12O2\\GXG501\\30-May-2010\\0\\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\\pe100h.freq\\0,1\\C,-0.04
08736953,0.0696540127,0.0277426926\\C,0.0211003685,-0.0288075269,1.5562
454933\\C,1.4476184395,-0.0024915808,2.1120635063\\C,-1.4660164336,-0.00
58243532,-0.5325149278\\C,-1.5253163967,-0.0064248364,-2.0632531072\\H,-
0.4820122413,-0.9589270478,1.8538271825\\H,0.5666502895,-0.7362136048,-
0.4124313731\\H,1.9565383418,0.9241475196,1.8316463806\\H,1.4422416912,-
0.0734521306,3.2053823959\\H,2.0411593624,-0.8407792055,1.7261196855\\H,
-1.9370795237,-0.9177545447,-0.1429302063\\H,-0.9994081683,-0.873581887
2,-2.4809556889\\H,-1.0545002002,0.890244852,-2.4805593637\\H,-2.5610712
028,-0.0414332681,-2.4184338307\\H,-0.5630767343,0.7946887556,1.9830903
263\\H,-2.0423862105,0.8358746078,-0.1297539641\\O,0.6746729511,1.217845
4397,-0.4667700127\\O,0.0301022279,2.418462419,0.0616844673\\H,-0.304991
0455,2.802229047,-0.7679001451\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-
348.1120265\\RMSD=7.077e-09\\RMSF=6.882e-06\\Dipole=-0.5646405,-0.234071
2,-0.2857109\\Quadrupole=-1.3657346,1.3580271,0.0077075,-1.6385515,0.66
14274,-1.9457078\\PG=C01 [X(C5H12O2)]\\@

PE_1R

1\\1\\GINC-V1285\\FOpt\\UB3LYP\\6-31G(d)\\C5H11(2)\\GXG501\\30-May-2010\\0\\#B3
LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pe1r.freq\\0,2\\C,-0.181
2559799,0.2626589476,0.1281673326\\C,0.004434855,0.0663559448,1.5990202
62\\C,1.4747175309,-0.0383866379,2.0267940234\\C,-1.5060924757,0.0663559
448,-0.5371879754\\C,-1.4193072204,-0.0383866379,-2.0659750297\\H,-0.542
0074974,-0.8332359174,1.9228572229\\H,0.588867366,0.810088146,-0.416392
1077\\H,2.0308982937,0.8634720431,1.7435735512\\H,1.5663086765,-0.159623
5413,3.1119284147\\H,1.9635971889,-0.8939187193,1.5471556454\\H,-1.99355
63412,-0.8332359174,-0.1299428385\\H,-0.8041399348,-0.8939187193,-2.367
0157322\\H,-0.9668908108,0.8634720431,-2.4959404575\\H,-2.411851354,-0.1
596235413,-2.5140394537\\H,-0.4681849843,0.8982235569,2.157705166\\H,-2.
190365601,0.8982235569,-0.277826019\\Version=EM64L-G09RevA.02\\State=2-
A\\HF=-197.1051495\\S2=0.753915\\S2-1=0.\\S2A=0.750011\\RMSD=6.779e-09\\RMS
F=4.252e-06\\Dipole=-0.0653488,0.046145,0.0462086\\Quadrupole=-0.0027291
0,0.0374532,-0.0347241,0.2570474,-0.0452477,-0.18176\\PG=CS [SG(C1H1),X(
C4H10)]\\@

PE_200

1\1\GINC-V1281\FOpt\UB3LYP\6-31G(d)\C7H15O2(2)\GXG501\30-May-2010\0\#\nB3LYP/6-31G* OPT Freq=normal maxdisk=268435456\pe200.freq\0,2\C,-0.0704277643,-0.0177712724,-0.0134597833\C,-0.0097942902,0.0069079999,1.5126540706\C,1.4134346549,-0.0121611335,2.0862944838\C,1.4308679238,0.0105190509,3.6178122902\C,-1.4820775352,-0.1039979687,-0.5906799549\C,-1.5301790939,-0.2334136764,-2.1190525374\C,-2.9616171636,-0.3202478789,-2.6574071921\O,0.6226447868,1.1748151488,-0.5613167994\O,0.0277873375,2.3009243088,-0.2044712214\H,2.4564556656,-0.0049349973,4.0029649507\H,0.9045613348,-0.8566076847,4.0359158052\H,0.9430213621,0.9128349563,4.0058398\H,1.9710292486,0.8486491529,1.6983045615\H,-0.5453310195,0.8989296198,1.8602214436\H,-0.5691095169,-0.8632736717,1.882889571\H,-1.9781075811,-0.9697740918,-0.1307706248\H,-2.0364137214,0.7863281378,-0.2692416399\H,-1.017652223,0.6243517683,-2.5707066011\H,-3.5380372108,0.5751525777,-2.3952393148\H,-3.4913411899,-1.1879450697,-2.2448362628\H,-2.969754104,-0.4132914723,-3.7490514509\H,0.5602976104,-0.8217196171,-0.4126251566\H,1.9386341042,-0.908136448,1.7257550766\H,-0.967000896,-1.1262455113,-2.426092696\Version=EM64L-G09RevA.02\State=2-A\HF=-426.1094489\S2=0.753288\S2-1=0.\S2A=0.750007\RMSD=4.193e-09\RMSF=3.798e-06\Dipole=-0.269245,-0.9486597,0.2384125\Quadrupole=0.5724009,-1.8473543,1.2749534,-1.0396195,1.1391083,0.9368578\PG=C01 [X(C7H15O2)]\@

PE_200H

1\1\GINC-V1284\FOpt\UB3LYP\6-31G(d)\C7H15O2(2)\GXG501\30-May-2010\0\#\nB3LYP/6-31G* OPT Freq=normal maxdisk=268435456\pe200h.freq\0,2\C,-0.0626480517,-0.1661503859,0.0177618784\C,-0.0060110553,0.0195571621,1.5364228252\C,1.4097521062,-0.0794955902,2.1167509293\C,1.4515818414,0.1621027832,3.6287374531\C,-1.4994337121,-0.2450303574,-0.5256024805\C,-1.5987349031,-0.1587778994,-2.0160990818\C,-2.926723625,-0.1787376979,-2.6979711024\O,0.7205818773,0.8220842716,-0.6751093931\H,2.4738956889,0.0855757101,4.0162165311\H,0.8356313061,-0.5687501548,4.1679554885\H,1.0746022311,1.1610813819,3.8798295911\H,2.0522369451,0.6462221725,1.6047372538\H,-0.4402984183,0.9984218388,1.7764362259\H,-0.6545449807,-0.7361571197,2.0033082606\H,-1.9425278975,-1.1903436898,-0.1599226215\H,-2.1087306527,0.5461725944,-0.06165945\H,-3.6636681511,0.4441143588,-2.1723696584\H,-3.356082684,-1.1967657379,-2.7347310458\H,-2.8605212785,0.1722150941,-3.7340419452\H,0.4808351022,-1.0798789007,-0.2655778185\H,1.8259028676,-1.0725285489,1.8926500034\H,-0.7033004519,-0.3424639421,-2.605530845\O,0.0612108478,2.1123581867,-0.5389358541\H,-0.4580537566,2.1187795968,-1.3667825658\Version=EM64L-G09RevA.02\State=2-A\HF=-426.074286\S2=0.753878\S2-1=0.\S2A=0.750011\RMSD=6.236e-09\RMSF=6.123e-06\Dipole=-0.7612612,-0.5265182,-0.2289824\Quadrupole=-0.658417,-0.7356844,1.3941014,-1.6509894,1.9221647,-0.7363746\PG=C01 [X(C7H15O2)]\@

PP_1

1\1\GINC-V1283\FOpt\RB3LYP\6-31G(d)\C8H18\GXG501\30-May-2010\0\#\nB3LYP/6-31G* OPT Freq=normal maxdisk=268435456\pp1.freq\0,1\C,0.0357221908,-0.3615228125,0.0559100462\C,-0.0090309355,-0.2532157673,1.5955051207\C,1.3490440583,0.0387107417,-0.6479605259\C,0.2296264195,1.186193203,2.0774560701\C,1.1720185629,-0.0345682206,-2.1727556513\C,2.5411442052,-0.823050121,-0.2043017743\C,-1.3500170653,-0.8171640507,2.1135526696\C,-1.4473696145,-0.9685276695,3.6362046657\H,3.4527136409,-0.5372952253,-0.7427911123\H,2.3531817979,-1.8851043144,-0.4114404102\H,2.7474653692,-0.7250209125,0.8671341668\H,0.9482727382,-1.0605359223,-2.4938774113\H,0.3484870256,0.6058922395,-2.5108760506\H,1.2047324366,1.5660739172,1.7546069511\H,-0.5390784487,1.8622143818,1.6790878636\H,0.2012703212,1.2569030771,3.1698513075\H,2.0820295517,0.2850467901,-2.6945908848\H,-0.7802181371,0.2530310276,-0.3551602227\H,-0.1983411467,-1.399

5594952,-0.2270014431\H,-1.5134193213,-1.8013115672,1.6525925099\H,-2.169545913,-0.1760984666,1.7555450702\H,-2.3929446084,-1.4441599667,3.9211389828\H,-1.4000424001,-0.0034610822,4.1522956377\H,-0.6326575901,-1.5930767004,4.0241044106\H,0.7889044101,-0.8874290641,2.0106180291\H,1.575338116,1.0845738276,-0.3955580004\\Version=EM64L-G09RevA.02\State=1-A\HF=-315.7097914\RMSD=4.556e-09\RMSF=2.025e-06\Dipole=0.0077495,0.008364,0.0155612\Quadrupole=0.1463066,0.293058,-0.4393646,0.0585431,0.0539782,-0.099827\PG=C01 [X(C8H18)]\\@

PP_100

1\1\GINC-V1287\FOpt\UB3LYP\6-31G(d)\C8H17O2(2)\GXG501\31-May-2010\0\#B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pp100.freq\0,2\C,0.3605826411,-0.722462865,0.3389334429\C,-0.0095446008,-0.2445417585,1.7562430196\C,1.4666284532,0.0150042129,-0.4451306886\C,-0.1270136079,1.2720711779,1.8918769609\C,1.5234526724,-0.5452117377,-1.8766968802\C,2.8529058868,-0.0698858215,0.213005233\C,-1.2633980362,-0.9963923887,2.2465906033\C,-1.6767646934,-0.7423481545,3.7005354939\H,3.604907457,0.4193460027,-0.4175760279\H,3.1571249371,-1.1150839553,0.3491247136\H,2.8769457794,0.4048525358,1.1978185494\H,1.7973702994,-1.6080746263,-1.8707858872\H,0.5566021539,-0.4526730441,-2.386101689\H,0.8039731216,1.7702989747,1.6096325596\H,-0.9248953255,1.6418955391,1.2387621183\H,-0.3636709433,1.5594987605,2.9196543502\H,2.2713298874,-0.0133664008,-2.476132543\H,-0.5638716339,-0.6787583722,-0.2530480307\H,0.6224011938,-1.7851217153,0.4208266266\H,-1.077292948,-2.0667719176,2.1058400983\H,-2.0880128636,-0.7283594485,1.5735660136\H,-2.5325445919,-1.3750515548,3.9597683128\H,-1.975401603,0.2970575695,3.8736410458\H,-0.8632122765,-0.9822779639,4.3919457738\H,1.1890702895,1.0761122745,-0.5233388012\O,1.1142002484,-0.5697451301,2.6950130181\O,1.3770783738,-1.8614186317,2.7589604922\\Version=EM64L-G09RevA.02\State=2-A\HF=-465.4221752\S2=0.753389\S2-1=0.\S2A=0.750008\RMSD=8.168e-09\RMSF=3.535e-06\Dipole=-0.7237082,0.551563,-0.5493994\Quadrupole=0.8540583,0.1308422,-0.9849004,0.7988126,-2.0583639,1.2268793\PG=C01 [X(C8H17O2)]\\@

PP_100H

1\1\GINC-V1338\FOpt\RB3LYP\6-31G(d)\C8H18O2\GXG501\31-May-2010\0\#B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pp100h.freq\0,1\C,0.1993653349,-0.4989992597,0.1570887706\C,0.1094064904,-0.1569143446,1.6700120897\C,1.4598752714,-0.0529418579,-0.6254475135\C,0.0002510046,1.3551308695,1.8974162222\C,1.0891170498,0.2776493632,-2.0809482467\C,2.5736378183,-1.1118207425,-0.5884482143\C,-1.0917818808,-0.935745877,2.2614808179\C,-1.5237397899,-0.6212287473,3.699663402\H,3.4661935643,-0.7576008616,-1.1186792301\H,2.2427186781,-2.0363776092,-1.0803665741\H,2.8546877636,-1.3584008213,0.4380031601\H,0.6488462578,-0.5950881874,-2.5811958343\H,0.3597838223,1.0950601786,-2.1358205129\H,0.8082333096,1.8915729883,1.3895507507\H,-0.9529300023,1.7291533341,1.507586637\H,0.0471048064,1.5931281274,2.9622026729\H,1.973400872,0.5762124933,-2.6565200786\H,-0.6890048465,-0.0415217606,-0.2971754121\H,0.0754573598,-1.5839064988,0.0394833859\H,-0.8469458705,-2.0021740587,2.1801267425\H,-1.9482487691,-0.7641570829,1.594037231\H,-2.3933166663,-1.2343132302,3.9644715065\H,-1.8183385042,0.4276029619,3.8178213058\H,-0.726706538,-0.8309071067,4.4158329465\H,1.8547031314,0.864684659,-0.1686422838\O,1.3648656583,-0.6637275176,2.1857753914\O,1.5031223775,-0.3441429933,3.6020961975\H,2.2296475398,0.3023765466,3.5544759781\\Version=EM64L-G09RevA.02\State=1-A\HF=-466.0474589\RMSD=3.388e-09\RMSF=5.520e-06\Dipole=-0.0605275,0.6196542,-0.1952881\Quadrupole=1.5090812,0.0283383,-1.5374195,2.0477643,1.4577884,2.3132336\PG=C01 [X(C8H18O2)]\\@

PP_1R

1\1\GINC-V1283\FOpt\UB3LYP\6-31G(d)\C8H17(2)\GXG501\30-May-2010\0\#B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pp1r.freq\0,2\C,-0.169

817139,-0.0055250921,-0.156551197\C,-0.4430037641,0.1791499964,1.31116
 4415\C,1.3325308774,-0.0401233309,-0.5522674173\C,-0.234479326,1.53673
 96577,1.9167178816\C,1.4876501052,-0.061327051,-2.0791851251\C,2.06008
 12434,-1.2264243182,0.0934020319\C,-1.2384733104,-0.8458552653,2.07299
 25577\C,-0.7705107035,-1.1047360609,3.5167105647\H,3.128506394,-1.2190
 382763,-0.1535845058\H,1.6442680292,-2.1795976958,-0.2600677545\H,1.96
 3823287,-1.2039647646,1.1846516812\H,1.0346476345,-0.9658992058,-2.506
 1113216\H,1.001976748,0.8050885693,-2.5443219195\H,0.4090767409,2.1668
 157873,1.2926661131\H,-1.1906841884,2.0781550705,2.0418758336\H,0.2198
 583797,1.490365049,2.915538167\H,2.5445560414,-0.0512698903,-2.3714454
 488\H,-0.640910313,0.8123049545,-0.7308898153\H,-0.6377752201,-0.93484
 45606,-0.5124007185\H,-1.2290126368,-1.7946738694,1.5211143029\H,-2.30
 27444809,-0.5399086536,2.1141165523\H,-1.3830498477,-1.8821293852,3.98
 75650891\H,-0.8480377034,-0.2051100519,4.13696038\H,0.2739288632,-1.43
 72733079,3.538976628\H,1.7963245027,0.8850188558,-0.1786739058\\Versio
 n=EM64L-G09RevA.02\State=2-A\HF=-315.0502773\S2=0.754128\S2-1=0.\S2A=0
 .750013\RMSD=5.738e-09\RMSF=2.153e-06\Dipole=-0.0488345,0.0584992,0.01
 18468\Quadrupole=0.02535,0.3096275,-0.3349776,0.2803019,-0.2106982,0.1
 324173\PG=C01 [X(C8H17)]\@

PP_200

1\1\GINC-V1297\FOpt\UB3LYP/6-31G(d)\C8H17O2(2)\GXG501\31-May-2010\0\#
 B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pp2oo.freq\0,2\C,0.0
 808846694,-0.4297024009,0.0539185109\C,0.0084428962,-0.30532244,1.5891
 881311\C,1.3667722354,0.0675548308,-0.6387404148\C,0.3207405025,1.1301
 352965,2.0446268784\C,1.2507148693,-0.0439174557,-2.1675772181\C,2.635
 7537171,-0.635277852,-0.1294208833\C,-1.3734222493,-0.7750554688,2.098
 3237581\C,-1.4453664432,-1.0018260242,3.612605328\H,3.5180069357,-0.24
 43360322,-0.6483214376\H,2.5872597279,-1.7132133143,-0.3175534161\H,2.
 7914990864,-0.4867160212,0.944628015\H,1.1835503387,-1.0883273415,-2.4
 891278981\H,0.3621073642,0.4767697877,-2.542248245\H,1.3481329024,1.42
 59788242,1.8119829818\H,-0.3550824752,1.8510270979,1.5664781313\H,0.19
 28099718,1.2271027051,3.1268641184\H,2.1304660309,0.4003532959,-2.6468
 51558\H,-0.7914804607,0.0487965111,-0.4039041997\H,-1.6378476426,-1.70
 97440843,1.5922411751\H,-2.131918968,-0.0370972643,1.7979617512\H,-2.4
 345120836,-1.3756916156,3.8994646944\H,-1.2666750957,-0.0835646042,4.1
 831697392\H,-0.705122772,-1.7443128307,3.9355053717\H,0.7685109294,-0.
 9777401526,2.0115690291\H,1.4407963988,1.1358789948,-0.3941588172\O,-0.
 .0680270547,-1.8670055453,-0.2487349525\O,-0.9536487461,-2.1005422856,
 -1.2042430648\\Version=EM64L-G09RevA.02\State=2-A\HF=-465.4181356\S2=0
 .753403\S2-1=0.\S2A=0.750007\RMSD=7.100e-09\RMSF=3.922e-06\Dipole=0.41
 40647,0.8691666,0.5392149\Quadrupole=1.1359907,-1.1279358,-0.008055,-1
 .1211057,-2.0137632,-2.2845219\PG=C01 [X(C8H17O2)]\@

PP_200H

1\1\GINC-V1298\FOpt\RB3LYP/6-31G(d)\C8H18O2\GXG501\31-May-2010\0\#B3L
 YP/6-31G* OPT Freq=norman maxdisk=268435456\pp2ooh.freq\0,1\C,-0.05
 76890949,-0.2510063921,0.0447334918\C,-0.0572443338,-0.2371840653,1.59
 52147229\C,1.2712129325,0.1409378159,-0.640600054\C,0.5321593353,1.067
 9949693,2.1550636414\C,1.1238560221,0.2226681437,-2.1689481119\C,2.425
 7111621,-0.798833192,-0.258752899\C,-1.4855420325,-0.4822138475,2.1312
 822272\C,-1.5542702659,-0.839857213,3.6204513519\H,3.3452498629,-0.507
 0697165,-0.7789526889\H,2.1881635315,-1.8292713718,-0.5432848942\H,2.6
 369515947,-0.7858453878,0.8165673278\H,0.9204043995,-0.760844448,-2.60
 26501097\H,0.3026858212,0.8883388638,-2.4590148137\H,1.5924926751,1.18
 30337041,1.9129506591\H,-0.0008919234,1.9423400946,1.7591588816\H,0.44
 44342593,1.0950040474,3.2457796047\H,2.0471497523,0.6091870386,-2.6169
 367659\H,-0.8530362598,0.4194820746,-0.3090592707\H,-1.935355177,-1.29
 84319677,1.5555213556\H,-2.096569998,0.41255967,1.9388492018\H,-2.5880
 623319,-1.0400323292,3.9245232138\H,-1.1772091594,-0.0348144555,4.2610
 762036\H,-0.9654359324,-1.7399380388,3.8362048373\H,0.5726259006,-1.07
 38642173,1.9298099626\H,1.5141779406,1.1526430375,-0.287215081\O,-0.44
 21873651,-1.5982910517,-0.3093327194\O,-1.1993218322,-1.5650051771,-1.

5537716883\H,-2.0689248063,-1.852347127,-1.2208384106\\Version=EM64L-G
09RevA.02\\State=1-A\\HF=-466.0463415\\RMSD=4.060e-09\\RMSF=4.002e-06\\Dipo
le=-0.3979473,0.3343468,0.4112768\\Quadrupole=3.3249652,-0.899234,-2.42
57312,1.5914985,1.0076233,-0.5870532\\PG=C01 [X(C8H18O2)]\\@

PP_2R

1\1\GINC-V1281\FOpt\UB3LYP\6-31G(d)\C8H17(2)\GXG501\31-May-2010\0\#B3
LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pp2.freq\\0,2\C,0.19542
56179,-0.2368094973,0.1634728651\C,0.0070686509,0.0004765293,1.6344187
981\C,1.5232574135,-0.1119120176,-0.5255867717\C,-0.293110137,1.493944
5595,1.9159290002\C,1.3732386829,0.4171476175,-1.962354722\C,2.2903983
427,-1.457328116,-0.5204296034\C,-1.0829519055,-0.9302983703,2.2117802
104\C,-1.2409552778,-0.8773321276,3.7355073709\H,3.2823242039,-1.34556
88195,-0.977074467\H,1.7402028875,-2.2188092173,-1.0863992669\H,2.4274
9442,-1.8320375769,0.5001794456\H,0.7653272424,-0.2684804803,-2.566800
9643\H,0.8833841003,1.3972053606,-1.9757535702\H,0.4834363871,2.134801
9639,1.4835165463\H,-1.2526760659,1.7860278002,1.4716302719\H,-0.33695
3899,1.7043258361,2.9909970284\H,2.3489026272,0.5163303384,-2.45314318
35\H,-0.6729503286,-0.5194703731,-0.4325049563\H,-0.8477954004,-1.9602
806626,1.9122547466\H,-2.0434333772,-0.6868999623,1.7336845025\H,-1.97
97387958,-1.6120219323,4.0759514083\H,-1.5746476208,0.1069336693,4.081
8327286\H,-0.2929652946,-1.1035457339,4.2399461911\H,0.9555756283,-0.2
366921003,2.1458529062\H,2.1378595696,0.6074410582,0.0396841405\\Versi
on=EM64L-G09RevA.02\\State=2-A\\HF=-315.044656\\S2=0.75405\\S2-1=0.\\S2A=0.
750011\\RMSD=7.143e-09\\RMSF=5.496e-06\\Dipole=0.0267981,0.000409,0.02925
92\\Quadrupole=0.5332323,-0.3784042,-0.1548282,0.3040646,0.1372168,0.08
17\\PG=C01 [X(C8H17)]\\@

PP_300

1\1\GINC-V1362\FOpt\UB3LYP\6-31G(d)\C8H17O2(2)\GXG501\31-May-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pp3oo.freq\\0,2\C,0.0
001764631,-0.3777249007,0.07441278\C,-0.0392538245,-0.3125206622,1.617
7486828\C,1.2966426443,0.0762592309,-0.6292428691\C,0.2544603359,1.094
5656765,2.1522330847\C,1.1180556457,-0.0112989388,-2.1530349821\C,2.52
72445741,-0.7292337312,-0.1847061296\C,-1.3686992131,-0.8959883895,2.1
442487391\C,-1.4617145968,-1.0365153652,3.6678483233\H,3.4211581463,-0
.4099303612,-0.7331237763\H,2.3840193632,-1.800456668,-0.3791906406\H,
2.7403774076,-0.6124579562,0.8840754059\H,0.9448342713,-1.048435231,-2
.4689965527\H,0.2633363628,0.5870426229,-2.4895382878\H,0.2000741714,1
.1510279551,3.2408962834\H,1.2310161657,1.4539770315,1.8160063327\H,2
.00989967,0.3510675466,-2.6776761623\H,-0.8358293148,0.2173765846,-0.31
65887938\H,-0.2037086267,-1.4175589342,-0.2201706591\H,-1.4960002676,-
1.8852324385,1.6844269138\H,-2.2026092981,-0.2815094709,1.7828910587\H
,-2.3724313571,-1.5772000462,3.9485413141\H,-1.4987026481,-0.060498491
4,4.1617560843\H,-0.6081143373,-1.5952363193,4.0731144482\H,0.77355350
29,-0.9372002931,2.0192929882\H,1.4750848065,1.1340046365,-0.385471436
6\O,-0.679063437,2.0868322281,1.6268376033\O,-1.7530483971,2.207608626
9,2.3934046686\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-465.4144244\\S2=
0.753198\\S2-1=0.\\S2A=0.750007\\RMSD=5.004e-09\\RMSF=4.656e-06\\Dipole=0.7
765503,-0.6886165,-0.0503737\\Quadrupole=-0.0686222,-1.5638335,1.632455
7,3.4927896,1.4933847,-0.8869515\\PG=C01 [X(C8H17O2)]\\@

PP_300H

1\1\GINC-V1298\FOpt\RB3LYP\6-31G(d)\C8H18O2\GXG501\31-May-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\\pp3ooh.freq\\0,1\C,0.024
0867921,-0.4466707116,-0.0058795887\C,-0.0237459931,-0.262854764,1.528
0049325\C,1.3093080786,-0.0041464572,-0.7341574176\C,0.2533709025,1.18
42077831,1.9597284527\C,1.1375555561,-0.1880635544,-2.2501811328\C,2.5
582916175,-0.7503287785,-0.2402944129\C,-1.3602177959,-0.8046568695,2.
0832312751\C,-1.4630074029,-0.8502280604,3.6120385002\H,3.449022193,-0

.4349058341,-0.7965780002\H,2.4469030744,-1.8339902782,-0.3803469013\H
 ,2.7565069473,-0.5716746123,0.8226521797\H,0.9871612283,-1.2459300161,
 -2.5035670188\H,0.2707925454,0.370293897,-2.6230415729\H,0.2344431865,
 1.2828750633,0.0539587855\H,1.2375697435,1.5182721719,1.6103728407\H,2
 .0222916756,0.1614597335,-2.7955113293\H,-0.8247392122,0.0934520962,-0
 .4440324734\H,-0.1453378122,-1.512467424,-0.2216113702\H,-1.498749841,
 -1.8207927861,1.6901266009\H,-2.1852937418,-0.2052683252,1.6781958372\
 H,-2.3982629137,-1.3297848108,3.9225529415\H,-1.449745557,0.1509703714
 ,4.0569385002\H,-0.6362020098,-1.4217473475,4.0526119775\H,0.786122634
 7,-0.8556281933,1.9796864964\H,1.4563056473,1.0696148758,-0.5515627435
 \O,-0.7576119473,2.0081202129,1.3816677864\O,-0.424895559,3.3828168808
 ,1.7227407949\H,-1.1614769576,3.5885245379,2.3264999868\Version=EM64L
 -G09RevA.02\State=1-A\HF=-466.0450467\RMSD=3.214e-09\RMSF=2.947e-06\Di
 pole=-0.1143719,-0.2634506,0.5636407\Quadrupole=0.240711,-1.0666512,0.
 8259403,-1.7418942,-1.7023236,2.7053778\PG=C01 [X(C8H18O2)]\@

PP_3R

1\1\GINC-V1338\FOpt\UB3LYP\6-31G(d)\C8H17(2)\GXG501\31-May-2010\0\#B3
 LYP/6-31G* OPT Freq=norman maxdisk=268435456\pp3.freq\0,2\C,0.03586
 34144,-0.4188012176,0.0082202269\C,0.0053480337,-0.2590111998,1.547074
 6721\C,1.3403664746,0.0099778096,-0.6920437327\C,0.1994067293,1.167653
 4708,1.9565026379\C,1.1611985536,-0.018566454,-2.2174027541\C,2.541291
 5618,-0.8523445934,-0.2746515922\C,-1.3250316392,-0.8436714874,2.10501
 41687\C,-1.4050057815,-0.872081964,3.6339049925\H,3.450992105,-0.53702
 62935,-0.799540584\H,2.3679692301,-1.9093994032,-0.5176373184\H,2.7417
 989848,-0.7845180705,0.8000385881\H,0.939684876,-1.0351828217,-2.56884
 49771\H,0.3357281582,0.6294717221,-2.5360150339\H,0.78537275,1.4442120
 202,2.826988837\H,-0.3648524969,1.9561877546,1.4632041925\H,2.06966026
 58,0.3181480147,-2.7311333411\H,-0.7966369728,0.1665094728,-0.41110970
 21\H,-0.1740598766,-1.4693851076,-0.2440423012\H,-1.4433294924,-1.8643
 90783,1.7144257846\H,-2.1637941036,-0.2589678008,1.7019050268\H,-2.349
 2186823,-1.3154474419,3.9704995104\H,-1.3395011229,0.1368872718,4.0561
 339605\H,-0.5881452301,-1.4661513269,4.0628561929\H,0.8178757996,-0.86
 04232733,1.9802135249\H,1.5523107329,1.047861697,-0.3954184844\Versio
 n=EM64L-G09RevA.02\State=2-A\HF=-315.0386566\S2=0.753897\S2-1=0.\S2A=0
 .75001\RMSD=5.862e-09\RMSF=6.174e-06\Dipole=-0.0360308,-0.0207241,0.03
 4882\Quadrupole=-0.0279107,0.4195323,-0.3916216,-0.107712,0.4190514,-0
 .0835718\PG=C01 [X(C8H17)]\@

PVC_1

1\1\GINC-V1303\FOpt\RB3LYP\6-31G(d)\C6H13Cl1\GXG501\31-May-2010\0\#B3
 LYP/6-31G* OPT Freq=norman maxdisk=268435456\pvc1.freq\0,1\C,-0.000
 0269769,-0.0187396429,0.0090101912\C,0.0150718226,-0.011298593,1.54214
 33748\C,1.4363999634,0.0211466744,2.1136067435\C,-1.3843765986,-0.1161
 666417,-0.6328824877\C,-1.3356498229,-0.2865792435,-2.152267063\C,-2.6
 911418358,-0.5289966002,-2.820375659\Cl,-2.3719503862,1.3870167069,-0.
 2118564348\H,-2.5652023003,-0.6902151358,-3.8965367142\H,-3.3613151552
 ,0.3242830632,-2.6813257793\H,-0.8452367361,0.5911136719,-2.5917815653
 \H,-0.6756313701,-1.1441201408,-2.3486011409\H,0.573876943,-0.88694482
 65,-0.3496225913\H,0.5112727315,0.8727683286,-0.3780568291\H,-0.550056
 8124,0.8535736013,1.9074745579\H,1.9749089844,0.9186525669,1.785485461
 3\H,1.4223026122,0.0245224132,3.2091213805\H,2.0184945126,-0.850983257
 6,1.7905591942\H,-0.509819798,-0.9034688359,1.9124742843\H,-1.95313120
 36,-0.9356105627,-0.1810568173\H,-3.1841211816,-1.4164978728,-2.404990
 9271\Version=EM64L-G09RevA.02\State=1-A\HF=-696.6839308\RMSD=5.984e-0
 9\RMSF=6.118e-06\Dipole=0.5148491,-0.6760246,-0.2100656\Quadrupole=-1.
 0676921,-0.1768644,1.2445565,1.2465655,0.3352879,0.166884\PG=C01 [X(C6
 H13Cl1)]\@

PVC_100

1\1\GINC-V1289\FOpt\UB3LYP\6-31G(d)\C6H12Cl1O2(2)\GXG501\31-May-2010\0
 \#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvcloo.freq\0,2\C
 , -0.0457320783, -0.0697136754, -0.0051139222\C, -0.0249354857, -0.00565990
 99, 1.5272938342\C, 1.4073155279, 0.0083914119, 2.0726216795\C, -1.42208099
 86, -0.1292236078, -0.6685478008\C, -1.3592350442, -0.262446491, -2.1915154
 25\C, -2.704211378, -0.3922144854, -2.9106756794\Cl, -2.4372904843, 1.29835
 51284, -0.1885700185\H, -2.5342436594, -0.5271931134, -3.9838662603\H, -3.3
 220955989, 0.499591871, -2.7744701998\H, -0.8028371447, 0.6030543301, -2.56
 86059167\H, -0.7464474512, -1.149913309, -2.387981157\H, 0.4881780037, -0.9
 67266423, -0.3411167136\H, 0.4815345884, 0.7940017166, -0.4283191412\H, -0.
 5581586074, 0.8891978916, 1.8661610773\H, 1.9664335923, 0.8769869102, 1.703
 4343382\H, 1.4081831042, 0.0533827612, 3.1669840959\H, 1.9579631409, -0.892
 5683048, 1.7759977191\H, -0.5668626093, -0.8670665796, 1.9340167352\H, -3.2
 659475776, -1.257416387, -2.5466399974\O, -2.20363915, -1.258694951, -0.101
 9424276\O, -1.6111019401, -2.413019049, -0.3552426168\Version=EM64L-G09R
 evA.02\State=2-A\HF=-846.3887652\S2=0.753347\S2-1=0.\S2A=0.750007\RMSD
 =2.457e-09\RMSF=1.878e-06\Dipole=0.7484613, 0.3443719, -0.4382168\Quadru
 pole=0.0922401, -3.2330876, 3.1408475, -0.129153, 1.0235687, 0.3335951\PG=C
 01 [X(C6H12Cl1O2)]\@

PVC_100H

1\1\GINC-V1351\FOpt\RB3LYP\6-31G(d)\C6H13Cl1O2\GXG501\01-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvclooh.freq\0,1\C, -
 0.02401703, -0.0982939915, 0.1118996098\C, 0.114124796, 0.0410244353, 1.633
 0598574\C, 1.5811141767, 0.1716547827, 2.0568658484\C, -1.4538442078, -0.20
 55484506, -0.4451245686\C, -1.4457256359, -0.4506932343, -1.9634930503\C, -
 2.7402120891, -0.3258881749, -2.7735568381\Cl, -2.3393031422, 1.4372879426
 , -0.101881401\H, -2.5061878174, -0.4592659839, -3.8360008001\H, -3.1898111
 091, 0.6636979764, -2.6526012023\H, -0.702712615, 0.2419429859, -2.37644241
 35\H, -1.031459778, -1.4611984541, -2.0816504469\H, 0.5045373174, -1.001556
 812, -0.2238125374\H, 0.452249959, 0.7518645365, -0.3890472763\H, -0.448061
 7322, 0.9195902339, 1.9686440341\H, 2.049902316, 1.0560896197, 1.6079704587
 \H, 1.667094668, 0.266569542, 3.1447942797\H, 2.166670183, -0.7049245985, 1.
 7529684843\H, -0.3377439026, -0.8279914044, 2.122896282\H, -3.4741111087, -
 1.0783918835, -2.483798868\O, -2.0591646827, -1.189171807, 0.3331494642\O,
 -3.4154539548, -1.453102256, -0.0934986975\H, -3.8807029885, -0.7093728766
 , 0.3409540697\Version=EM64L-G09RevA.02\State=1-A\HF=-847.0253019\RMSD
 =3.090e-09\RMSF=6.428e-06\Dipole=0.4267172, -0.0309974, -0.2060774\Quad
 upole=2.6157169, -4.08521, 1.4694931, -0.7534311, -0.7566073, 0.5818361\PG=
 C01 [X(C6H13Cl1O2)]\@

PVC_1R

1\1\GINC-V1444\FOpt\UB3LYP\6-31G(d)\C6H12Cl1(2)\GXG501\31-May-2010\0\#
 B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc1r.freq\0,2\C, 0.
 1624429968, 0.2438385036, -0.0897631381\C, -0.0422233961, -0.0388621996, 1.
 4125036314\C, 1.2841374666, -0.1630989981, 2.1680255754\C, -1.0977730249, 0.
 3815673137, -0.8870328812\C, -1.2976032718, -0.1765397581, -2.2631731875\
 C, -2.7116986977, -0.7097724664, -2.5483939153\Cl, -2.1392866069, 1.7346658
 281, -0.446883061\H, -2.7714306418, -1.1031954928, -3.569150693\H, -3.45935
 17163, 0.0824650663, -2.4459184956\H, -1.0476385094, 0.5874286895, -3.02045
 37987\H, -0.5681245108, -0.9859719568, -2.3959410435\H, 0.7474931564, -0.57
 33493583, -0.5333588085\H, 0.7794773977, 1.1541598668, -0.1931588055\H, -0.
 6448970768, 0.7657208851, 1.8498418409\H, 1.8726232222, 0.7594557392, 2.091
 2720014\H, 1.1154357646, -0.3625353649, 3.232073438\H, 1.897150016, -0.9810
 862762, 1.7694220283\H, -0.6263585425, -0.9612159935, 1.5252318293\H, -2.97
 45754295, -1.5146077919, -1.8535645208\Version=EM64L-G09RevA.02\State=2
 -A\HF=-696.0227574\S2=0.754105\S2-1=0.\S2A=0.750013\RMSD=1.976e-09\RMS
 F=7.164e-06\Dipole=0.4588455, -0.4581732, -0.1960182\Quadrupole=-0.59832
 52, -0.6879887, 1.2863139, 0.5246236, 0.2748352, 0.5127536\PG=C01 [X(C6H12C
 l1)]\@

PVC_200

1\1\GINC-V1297\FOpt\UB3LYP\6-31G(d)\C6H12Cl1O2(2)\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc11oo.freq\0,2\C,-0.126061092,0.3222013916,0.2022228706\C,0.0044060556,-0.2910019858,1.5947966981\C,1.422975267,-0.1904940784,2.1661633301\C,-1.5359230587,0.3042733154,-0.4175191183\C,-1.5886613522,0.8419419084,-1.8489798812\C,-2.9575296529,0.7056032518,-2.5206998621\Cl,-2.6385580756,1.2997311549,0.660356768\H,-2.9095758935,1.0645180701,-3.5541699403\H,-3.7226069246,1.2852840708,-1.9959938209\H,-1.2668898307,1.8910769095,-1.8465663599\H,-0.8431350728,0.2836542801,-2.426783884\H,0.2732354332,1.3420662965,0.1779949096\H,-0.7027269484,0.2194581717,2.2552109476\H,1.7445469938,0.8544089752,2.2525962127\H,1.4627599416,-0.6343500425,3.1662340351\H,2.1474281187,-0.7155904531,1.5359869699\H,-0.3092623636,-1.3394152081,1.533315622\H,-1.9330758347,-0.7125497604,-0.3721135681\H,-3.2825986243,-0.3413830289,-2.5460095067\O,0.786931186,-0.3761209151,-0.7308568827\O,0.48172272,-1.6587894355,-0.856162021\Version=EM64L-G09RevA.02\State=2-A\HF=-846.3893219\S2=0.753349\S2-1=0.\S2A=0.750007\RMSD=4.652e-09\RMSF=7.108e-06\Dipole=0.0279382,0.2812785,0.0782487\Quadrupole=-1.7467273,-0.9568074,2.7035347,3.044313,3.47055,-2.0936432\PG=C01 [X(C6H12Cl1O2)]\@

PVC_200H

1\1\GINC-V1302\FOpt\RB3LYP\6-31G(d)\C6H13Cl1O2\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc11ooh.freq\0,1\C,-0.0388476893,-0.002724154,-0.0064877311\C,-0.0821636266,0.0252889879,1.5247733833\C,1.3109956839,-0.0054148075,2.1619346689\C,-1.4162408112,0.1126927357,-0.6965757387\C,-1.3653103731,-0.0795643061,-2.2112653665\C,-2.7361505231,-0.0868162995,-2.8924763958\Cl,-2.1117978426,1.7713045064,-0.2969618374\H,-2.6266635174,-0.2816708403,-3.9648109591\H,-3.2510966016,0.871243445,-2.7734114728\H,-0.7255207415,0.6978297443,-2.6483300437\H,-0.8612367304,-1.0364085536,-2.3852807821\H,0.6047068151,0.8057178919,-0.3800641396\H,-0.614723638,0.9274714444,1.8400764318\H,1.9010910027,0.8706512201,1.8671816344\H,1.2388858716,-0.0056460991,3.2547603873\H,1.8748503988,-0.8948884826,1.8601234477\H,-0.6785649836,-0.8281708799,1.8693675669\H,-2.1159328966,-0.5947181299,-0.2453772293\H,-3.3800498794,-0.8709706531,-2.4757787306\O,0.6633353116,-1.1550044873,-0.5013462682\O,-0.0965292912,-2.346635453,-0.1283764491\H,0.5299394786,-2.7550144094,0.4954744569\Version=EM64L-G09RevA.02\State=1-A\HF=-847.0218106\RMSD=4.214e-09\RMSF=8.801e-06\Dipole=0.4544559,-0.5638384,0.4287589\Quadrupole=-1.1688985,-0.6285896,1.7974881,0.7997779,2.1847207,-2.5751507\PG=C01 [X(C6H13Cl1O2)]\@

PVC_2R

1\1\GINC-V1289\FOpt\UB3LYP\6-31G(d)\C6H12Cl1(2)\GXG501\31-May-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc11r.freq\0,2\C,0.5741607303,-0.843846888,0.550392295\C,0.2649822719,0.2502122718,1.5189207797\C,1.4800585247,0.6915005952,2.3488492597\C,-0.426981642,-1.7908976128,0.0652377219\C,0.1279042193,-3.0767160531,-0.54292569\C,-0.926948263,-4.098463376,-0.9718492927\Cl,-1.4767618322,-0.8850752676,-1.2906621158\H,-0.4465723139,-5.0096070034,-1.3444906808\H,-1.5654539683,-3.6998421759,-1.7649787145\H,0.7765126716,-2.8162911117,-1.3882797809\H,0.7779027206,-3.5227018559,0.2240600969\H,1.5228779907,-0.8022754469,0.0153833381\H,-0.1243233204,1.122162512,0.9637521714\H,2.2962468992,1.0324478867,1.7009986222\H,1.2170850393,1.5181118286,3.017422295\H,1.8620183563,-0.1324074531,2.9618768024\H,-0.5546074058,-0.0600031443,2.1821640927\H,-1.1979669808,-1.9958049415,0.8123703619\H,-1.5699864639,-4.3809087298,-0.1293220949\Version=EM64L-G09RevA.02\State=2-A\HF=-696.0220355\S2=0.755364\S2-1=0.\S2A=0.750021\RMSD=3.330e-09\RMSF=2.410e-06\Dipole=0.6594308,-0.32475,0.7636835\Quadrupole=-0.8808455,1.6866093,-0.8057638,0.9133255,-1.8194173,1.4968673\PG=C01 [X(C6H12Cl1)]\@

PVC_3

1\1\GINC-V1303\FOpt\RB3LYP\6-31G(d)\C5H10Cl2\GXG501\31-May-2010\0\#B3
LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc2.freq\0,1\C,0.0077
717072,-0.0006971288,-0.0049817627\C,0.0271546552,0.0011456677,1.52297
00296\C,1.4373894062,0.0091139904,2.0974494151\C,-1.3648873011,0.11883
24331,-0.6656888604\C,-1.3070954057,-0.0207989426,-2.1809496503\Cl,-0.
8675848064,-1.4805987223,2.1560276538\Cl,-2.1160430424,1.7481920754,-0
.2439788551\H,2.0115152074,-0.8554050879,1.7482197407\H,1.9554943724,0
.9219945775,1.7783490143\H,1.4159337999,-0.0091058966,3.1902615683\H,-
2.0534255282,-0.6116656965,-0.2369882294\H,-0.5498815301,0.8451492499,
1.9053099418\H,0.4729728242,-0.9288650429,-0.3635906832\H,0.6396925057
,0.8290748508,-0.349459921\H,-0.9219606992,-1.014688289,-2.4406880217\
H,-0.6470679599,0.7330327464,-2.6226244016\H,-2.3008406048,0.088470952
4,-2.6231727586\Version=EM64L-G09RevA.02\State=1-A\HF=-1116.9692325\R
MSD=9.090e-09\RMSF=9.679e-06\Dipole=0.8583724,-0.0769847,-0.5500857\Qu
adrapole=1.2371604,-2.6365759,1.3994155,1.9153258,0.8848695,3.4274725\
PG=C01 [X(C5H10Cl2)]\@

PVC_300

1\1\GINC-V1292\FOpt\UB3LYP\6-31G(d)\C5H9Cl2O2(2)\GXG501\31-May-2010\0\
#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc2oo.freq\0,2\C,
0.019077073,0.0445523675,0.0231865013\C,0.0018427461,0.0256090907,1.55
5296802\C,1.3991443174,-0.0028795294,2.163005123\C,-1.3465502045,0.089
0402194,-0.6823914824\C,-1.2572639017,-0.0055650788,-2.1993051734\Cl,-
0.967272883,-1.3993532757,2.1757174096\Cl,-2.1511484546,1.6708176703,-
0.2176985317\H,1.9432157683,-0.9007486227,1.859977869\H,1.9624714503,0
.8770476111,1.8285482474\H,1.3394043114,0.0208263963,3.2538145612\H,-1
.9953121188,-0.6887550006,-0.2773107964\H,-0.5493541477,0.9049121854,1
.8920359213\H,0.632668433,0.8872497381,-0.3086446661\H,-0.8424802623,-
0.9767043411,-2.4858162101\H,-0.6175527754,0.7807848961,-2.6111868442\
H,-2.2539680361,0.0885588943,-2.6378703585\O,0.7157211322,-1.164997995
4,-0.4269415902\O,1.6395991617,-0.8949455396,-1.3369744057\Version=EM
64L-G09RevA.02\State=2-A\HF=-1266.6683062\S2=0.753263\S2-1=0.\S2A=0.75
0007\RMSD=8.804e-09\RMSF=2.892e-06\Dipole=0.1729211,0.4779178,-0.00854
48\Quadrupole=-0.6160921,-1.4732803,2.0893724,3.6195752,4.403964,1.636
8511\PG=C01 [X(C5H9Cl2O2)]\@

PVC_300H

1\1\GINC-V1292\FOpt\RB3LYP\6-31G(d)\C5H10Cl2O2\GXG501\01-Jun-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc2ooh.freq\0,1\C,-
0.0059330472,0.036319538,-0.0229836907\C,-0.0098498501,-0.0134003725,1
.5136180511\C,1.3834296612,0.0976846535,2.1179457473\C,-1.3994109193,0
.027289672,-0.6815674612\C,-1.3741737463,-0.0560005796,-2.2004682011\C
l,-0.8077510676,-1.5539851393,2.1131474906\Cl,-2.275498397,1.565437341
9,-0.175814672\H,2.0179230665,-0.7296634936,1.790906693\H,1.8442315817
,1.0429270126,1.8043079173\H,1.3300134603,0.0884422928,3.209489298\H,-
1.9935524927,-0.7844650481,-0.2589031775\H,-0.6544319874,0.7883044705,
1.8759457595\H,0.5229883112,0.9514546502,-0.3144338693\H,-0.8957926387
, -0.9914462116,-2.5044845706\H,-0.8143398049,0.7761091824,-2.637091060
1\H,-2.3944426909,-0.037607287,-2.5930994213\O,0.7557456906,-1.0872625
464,-0.4794785679\O,1.4919669354,-0.677240874,-1.6701383622\H,2.395901
4052,-0.8863569943,-1.3719426711\Version=EM64L-G09RevA.02\State=1-A\H
F=-1267.3006377\RMSD=5.340e-09\RMSF=1.072e-05\Dipole=1.1716692,0.2705,
-0.200717\Quadrupole=4.3021346,-3.518077,-0.7840576,1.9245037,0.855639
6,2.5988402\PG=C01 [X(C5H10Cl2O2)]\@

PVC_3R

1\1\GINC-V1318\FOpt\UB3LYP\6-31G(d)\C5H9Cl2(2)\GXG501\31-May-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc2r.freq\0,2\C,-0.

0768445283,-0.0636656878,0.0465000967\C,-0.0162162797,-0.2122082545,1.5081507524\C,1.3435416887,0.0594085736,2.1297565898\C,-1.320408319,0.2723232965,-0.6625905634\C,-1.3917937718,-0.2042193698,-2.1037313264\Cl,-0.5096324776,-2.0036415197,1.9169181388\Cl,-1.4832290161,2.1679092582,-0.6544070928\H,2.1150391757,-0.5686799351,1.6736095829\H,1.6078039899,1.1111529624,1.9654241509\H,1.3292346801,-0.1330994331,3.2054673267\H,-2.2005547968,-0.0336103343,-0.0932529431\H,-0.8056521945,0.3588643565,2.0011846479\H,0.8327567708,-0.2079234779,-0.5322751548\H,-1.3734169559,-1.300787569,-2.1186672313\H,-0.5390736975,0.1660667614,-2.6812502136\H,-2.3121089232,0.1362179519,-2.5849123268\\Version=EM64L-G09RevA.02\State=2-A\HF=-1116.3077443\S2=0.755947\S2-1=0.\S2A=0.750028\RMSD=4.469e-09\RMSF=7.211e-06\Dipole=0.4263335,-0.067734,-0.2709761\Quadrupole=3.1426909,-5.6550584,2.5123676,1.6706291,0.842144,4.6212706\PG=C01[X(C5H9Cl2)]\@

PVC_4

1\1\GINC-V1458\FOpt\RB3LYP\6-31G(d)\C5H11Cl\GXG501\31-May-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pvc3.freq\0,1\C,-0.0060670189,0,-0.0123745213\C,0.0091199542,0,1.5240081433\C,1.4284003452,0,2.1080379514\C,1.4471198804,0,3.6397182931\C,-1.4262621032,0,-0.5611170337\Cl,-1.4497189964,0,-2.382961595\H,-1.9817754902,-0.8882588696,-0.2516579227\H,-1.9817754902,0.8882588696,-0.2516579227\H,0.5269421494,0.8804090246,-0.3922913573\H,0.5269421494,-0.8804090246,-0.3922913573\H,-0.5358372062,-0.8793476046,1.8978076116\H,-0.5358372062,0.8793476046,1.8978076116\H,1.9726775731,0.8782360863,1.7337647741\H,1.9726775731,-0.8782360863,1.7337647741\H,0.9396231411,-0.8849295899,4.0429822658\H,0.9396231411,0.8849295899,4.0429822658\H,2.4727514163,0,4.0252959814\\Version=EM64L-G09RevA.02\State=1-A\HF=-657.3676784\RMSD=6.524e-09\RMSF=2.552e-05\Dipole=0.1681517,0,0.9624753\Quadrupole=1.5917083,2.1024876,-3.6941959,0,-1.9609502,0\PG=CS [SG(C5H1Cl),X(H10)]\@

PVC_400

1\1\GINC-V1292\FOpt\UB3LYP\6-31G(d)\C5H10Cl1O2(2)\GXG501\31-May-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pvc3oo.freq\0,2\C,0.0068396788,-0.0595866748,0.0742317716\C,0.0362946482,0.0130450028,1.6020254932\C,1.4454090088,0.0279723072,2.1925716057\C,1.4722311727,0.1833814291,3.7163608254\C,-1.4102097807,-0.0128032579,-0.4872583471\Cl,-1.3917942582,-0.0336659176,-2.3034321829\H,-1.9984239366,-0.8751826641,-0.1721602315\H,-1.933636534,0.9008738986,-0.1959461061\H,0.585295699,0.7831057996,-0.3208300489\H,0.5044481138,-0.9802947951,-0.245547768\H,-0.5435213408,0.8706219945,1.9648228732\H,1.9934548631,0.8533683319,1.7203795194\H,1.9468638915,-0.8996369039,1.8939051127\H,0.9460854117,-0.6411917497,4.207038685\H,0.9980413307,1.1210302755,4.0305130125\H,2.5035211087,0.1913965086,4.0840288104\O,-0.7412422014,-1.1120788643,2.1726978432\O,-0.2205400204,-2.2852522197,1.8509144796\\Version=EM64L-G09RevA.02\State=2-A\HF=-807.075842\S2=0.753271\S2-1=0.\S2A=0.750007\RMSD=3.567e-09\RMSF=4.037e-06\Dipole=0.4873656,0.9189651,0.6512086\Quadrupole=3.2277338,0.3618915,-3.5896253,-0.1918569,-0.3335564,2.7000747\PG=C01 [X(C5H10Cl1O2)]\@

PVC_400H

1\1\GINC-V1477\FOpt\RB3LYP\6-31G(d)\C5H11Cl1O2\GXG501\01-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pvc3ooh.freq\0,1\C,0.0087533829,0.0259312408,0.0043101587\C,-0.0014109091,-0.012048994,1.5393631894\C,1.4058801061,-0.0217742996,2.1463132282\C,1.4095344841,0.0585942555,3.6759499802\C,-1.398635816,-0.0023258595,-0.5779426113\Cl,-1.3612228463,0.1316746931,-2.3934512557\H,-1.910320806,-0.9353533849,-0.3447860926\H,-2.0046995238,0.8349834573,-0.2241391958\H,0.5239639363,0.938286854,-0.318359691\H,0.5807130692,-0.8246223349,-0.3791522138\H,-0.5587840933,0.8558492193,1.9233201232\H,1.9645645475,0.8250461476,1

.7271437516\H,1.9210663878,-0.9295298793,1.8102535782\H,0.8422225062,-
0.767025182,4.1187112482\H,0.9542827085,0.9927815693,4.0262968189\H,2.
4309514097,0.0171564122,4.0690544083\O,-0.8235064507,-1.0809002135,2.0
424747652\O,-0.2649006055,-2.3434881552,1.5635214602\H,-0.0239551681,-
2.7490104674,2.4151995574\Version=EM64L-G09RevA.02\State=1-A\HF=-807.
7075399\RMSD=7.288e-09\RMSF=4.670e-06\Dipole=0.6659362,0.0890185,1.277
1302\Quadrupole=0.6533664,3.0088533,-3.6622197,-1.0473778,-0.126419,-1
.0186492\PG=C01 [X(C5H11ClO2)]\@

PVC_4R

1\1\GINC-V1414\FOpt\UB3LYP\6-31G(d)\C5H10Cl1(2)\GXG501\31-May-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pvc3r.freq\0,2\C,0.
069504977,0.4819039916,-0.1455638444\C,0.3685649228,0.6997544071,1.305
2231938\C,1.4045409382,-0.0842808563,2.0454501667\C,1.2040554685,-0.09
52006312,3.5666766183\C,-1.245797143,-0.2912086489,-0.3179368242\Cl,-1
.647546073,-0.5633792095,-2.07870825\H,-1.193497157,-1.2803397784,0.14
04476682\H,-2.0904639399,0.2543702853,0.1067731022\H,-0.0209562326,1.4
366996058,-0.6811932086\H,0.8755247365,-0.0836292384,-0.629038088\H,-0
.165746433,1.4891092429,1.8315661552\H,2.4106101287,0.3194507584,1.822
5162625\H,1.4300070063,-1.1174994302,1.6648350686\H,0.2454265644,-0.55
36103619,3.8349376421\H,1.2101494829,0.9242178069,3.9707032734\H,2.000
0637714,-0.6570103386,4.0673214149\Version=EM64L-G09RevA.02\State=2-A
\HF=-656.7012535\S2=0.754133\S2-1=0.\S2A=0.750012\RMSD=8.524e-09\RMSF=
7.237e-06\Dipole=0.3872627,0.1698064,0.9399167\Quadrupole=0.9553093,1.
6748171,-2.6301264,-0.806284,-2.0576365,-0.7968814\PG=C01 [X(C5H10Cl1)
]\@

PMMA_1

1\1\GINC-V1438\FOpt\RB3LYP\6-31G(d)\C9H18O2\GXG501\07-Jun-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma1.freq\0,1\C,-0.132
2229613,-0.0122155783,0.051419039\C,0.0597688847,-0.066424102,1.574012
1036\C,1.5323864609,-0.2348209369,1.9651944325\C,-1.5978393505,0.10567
67063,-0.4597422237\C,-1.5664243995,0.0350097408,-2.0149986105\C,-2.92
94879907,0.0386094149,-2.7170940223\C,-2.4157464083,-1.0723617374,0.08
0161719\O,-1.8943059442,-2.2633572871,-0.3086305489\O,-3.4095459523,-0
.9905927116,0.7700431892\C,-2.5985097361,-3.4252259098,0.1561604501\C,
-2.2444573469,1.4169333898,0.0170650837\H,-2.2808968417,1.4741757039,1
.1076233262\H,-1.6686842623,2.2716351543,-0.3572651054\H,-3.5500378939
,-0.8084408293,-2.4014998288\H,-3.4939624666,0.9560126719,-2.521212583
2\H,-2.7955760888,-0.0395375789,-3.8018736787\H,-3.2735491191,1.509203
0733,-0.3385366592\H,-2.6074878432,-3.4589840689,1.2490521894\H,-3.630
8070257,-3.4209952983,-0.2041168349\H,-2.0546553845,-4.2794309342,-0.2
489106787\H,-0.5222128942,-0.89910853,1.9921341414\H,-0.3343778365,0.8
454865176,2.0387950559\H,1.653282857,-0.2719585595,3.0537110693\H,1.94
97852173,-1.1606937132,1.550709969\H,2.1403944798,0.5981110069,1.59086
77842\H,0.3165750589,-0.9100693232,-0.3909676099\H,0.426542623,0.84502
51986,-0.3508175671\H,-1.0178047964,-0.8676028463,-2.3066116487\H,-0.9
732513995,0.8893281676,-2.3686071227\Version=EM64L-G09RevA.02\State=1
-A\HF=-504.2675955\RMSD=5.392e-09\RMSF=2.672e-06\Dipole=0.5030048,-0.3
002785,-0.3416961\Quadrupole=-3.679497,4.3022813,-0.6227842,1.6011703,
2.2049745,-0.7307588\PG=C01 [X(C9H18O2)]\@

PMMA_100

1\1\GINC-V1279\FOpt\UB3LYP\6-31G(d)\C9H17O4(2)\GXG501\07-Jun-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma100.freq\0,2\C,0
.0343825554,-0.0241054905,0.0086428298\C,0.0312969588,-0.0170985893,1.
5438670966\C,1.4522745962,-0.0706357268,2.1165377775\C,-1.3533392465,-
0.0738468689,-0.6926484423\C,-1.1226214429,-0.159917938,-2.2303171093\
C,-2.3813398348,-0.2833811567,-3.0976368393\C,-2.1265507317,-1.3078599
709,-0.2188919781\O,-1.4593995808,-2.450553914,-0.4860045441\O,-3.2092

268338,-1.2854297427,0.3301907416\C,-2.1131863336,-3.6617413574,-0.067
 6740354\C,-2.2334638326,1.1407939021,-0.3288076901\H,-2.3600927728,1.2
 612118133,0.7462065668\H,-2.9866884709,-1.1552125936,-2.8220042648\H,-
 3.0201015895,0.6035976437,-3.0300187691\H,-2.0997017547,-0.3993594359,
 -4.1497870662\H,-3.2148003592,1.0739430389,-0.8007250277\H,-2.26092720
 67,-3.6623194727,1.0153445905\H,-3.0844299229,-3.7626840515,-0.5587171
 863\H,-1.4454590019,-4.470555389,-0.3651149602\H,-0.5452836037,-0.8713
 938964,1.9250930462\H,-0.4663747059,0.8882791937,1.9087403208\H,1.4387
 14607,-0.0578769076,3.2120080134\H,1.9763870658,-0.9803967408,1.798653
 7392\H,2.0447123648,0.7888961482,1.7806903681\H,0.608413549,-0.8890424
 842,-0.3443298043\H,0.5601235959,0.8685609305,-0.3514271468\H,-0.47020
 75772,-1.0195202959,-2.4163218093\H,-0.5609167411,0.7327387913,-2.5286
 742071\O,-1.6617478958,2.3752202168,-0.8487255094\O,-0.8606591074,2.96
 26683825,0.028722548\Version=EM64L-G09RevA.02\State=2-A\HF=-653.97167
 45\S2=0.75322\S2-1=0.\S2A=0.750007\RMSD=4.195e-09\RMSF=6.505e-06\Dipol
 e=0.1389966,-1.2719781,-0.2803654\Quadrupole=-1.5852526,-0.2765588,1.8
 618114,-1.155419,1.5818392,0.0759525\PG=C01 [X(C9H17O4)]\@

PMMA_10OH

1\1\GINC-V1349\FOpt\RB3LYP\6-31G(d)\C9H18O4\GXG501\08-Jun-2010\0\#B3L
 YP/6-31G* OPT Freq=norman maxdisk=268435456\pmma10oh.freq\0,1\C,0.0
 806319463,-0.0988248961,-0.0560973028\C,0.0789773152,-0.0202183952,1.4
 767928816\C,1.4983684947,-0.0715006858,2.0535277436\C,-1.3106757346,-0
 .1353385521,-0.7535225713\C,-1.0781345587,-0.2770528179,-2.28564204\C,
 -2.3355375298,-0.4390372296,-3.1485757865\C,-2.1006374771,-1.340457005
 3,-0.2383431443\O,-1.4569085712,-2.5064896466,-0.4750982661\O,-3.17862
 62916,-1.2887349651,0.3192826226\C,-2.1326029531,-3.689233359,-0.01774
 02981\C,-2.1729799863,1.1133080921,-0.4479403056\H,-2.30949907,1.26142
 5813,0.6266955513\H,-2.9341639735,-1.3064253329,-2.8450349264\H,-2.980
 3181106,0.4450652646,-3.1079748081\H,-2.0537975133,-0.5866217951,-4.19
 70507968\H,-3.1665405296,0.9949317435,-0.8903544614\H,-2.2707480736,-3
 .6583637878,1.0663690143\H,-3.1111188013,-3.7830664757,-0.4960610357\H
 ,-1.4865642108,-4.5216772335,-0.2983655538\H,-0.5122487196,-0.84530443
 12,1.8983685725\H,-0.4045547073,0.9087543792,1.7993931512\H,1.48635222
 91,-0.01082352,3.1477570298\H,2.0075727585,-1.0028696561,1.776302013\H
 ,2.1055925173,0.7616539118,1.6793251489\H,0.6255862593,-0.9995455844,-
 0.3638661836\H,0.6315980644,0.7587937628,-0.4570878538\H,-0.4182276711
 ,-1.1365161502,-2.4458111759\H,-0.5288788036,0.613431343,-2.6101833773
 \O,-1.6902873881,2.3145425493,-1.0467773607\O,-0.6211781262,2.85130972
 62,-0.2110557305\H,-1.0563743868,3.6651546042,0.1012914562\Version=EM
 64L-G09RevA.02\State=1-A\HF=-654.6022786\RMSD=8.995e-09\RMSF=6.757e-06
 \Dipole=0.1396645,-0.2247456,0.1503019\Quadrupole=-5.6873051,7.4683141
 ,-1.781009,-0.9582373,1.4583723,2.9573371\PG=C01 [X(C9H18O4)]\@

PMMA_1R

1\1\GINC-V1297\FOpt\UB3LYP\6-31G(d)\C9H17O2(2)\GXG501\07-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pmma1r.freq\0,2\C,0.
 0281017373,-0.0419504484,-0.0371216664\C,-0.0215446062,0.0074136081,1.
 4951039567\C,1.3735316558,0.0847922871,2.1238050189\C,-1.3660504386,-0
 .0745553935,-0.7471014437\C,-1.1164075434,-0.2014590909,-2.2875532241\
 C,-2.3860520625,-0.315631948,-3.1362007509\C,-2.1483481269,-1.30356873
 94,-0.2632536215\O,-1.4755619284,-2.4498378259,-0.5285068568\O,-3.2281
 139754,-1.2936525706,0.2873033214\C,-2.1279962589,-3.6584685347,-0.108
 437917\C,-2.1432503776,1.167558283,-0.4406790972\H,-3.1104410706,1.127
 6969384,0.042525605\H,-2.957501806,-1.2178333596,-2.8879906985\H,-3.04
 47914749,0.5466033095,-2.9867248612\H,-2.1327603599,-0.3687279969,-4.2
 009629133\H,-1.72338582,2.1304962796,-0.7155711155\H,-2.2808578734,-3.
 6569744858,0.9741703739\H,-3.0980827956,-3.7643754857,-0.6014074404\H,
 -1.4589721361,-4.4688016743,-0.4001306924\H,-0.5419729241,-0.881507475
 3,1.877231901\H,-0.6202739936,0.870778388,1.8126484329\H,1.3155105928,
 0.1143836611,3.2177566096\H,1.9846066136,-0.782996262,1.8459353211\H,1.
 9084881154,0.9842065216,1.7944644797\H,0.6055356104,-0.9175377061,-0.
 3580851101\H,0.5618652715,0.8430041047,-0.4108401083\H,-0.4717605311,-

1.0697456822,-2.4648069649\H,-0.5470208699,0.6850456267,-2.5962758464\
\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-503.5961635\\S2=0.753898\\S2-1=0
\\S2A=0.750009\\RMSD=8.520e-09\\RMSF=4.859e-06\\Dipole=0.5841287,-0.31096
37,-0.2625256\\Quadrupole=-4.3047984,4.7746371,-0.4698386,1.1244044,1.2
930419,-0.6718277\\PG=C01 [X(C9H17O2)]\\#@

PMMA_200

1\\GINC-V1307\\FOpt\\UB3LYP\\6-31G(d)\\C9H17O4(2)\\GXG501\\07-Jun-2010\\0\\#
B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\\pmma200.freq\\0,2\\C,-
0.0165110047,0.0057583529,-0.041242179\\C,-0.0127626506,0.080124843,1.4
873708298\\C,1.3857026269,-0.1065104971,2.0853602819\\C,-1.4186333686,-0
.0299062144,-0.7246158518\\C,-1.2231499221,-0.1369484172,-2.2678712924\\
C,-2.5057684208,-0.3538513762,-3.0801889857\\C,-2.1404425135,-1.2944822
661,-0.2374192129\\O,-1.3959351454,-2.4055864625,-0.4539711705\\O,-3.242
1047235,-1.3273002858,0.2647346914\\C,-2.0029613221,-3.6464929594,-0.05
38214466\\C,-2.2585158292,1.202864982,-0.3499108348\\H,-2.4435885245,1.2
527535679,0.7259916196\\H,-1.7409161564,2.1152247154,-0.6609803822\\H,-3
.0303080251,-1.2698887859,-2.7842833566\\H,-3.2081401392,0.4793703991,-
2.9767755284\\H,-2.2598365214,-0.4451415982,-4.1436964346\\H,-3.23524313
88,1.1693938513,-0.8367033701\\H,-2.2223345969,-3.639467179,1.017087793
1\\H,-2.9323146176,-3.8128635611,-0.6045574944\\H,-1.2716449846,-4.41922
00048,-0.291997495\\H,-0.6924040917,-0.6886667353,1.8759961749\\H,-0.426
2919274,1.0457415545,1.8000517566\\H,1.3544847091,-0.0238558474,3.17687
30215\\H,1.7966071404,-1.0914785402,1.8341744108\\H,2.0789084525,0.65231
00534,1.7088043258\\H,0.5823886842,-0.836209844,-0.3928944012\\H,-0.5261
285165,-0.9571696282,-2.4717554963\\H,-0.7300210161,0.780993503,-2.6050
30797\\O,0.6925951398,1.2098543936,-0.5074601692\\O,1.6416048411,0.93478
73688,-1.3885853207\\\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-653.974700
7\\S2=0.753361\\S2-1=0\\S2A=0.750007\\RMSD=1.724e-09\\RMSF=3.216e-06\\Dipol
e=-0.1869623,-0.8548269,0.2784619\\Quadrupole=-7.3078549,4.6880365,2.61
98184,-2.539435,4.5769174,0.6643399\\PG=C01 [X(C9H17O4)]\\#@

PMMA_200H

1\\GINC-V1282\\FOpt\\RB3LYP\\6-31G(d)\\C9H18O4\\GXG501\\08-Jun-2010\\0\\#B3L
YP/6-31G* OPT Freq=norman maxdisk=268435456\\pmma200h.freq\\0,1\\C,0.0
326438161,0.0023575327,0.0013773546\\C,-0.0097618355,0.0013254626,1.537
8878812\\C,1.3822527751,-0.0841651761,2.1704334175\\C,-1.3563396852,-0.2
20167975,-0.6901041546\\C,-1.1672259185,-0.2319752563,-2.2366992252\\C,-
2.4085624021,-0.6216656554,-3.0494808365\\C,-1.885412484,-1.5899375222,
-0.2520179042\\O,-1.0099993113,-2.5821564143,-0.5566243341\\O,-2.9467962
608,-1.8019659734,0.2935970022\\C,-1.4293131002,-3.9076718302,-0.194940
3366\\C,-2.3564612068,0.866916007,-0.2639452416\\H,-2.5639870965,0.82623
68435,0.8083621278\\H,-1.9492301052,1.8524040023,-0.5081316291\\H,-2.764
0842268,-1.6287200686,-2.8005744461\\H,-3.2416879711,0.0717285751,-2.89
51167521\\H,-2.1704742391,-0.6138402157,-4.1190115187\\H,-3.3139545073,0
.7438541171,-0.7750167446\\H,-1.5943428683,-3.9796133355,0.8835693719\\H
,-2.3558456657,-4.1720728241,-0.7114154437\\H,-0.6170348049,-4.56651619
41,-0.5039293489\\H,-0.6279353996,-0.8392220866,1.8762507206\\H,-0.51579
94174,0.9118389087,1.8793600387\\H,1.3190475324,-0.0517967614,3.2635502
62\\H,1.8895813646,-1.0160994605,1.8923720678\\H,2.0084805713,0.75340287
36,1.8460907847\\H,0.7265336092,-0.7684680771,-0.3475249625\\H,-0.349036
2615,-0.916962196,-2.482939918\\H,-0.8330292708,0.7669463506,-2.5340681
494\\O,0.5904495467,1.2827768697,-0.3472414589\\O,1.3937829419,1.1437475
256,-1.5554867381\\H,2.2743024715,1.33438909,-1.1841336501\\\\Version=EM6
4L-G09RevA.02\\State=1-A\\HF=-654.6042944\\RMSD=8.184e-09\\RMSF=9.210e-06\\
Dipole=0.968504,-0.5061647,0.1114491\\Quadrupole=-0.7584248,2.0589521,-
1.3005272,0.0341525,2.524507,0.8407607\\PG=C01 [X(C9H18O4)]\\#@

PMMA_2R

1\\GINC-V1409\\FOpt\\UB3LYP\\6-31G(d)\\C9H17O2(2)\\GXG501\\07-Jun-2010\\0\\#

B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma2r.freq\0,2\C,-0.0952981552,-0.1014372502,0.0981687447\C,0.0308083471,0.2995839856,1.5347116158\C,1.4103609114,-0.0113939965,2.128454171\C,-1.4110310676,-0.1243037888,-0.6527940074\C,-1.1248263805,-0.1777439886,-2.1771077045\C,-2.3514018818,-0.320480201,-3.0848585687\C,-2.1111738705,-1.4055370371,-0.151700908\O,-1.6631546383,-2.5170141205,-0.7854095297\O,-2.9150298949,-1.4479823537,0.7568829715\C,-2.1975971277,-3.7578771809,-0.2983802731\C,-2.2921828501,1.086489615,-0.2859550559\H,-2.4869085329,1.1249237109,0.7873144294\H,-1.7920328786,2.013095243,-0.5884941802\H,-2.9127314241,-1.2334061778,-2.8570004322\H,-3.0356551385,0.5299176557,-2.9957019152\H,-2.0397584462,-0.3797255991,-4.1337943055\H,-3.2625463977,1.0359645735,-0.7883160853\H,-1.9335271687,-3.9043935732,0.7526287763\H,-3.2865340795,-3.7731138752,-0.3938515203\H,-1.7471378322,-4.533819364,-0.9184630645\H,-0.7515382557,-0.1992844326,2.1319651278\H,-0.177311956,1.3765620867,1.6499872967\H,1.4723104818,0.3081509686,3.1743173877\H,1.6224141544,-1.0863974852,2.0923487694\H,2.2030169965,0.5032921208,1.5726850963\H,0.7489003996,-0.5974675314,-0.3780250478\H,-0.4393264375,-1.0097975914,-2.3704153556\H,-0.5813446066,0.7408767396,-2.4344606815\Version=EM64L-G09RevA.02\State=2-A\HF=-503.6020388\S2=0.754493\S2-1=0\S2A=0.750015\RMSD=6.628e-09\RMSF=2.415e-06\Dipole=0.4390395,-0.2473361,-0.3426033\Quadrupole=-2.7377281,4.1548591,-1.4171311,0.6174322,2.477405,0.3684002\PG=C01 [X(C9H17O2)]\@

PMMA_300

1\1\GINC-V1289\FOpt\UB3LYP\6-31G(d)\C9H17O4(2)\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma3oo.freq\0,2\C,-0.0032094305,0.000203604,-0.0487047143\C,0.0284954434,-0.1179044385,1.4823176829\C,1.4583787655,-0.064540563,2.0321996025\C,-1.4084740865,-0.0282557214,-0.7218763475\C,-1.2006112048,-0.0781165654,-2.2650642763\C,-2.4712133084,-0.2095274022,-3.1130879477\C,-2.1462113322,-1.2852670372,-0.2718019669\O,-1.4391676543,-2.424728807,-0.6165812555\O,-3.2034682016,-1.3368364031,0.3068730389\C,-1.9585527481,-3.6474427465,-0.1662676275\C,-2.2414273053,1.2006451472,-0.3195426923\H,-2.3915486354,1.2488424612,0.7615899632\H,-1.7267724864,2.1137816807,-0.639559081\H,-3.0289162104,-1.1221436237,-2.8706213689\H,-3.149184069,0.6398557374,-2.9813730046\H,-2.2103722118,-0.2593003279,-4.1760075444\H,-3.2330502089,1.182988024,-0.7785259524\H,-3.0438606363,-3.6149033299,-0.0713508483\H,-1.589363702,-4.4251368261,-0.8323762187\H,-0.4380301431,-1.0627331289,1.7915606683\H,-0.5639815894,0.684528301,1.9389849152\H,1.4655453236,-0.1554167678,3.1239101749\H,2.069681992,-0.8793911591,1.6262013832\H,1.9494188007,0.8815029411,1.7722881457\H,0.6010569852,-0.809804782,-0.474415871\H,0.4783337407,0.9410220496,-0.350870707\H,-0.5278579696,-0.911373941,-2.496315785\H,-0.6674908627,0.8396832894,-2.5466597867\O,-1.4836133786,-3.934481155,1.1702288713\O,-0.2305530785,-4.3748222918,1.1396321626\Version=EM64L-G09RevA.02\State=2-A\HF=-653.9746082\S2=0.752951\S2-1=0\S2A=0.750006\RMSD=5.033e-09\RMSF=4.413e-06\Dipole=0.0425944,0.3907854,-0.9590693\Quadrupole=-2.4412633,2.4012612,0.040002,3.8660599,1.2080778,3.2453604\PG=C01 [X(C9H17O4)]\@

PMMA_30OH

1\1\GINC-V1347\FOpt\RB3LYP\6-31G(d)\C9H18O4\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma3ooh.freq\0,1\C,0.0182713421,-0.0038996325,0.0213640872\C,0.0869099551,-0.0535966334,1.5549787393\C,1.5287501828,0.0273376996,2.069185279\C,-1.4039665839,-0.0698617041,-0.6145576811\C,-1.2354812771,-0.1952527183,-2.1571992934\C,-2.5284177214,-0.362221268,-2.9641437613\C,-2.1163094685,-1.3117161407,-0.0791540424\O,-1.4478501539,-2.4444184313,-0.3780707501\O,-3.1553955308,-1.2908737835,0.5605081721\C,-2.0042913273,-3.7314756171,0.0134292272\C,-2.2266815454,1.1776835064,-0.2506134672\H,-2.3384278024,1.2853183503,0.8308577066\H,-1.7264081992,2.0725097134,-0.6382971733\H,-3.0856926006,-1.2561517979,-2.658857978\H,-3.1974652897,0.4980277049,-2.8602640131\H,-2.2965741971,-0.4707126838,-4.0293914378\H,-3.2340420713,1.1349243534,-0.6720886074\H,-2.9739725723,-3.8730566798,-0.4688174732\H

, -1.252831405, -4.4346922749, -0.3500613542\H, -0.371050824, -0.9840422717
 , 1.9167066931\H, -0.4967771542, 0.7677354754, 1.9885980818\H, 1.5615259328
 , -0.0141993903, 3.1634433023\H, 2.1340990257, -0.8030956709, 1.6859479117\H,
 2.0110429463, 0.9615039932, 1.7558058774\H, 0.6169469275, -0.8290302644,
 -0.3832803276\H, 0.4868417301, 0.9250134648, -0.3331322493\H, -0.572675382
 6, -1.0429058572, -2.3637166896\H, -0.7065591063, 0.7044612772, -2.49854124
 59\O, -2.1111585836, -3.9079416466, 1.3834183871\O, -3.4839249812, -3.67748
 80623, 1.8004369711\H, -3.5573682915, -2.7100395363, 1.6187990315\Version
 =EM64L-G09RevA.02\State=1-A\HF=-654.616404\RMSD=7.702e-09\RMSF=5.750e-
 06\Dipole=0.6454728, 0.6500415, -1.1139349\Quadrupole=-0.7869703, 0.67776
 51, 0.1092052, -1.6792532, 2.6373682, 5.0888557\PG=C01 [X(C9H18O4)]\@

PMMA_3R

1\1\GINC-V1288\FOpt\UB3LYP\6-31G(d)\C9H17O2(2)\GXG501\07-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pmma3r.freq\0, 2\C, -0
 .01131696, -0.0116402524, -0.0047188863\C, -0.0264931151, -0.0178538281, 1.
 5309279373\C, 1.3882737957, -0.0342775175, 2.1209841272\C, -1.3976598706, -
 0.0527437715, -0.7137168743\C, -1.1462371895, -0.1349689589, -2.2490468257
 \C, -2.3923158986, -0.2908273408, -3.1287737282\C, -2.1562054133, -1.297812
 8066, -0.2585296351\O, -1.4552207309, -2.4456703916, -0.5658101089\O, -3.22
 76009095, -1.3294923084, 0.3000907033\C, -1.9861896437, -3.6496072527, -0.1
 930203136\C, -2.2358349704, 1.1875599311, -0.3606076338\H, -2.4319292819, 1.
 2483833526, 0.7124806533\H, -1.70230367, 2.0941801426, -0.6687699214\H, -2
 .9504543038, -1.2023066928, -2.8841465263\H, -3.0779453346, 0.5569425355, -
 3.0299410521\H, -2.102708612, -0.3575584328, -4.1834007496\H, -3.207707200
 3, 1.1706786685, -0.8599338587\H, -2.9980037033, -3.6684292685, 0.185512608
 3\H, -1.4567866216, -4.4971772018, -0.6025396033\H, -0.5796280503, -0.89450
 26864, 1.8946347551\H, -0.5638097335, 0.8609643525, 1.9075877912\H, 1.36187
 24446, -0.036850919, 3.2163800827\H, 1.9424264959, -0.9240736379, 1.7980927
 263\H, 1.9614149347, 0.8456534816, 1.8034436638\H, 0.5810976047, -0.8660069
 354, -0.3545852507\H, 0.5086246907, 0.8909124684, -0.3563735989\H, -0.46541
 90525, -0.971471496, -2.4427960128\H, -0.608103412, 0.77802314, -2.53758790
 52\Version=EM64L-G09RevA.02\State=2-A\HF=-503.5996323\S2=0.753512\S2-
 1=0.\S2A=0.750008\RMSD=2.830e-09\RMSF=9.876e-06\Dipole=0.5912297, 0.039
 1232, -0.3886929\Quadrupole=-3.5336092, 3.4767291, 0.0568801, 0.3038816, 1.
 4780642, 0.3784075\PG=C01 [X(C9H17O2)]\@

PVA_1

1\1\GINC-V1347\FOpt\RB3LYP\Gen\C8H16O2\GXG501\26-Jun-2010\0\#B3LYP/ge
 n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
 6\pva1.freq\0, 1\C, 0.1386845007, -0.0872954837, 0.0148189061\C, 0.250873
 1999, -0.2659714713, 1.5342261546\C, 1.7041308239, -0.3148041106, 2.0170135
 262\C, -1.293286955, -0.0998658935, -0.5247821099\C, -1.3597467835, 0.03916
 22109, -2.047276701\C, -2.7805254038, -0.0155250805, -2.6160869301\O, -2.01
 23015486, 1.0311750707, 0.0512514786\C, -3.0292550046, 0.781365741, 0.91110
 16885\O, -3.390355899, -0.3238370819, 1.2518502203\H, -3.389182096, 0.81133
 5256, -2.2357497458\H, -2.7660618229, 0.0558817554, -3.7091543401\H, -3.281
 5657444, -0.952879168, -2.3468832603\H, -0.874739045, 0.9807462256, -2.3377
 682381\H, -0.7562994719, -0.7699916415, -2.4798964292\H, -1.8094483897, -1.
 0096544691, -0.2040383339\H, 0.6234598067, 0.8525338, -0.2855594879\H, 0.68
 85719538, -0.8956325393, -0.4880499208\H, -0.2707737223, -1.1848691459, 1.8
 331657736\H, -0.2710605409, 0.5591885344, 2.0347233869\H, 2.2410870094, 0.6
 055905045, 1.7558440102\H, 2.2467268836, -1.1535487704, 1.5634616042\H, 1.7
 576090321, -0.4338003408, 3.1049951569\C, -3.6477860097, 2.0789866275, 1.38
 17846758\H, -4.0382181847, 2.6416520902, 0.5273148937\H, -4.4543520835, 1.8
 638117905, 2.0834245894\H, -2.8901566118, 2.7051036992, 1.8642998139\Vers
 ion=EM64L-G09RevA.02\State=1-A\HF=-464.9657677\RMSD=3.852e-09\RMSF=4.8
 35e-06\Dipole=0.4165877, 0.4908447, -0.3556536\Quadrupole=-1.0829361, 0.5
 897758, 0.4931603, -3.7539862, 0.8341758, 2.5958289\PG=C01 [X(C8H16O2)]\@

PVA_100

1\1\GINC-V1360\FOpt\UB3LYP\Gen\C8H15O4(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pvaloo.freq\0,2\C,0.1403682835,-0.2113057154,-0.2081712738\C,0.
1311570477,0.2170495481,1.2656046805\C,1.5244399122,0.1187591919,1.895
4894026\C,-1.2249656054,-0.2160426536,-0.8943433075\C,-1.1834779804,-0
.6055631224,-2.3720978276\C,-2.5419534707,-0.5845251481,-3.0797815152\
O,-1.987923294,0.9720470933,-0.6474212117\C,-1.5651434866,2.1752196054
,-1.1209085106\O,-0.5550633081,2.3425948638,-1.765329765\H,-2.97119230
13,0.4221577802,-3.1061286609\H,-2.4259269815,-0.9225168462,-4.1145873
692\H,-3.2604989874,-1.2458957263,-2.5862321029\H,-0.4803359959,0.0677
207557,-2.8697570115\H,-0.7566721423,-1.6136154806,-2.4071740842\H,0.8
011603109,0.4397582256,-0.7883860983\H,0.5264936007,-1.2335478487,-0.2
9531122\H,-0.5737320503,-0.4090646475,1.8251418352\H,-0.234767531,1.24
7632604,1.3508456396\H,2.2456156828,0.7554824564,1.3686966264\H,1.9035
312407,-0.9098067316,1.8631319441\H,1.5053897505,0.4336732509,2.944630
3558\O,-2.1218639745,-1.1658618519,-0.1737363337\O,-1.668125099,-2.402
5668606,-0.2287018975\C,-2.5404698408,3.2560899672,-0.7199738127\H,-2.
6143243798,3.3088246642,0.3711439626\H,-3.5394144965,3.0236311848,-1.1
026117923\H,-2.2012721656,4.2132719866,-1.1168576651\\Version=EM64L-G0
9RevA.02\State=2-A\HF=-614.6730067\S2=0.753282\S2-1=0\S2A=0.750007\RM
SD=1.701e-09\RMSF=2.566e-06\Dipole=-0.0793852,0.6473041,-0.0362047\Qua
drupole=0.4972434,-1.6610361,1.1637926,-5.4214953,2.4894523,3.7418779\
PG=C01 [X(C8H15O4)]\@

PVA_100H

1\1\GINC-V1283\FOpt\RB3LYP\Gen\C8H16O4\GXG501\26-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pvaloo.freq\0,1\C,0.0208064709,0.0292885675,-0.0194218914\C,0.036
1639503,-0.0437221871,1.5132990052\C,1.4572384011,0.0245914218,2.08198
27745\C,-1.366602829,-0.0944758082,-0.6599052303\C,-1.3418107155,-0.00
6073331,-2.1898863775\C,-2.7204659472,-0.1048185668,-2.8493414542\O,-2
.3142769506,0.8294780423,-0.0788969115\C,-2.160053527,2.1709201571,-0.
2019634081\O,-1.2406110632,2.7172910131,-0.7697799066\H,-3.3650395836,
0.7355271725,-2.5705065528\H,-2.6160885243,-0.0948238026,-3.9394784966
\H,-3.2286727858,-1.0294115207,-2.5613979448\H,-0.8476106299,0.9297461
264,-2.4652479344\H,-0.7049293468,-0.8258415685,-2.5385960191\H,0.4636
107986,0.9715220637,-0.3550115929\H,0.6348641344,-0.7779382508,-0.4361
909338\H,-0.4541430792,-0.9680388359,1.8455522519\H,-0.5627710244,0.77
60294172,1.9282283718\H,1.9541578078,0.9590988834,1.7950797696\H,2.075
7205254,-0.8035234296,1.7137969371\H,1.4494992449,-0.0265888915,3.1765
536004\O,-2.0371001422,-1.306098068,-0.2278152372\O,-1.2686152671,-2.4
32433063,-0.7242260797\C,-3.3084207305,2.8821298866,0.4773470483\H,-3.
3606633528,2.5935321646,1.532031938\H,-4.2565438895,2.5912334564,0.013
4768245\H,-3.1672398657,3.959944121,0.3911791065\H,-0.9360237818,-2.79
15283167,0.1181744708\\Version=EM64L-G09RevA.02\State=1-A\HF=-615.3027
843\RMSD=7.236e-09\RMSF=2.372e-06\Dipole=0.1058256,-0.196201,0.6013268
\Quadrupole=0.4850249,-0.9920513,0.5070264,-6.2403568,0.2954688,-0.119
7684\PG=C01 [X(C8H16O4)]\@

PVA_1R

1\1\GINC-V1378\FOpt\UB3LYP\Gen\C8H15O2(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pvalr.freq\0,2\C,0.1429059221,0.1524513647,0.006732503\C,0.2693
524025,0.1828611526,1.5513551992\C,1.7181354114,0.3598944301,2.0146507
337\C,-1.2586495235,-0.0333932937,-0.4875258323\C,-2.249636402,1.08480
59248,-0.5867380232\C,-3.3052191654,0.8878000346,-1.6876930315\O,-1.89
32132363,-1.2550308135,-0.2108624951\C,-1.3711651733,-2.4363719448,-0.
6565821622\O,-0.3842790488,-2.5302239298,-1.3476582709\H,-3.8780740058
,-0.029141326,-1.5174328818\H,-4.0078815188,1.7281481093,-1.7056669869
\H,-2.833845566,0.8133526388,-2.673737788\H,-2.7699074863,1.218450088,
0.3795973212\H,-1.6948713184,2.0142769905,-0.7633617685\H,0.5224572678
,1.0987903976,-0.4005952012\H,0.7829149607,-0.6441309813,-0.3883227691

\H,-0.1399829574,-0.7495720676,1.9613622312\H,-0.3508134823,0.99527255
77,1.953389154\H,2.1413802024,1.3013304978,1.6431560553\H,2.3529005352
,-0.4554773285,1.6471934999\H,1.7880817055,0.3718966718,3.1084142442\C
,-2.2070677438,-3.5904471389,-0.1541321608\H,-1.8513686807,-4.51718094
89,-0.6056403079\H,-3.2626346007,-3.4332484032,-0.396657476\H,-2.13002
26028,-3.6617176968,0.9365416396\\Version=EM64L-G09RevA.02\State=2-A\H
F=-464.3020972\S2=0.753648\S2-1=0.\S2A=0.75001\RMSD=4.245e-09\RMSF=1.6
26e-06\Dipole=-0.5154008,0.2307305,0.58916\Quadrupole=-0.4092357,2.511
1827,-2.1019469,2.9509032,1.8021532,-2.3511235\PG=C01 [X(C8H15O2)]\\@

PVA_200

1\1\GINC-V1361\FOpt\UB3LYP\Gen\C8H15O4(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva300.freq\0,2\C,-0.1110466318,0.0990067371,-0.0271346699\C,0.
0660601273,-0.1085239402,1.4762478296\C,1.5350465796,-0.0794428414,1.9
119557193\C,-1.5648556095,0.3292544189,-0.4768517449\C,-2.5276080069,-
0.8217331651,-0.185310774\C,-3.9696696819,-0.5192601152,-0.6050156995\
O,-1.5879345642,0.5340625073,-1.9088549656\C,-1.2096839784,1.753008642
3,-2.3704539363\O,-0.9093386342,2.6809063058,-1.6507764398\H,-4.035925
8899,-0.3380680413,-1.6817399805\H,-4.6268168103,-1.3608690916,-0.3617
420665\H,-4.3568662062,0.3676467121,-0.0884051126\H,-2.1645916641,-1.7
220832856,-0.6939232492\H,-2.4961926109,-1.0298888718,0.890899465\H,-1
.9055713958,1.2533143735,0.0044978491\H,0.5019406445,0.9295062984,-0.3
836277833\H,-0.3896191593,-1.0632594192,1.7648967069\H,-0.4963790271,0
.6784360289,1.9954484647\H,1.9959779673,0.8885799379,1.6839427792\H,2.
1111856497,-0.8563408783,1.399378217\H,1.6232786012,-0.2484145239,2.99
0246977\O,0.4140276869,-1.1031574882,-0.6855627771\O,0.9973150607,-0.8
256316911,-1.842150099\C,-1.1998571777,1.7686711968,-3.878483402\H,-1.
0231812828,2.7849821892,-4.2321245509\H,-2.1446867012,1.3859039638,-4.
2757699628\H,-0.4012411314,1.1090588864,-4.2354233852\\Version=EM64L-G
09RevA.02\State=2-A\HF=-614.6727172\S2=0.753098\S2-1=0.\S2A=0.750006\R
MSD=6.071e-09\RMSF=4.906e-06\Dipole=-0.653791,-0.1242332,0.5207335\Qua
drupole=-0.1684353,-0.044688,6.2131233,1.6966828,2.148324,-2.4880293\P
G=C01 [X(C8H15O4)]\\@

PVA_200H

1\1\GINC-V1398\FOpt\RB3LYP\Gen\C8H16O4\GXG501\26-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pva300h.freq\0,1\C,0.0152432931,-0.023296498,0.0045182294\C,0.0077
785158,0.0412737037,1.5371801012\C,1.4181653369,0.0599692422,2.1344422
307\C,-1.3637169491,0.2556595634,-0.6261324906\C,-2.4484648541,-0.7617
657037,-0.2790844459\C,-3.8053669086,-0.4532264547,-0.9198204595\O,-1.
2164650676,0.2299480565,-2.0824624384\C,-0.8618847887,1.3934491647,-2.
6942510434\O,-0.712645765,2.4427182735,-2.1107019541\H,-3.7397728824,-
0.4660595643,-2.0120692163\H,-4.5526799486,-1.1949600611,-0.6182835587
\H,-4.1737416971,0.5344661792,-0.616589548\H,-2.1037494503,-1.76101178
48,-0.5694685452\H,-2.555114327,-0.7760286399,0.8123486404\H,-1.674128
1046,1.2681300151,-0.3499571863\H,0.730466377,0.707197894,-0.390891927
2\H,-0.5491476358,-0.8189745982,1.928176267\H,-0.5449219874,0.93997007
41,1.8414017115\H,1.9713316358,0.9503058985,1.8130991607\H,1.982424414
4,-0.8214979456,1.8166615412\H,1.3777206859,0.0666400423,3.2290456174\
O,0.487751952,-1.336231591,-0.3313995122\O,1.0908164772,-1.3016316394,
-1.6527024653\H,0.2919515318,-1.3215711364,-2.2135548669\C,-0.66594932
16,1.1790439243,-4.1759663862\H,-1.4937235157,0.6042905414,-4.60124677
86\H,-0.5787361053,2.1453056968,-4.6739099936\H,0.2555369662,0.6076963
983,-4.3394079483\\Version=EM64L-G09RevA.02\State=1-A\HF=-615.3055826\
RMSD=7.466e-09\RMSF=8.167e-06\Dipole=-0.8270828,-0.0886088,-0.2121614\
Quadrupole=-1.7512751,-6.4973782,8.2486534,2.80386,-0.1579163,1.149250
9\PG=C01 [X(C8H16O4)]\\@

PVA_2R

1\1\GINC-V1348\FOpt\UB3LYP\Gen\C8H15O2(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva3r.freq\0,2\C,0.0288281365,0.0497945994,-0.0843459828\C,0.10
31213155,-0.0627700581,1.4041381763\C,1.532507473,0.1090778813,1.95999
04945\C,-0.763224116,1.0758849031,-0.818054178\C,-1.620781009,0.493910
6601,-1.9475141086\C,-2.4757378782,1.533958128,-2.6782441223\O,0.13353
98905,2.050090762,-1.4831740025\C,0.6784334648,3.0063695642,-0.7039255
667\O,0.4792550343,3.1149850449,0.4886097566\H,-1.8487500732,2.2964187
388,-3.1498124593\H,-3.0809450494,1.0603514424,-3.4590760316\H,-3.1603
82137,2.0402486909,-1.9866818428\H,-0.9602765826,-0.0206249468,-2.6576
966836\H,-2.2645848816,-0.2767078009,-1.5047596962\H,-1.3835215936,1.6
456833343,-0.1190370672\H,0.6379414623,-0.6244112767,-0.6871297441\H,-
0.5536645238,0.6835485089,1.8652708182\H,-0.2706475209,-1.0519240558,1
.7193931805\H,1.9044907306,1.1152166431,1.7461392175\H,2.2210304499,-0
.6179098574,1.5126822523\H,1.5453209441,-0.039789148,3.0460177356\C,1.
5687098255,3.9193995742,-1.5187723396\H,1.0064847499,4.3572609853,-2.3
497842331\H,1.9630976696,4.7089282313,-0.8780610477\H,2.3953666147,3.3
454800269,-1.9510371748\Version=EM64L-G09RevA.02\State=2-A\HF=-464.30
01992\S2=0.754013\S2-1=0.\S2A=0.750011\RMSD=2.345e-09\RMSF=3.093e-06\D
ipole=-0.0423613,-0.3013669,-0.5935506\Quadrupole=1.3191262,0.5422376,
-1.8613637,1.1460909,-1.0359808,-2.9883105\PG=C01 [X(C8H15O2)]\@

PVA_300

1\1\GINC-V1367\FOpt\UB3LYP\Gen\C8H15O4(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva4oo.freq\0,2\C,-0.0159822481,-0.0129012967,0.0476574872\C,-0
.0650179595,-0.0607160563,1.5806016061\C,1.3305476554,-0.0664509487,2.
2128034142\C,-1.3839710795,-0.0753619678,-0.6324328369\C,-1.3083674712
, -0.0275939972,-2.1586810001\C,-2.6684937415,-0.1131588433,-2.85774167
02\O,-2.1474844766,1.0953015285,-0.1859947587\C,-3.2820805082,0.898910
1993,0.4872197152\O,-3.8227808279,-0.1606865978,0.715337069\H,-3.29800
07213,0.746546805,-2.60518794\H,-2.5446918007,-0.1245048339,-3.9459096
154\H,-3.2094141972,-1.0220695665,-2.569996158\H,-0.7878799336,0.89162
20021,-2.4576647232\H,-0.6739859713,-0.8648970858,-2.4784207771\H,-1.9
361564055,-0.9616418326,-0.3066032845\H,0.5011304154,0.8998908742,-0.2
787664018\H,0.5750582633,-0.8599467888,-0.3286487341\H,-0.6181951427,-
0.9550194307,1.8998217166\H,-0.628629868,0.8045140341,1.949929626\H,1.
8957496997,0.8309095205,1.9329612132\H,1.9121642446,-0.9391181039,1.89
03881199\H,1.2693705915,-0.092435262,3.3063670906\C,-3.9162922129,2.20
68002596,0.9566222302\H,-4.2327468485,2.0901734779,1.9950386929\H,-4.7
83699583,2.434602987,0.3298012345\O,-3.0613174074,3.3642906558,0.85004
25393\O,-2.1050097617,3.3286655502,1.7673875061\Version=EM64L-G09RevA
.02\State=2-A\HF=-614.662143\S2=0.752956\S2-1=0.\S2A=0.750006\RMSD=9.5
27e-09\RMSF=1.841e-06\Dipole=0.0148023,-0.3134194,-0.54674\Quadrupole=
2.672983,-4.2387348,1.5657518,-5.392701,-0.7239535,0.3687811\PG=C01 [X
(C8H15O4)]\@

PVA_300H

1\1\GINC-V1286\FOpt\RB3LYP\Gen\C8H16O4\GXG501\26-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pva4ooh.freq\0,1\C,0.0356227593,-0.054112432,0.0326770843\C,0.0354
736094,-0.1425118544,1.5642045479\C,1.4471197648,-0.261161101,2.147608
4122\C,-1.3545171897,0.0031576053,-0.6001329404\C,-1.3273836086,0.0436
1584,-2.1294664316\C,-2.7132112761,0.1351374571,-2.7772986946\O,-2.013
8453069,1.2293146419,-0.1397966787\C,-3.1509902576,1.1162261868,0.5816
239565\O,-3.6616356923,0.0775017736,0.9336432646\H,-3.2236380669,1.063
1508953,-2.4980848369\H,-2.6326251582,0.1150718624,-3.8692541542\H,-3.
3512779732,-0.7019874836,-2.4712953497\H,-0.7024472708,0.8879186451,-2
.452740122\H,-0.81642958,-0.8660725416,-2.4712208629\H,-1.9667677733,-
0.8341498063,-0.2538272705\H,0.6107403434,0.8253122895,-0.2897021303\H
,0.5495037238,-0.9316905964,-0.3845299021\H,-0.5693769883,-1.003446711
7,1.8793438446\H,-0.4556723226,0.7473395881,1.977054325\H,2.0647809295

,0.6024475783,1.8721130732\H,1.9552820419,-1.1619784351,1.7819080116\H
,1.4202976015,-0.3152444389,3.2414943691\C,-3.7625362265,2.4770694121,
0.9160272501\H,-3.8009118089,2.5752142936,2.0072539664\H,-4.7906122533
,2.4874366096,0.5336824078\O,-3.0359862738,3.6013224159,0.4749182059\O
, -3.1285130578,3.6343506861,-0.9746123342\H,-2.3444250082,3.0944044311
, -1.1947226787\Version=EM64L-G09RevA.02\State=1-A\HF=-615.2998745\RMS
D=3.446e-09\RMSF=1.685e-06\Dipole=0.7867278,-0.6338541,-0.2936067\Quad
rupole=0.9760399,-5.057383,4.0813431,-1.0210914,-0.8952681,2.8779975\PG
G=C01 [X(C8H16O4)]\@

PVA_3R

1\1\GINC-V1283\FOpt\UB3LYP\Gen\C8H15O2(2)\GXG501\26-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva4r.freq\0,2\C,-0.0266613516,0.0083186277,0.0179242075\C,-0.0
542397988,-0.0246232232,1.5513191936\C,1.3489206528,-0.0232287297,2.16
66041417\C,-1.404431297,-0.0623743814,-0.6461076288\C,-1.3315286142,-0
.058705826,-2.1751533779\C,-2.6952235076,-0.1743818845,-2.8622343055\O
, -2.1722063903,1.1065897003,-0.2418688592\C,-3.2602900632,0.9198807283
,0.5551889178\O,-3.6416243719,-0.16554036,0.970768581\H,-3.337155893,0
.675236613,-2.6079103495\H,-2.5826724165,-0.1946657031,-3.9517584973\H
, -3.2162338019,-1.0909541614,-2.5610655792\H,-0.822537242,0.85791728,-
2.5021477602\H,-0.6907938278,-0.8976130078,-2.4780154521\H,-1.94597124
18,-0.9459234126,-0.2949293975\H,0.4865893695,0.9180476319,-0.32485475
76\H,0.563372643,-0.8412916182,-0.3545577087\H,-0.6062394661,-0.912429
7278,1.8873895951\H,-0.6147752238,0.842894741,1.9210996506\H,1.9127754
13,0.8696466617,1.8690496216\H,1.9256071323,-0.8998179501,1.846168653\
H,1.3026763239,-0.0378138536,3.2613160014\C,-3.9167405862,2.177453355,
0.8533157096\H,-3.5382147899,3.1150157246,0.4640656525\H,-4.7994325225
,2.160197841,1.479827156\Version=EM64L-G09RevA.02\State=2-A\HF=-464.3
009838\S2=0.757179\S2-1=0.\S2A=0.750032\RMSD=5.412e-09\RMSF=1.100e-06\
Dipole=0.3750977,0.5165437,-0.3254629\Quadrupole=-0.9848219,1.2992403,
-0.3144184,-4.2847713,0.3190212,2.3130123\PG=C01 [X(C8H15O2)]\@

PVA_4

1\1\GINC-V1296\FOpt\RB3LYP\Gen\C9H16O4\GXG501\27-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pva2.freq\0,1\C,-0.0469492177,-0.0023664655,-0.0537365946\C,-0.063
3576555,0.0046881817,1.4767763584\C,1.3560130152,-0.0069497774,-0.6657
001936\C,-1.4618297605,0.1550895107,2.0633551315\C,1.3511962239,-0.160
0233317,-2.1819200262\O,0.7444070427,1.1331928136,1.9183694966\C,1.708
7451543,0.8977378686,2.8429247414\O,1.8957895069,-0.1773389096,3.37413
26482\O,2.0804684556,-1.1327654804,-0.0921647355\C,3.306945689,-0.8933
074618,0.4354302934\O,3.8662559725,0.1832119255,0.3991799867\H,0.78948
46415,0.6586932424,-2.6458869422\H,0.8882665071,-1.1079960333,-2.47791
1314\H,2.3735548915,-0.1358206362,-2.571902604\H,-0.6027531329,-0.8861
589795,-0.3941038965\H,-0.5792553132,0.8795514686,-0.4342827002\H,0.40
7947508,-0.9027300575,1.8568811439\H,1.8876500378,0.9022117384,-0.3814
575307\H,-1.4222143562,0.1326323728,3.1568893228\H,-1.9172942195,1.101
4483171,1.7510622256\H,-2.1060351825,-0.6657639357,1.7282732451\C,3.85
05900408,-2.1254657585,1.1142959517\C,2.5427781442,2.132361519,3.07674
49788\H,4.9400396808,-2.0719938357,1.1506628327\H,3.4645880577,-2.1376
647265,2.1404209915\H,3.5240278846,-3.0383449136,0.6108778042\H,3.0003
644891,2.0822317705,4.0662898566\H,1.9498508896,3.0436196596,2.9697237
378\H,3.3377967685,2.1446116816,2.3218482012\Version=EM64L-G09RevA.02
\State=1-A\HF=-653.536359\RMSD=9.730e-09\RMSF=9.905e-06\Dipole=-0.7654
923,-0.0012896,-0.507555\Quadrupole=-0.1769403,1.5968714,-1.4199311,-1
.6562929,1.457636,2.496758\PG=C01 [X(C9H16O4)]\@

PVA_400

1\1\GINC-V1364\FOpt\UB3LYP\Gen\C9H15O6(2)\GXG501\27-Jun-2010\0\#B3LYP

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/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva2oo.freq\0,2\C,-0.1360927274,-0.0598470709,0.0404862187\C,-0
.2035913566,-0.2456360766,1.565242415\C,1.2787767333,0.1265052281,-0.5
174014628\C,-1.6272043938,-0.2660362474,2.1055924495\C,1.3477121645,0.
1303140543,-2.0397604976\O,0.5020283241,0.8831113985,2.1357163845\C,1.
451445184,0.6248724314,3.0788462774\O,1.7087460112,-0.4860469057,3.488
0211829\O,2.1036609543,-0.951872284,-0.0107422715\C,3.2841103021,-0.61
81844402,0.575689814\O,3.6936412003,0.5199948825,0.66679744\H,0.696970
7789,0.9087477876,-2.4520246979\H,1.0354851986,-0.8332532159,-2.450688
3496\H,2.3742818714,0.3345442978,-2.3581113288\H,-0.7602988133,0.77706
18959,-0.2847575069\H,0.3263683939,-1.1590030166,1.8402088571\H,1.6682
691933,1.0656201229,-0.1188171683\H,-1.6121711561,-0.4253865279,3.1879
212683\H,-2.1371470262,0.6813323539,1.8991573793\H,-2.1973677032,-1.07
82368115,1.6449564778\O,-0.7430493713,-1.2670787674,-0.5262313595\O,-1
.574116781,-0.9888424513,-1.5196699127\C,2.1526182927,1.8925774214,3.4
919557935\C,3.9715969675,-1.8388332877,1.1298034023\H,2.9526487843,2.0
834045885,2.7671124685\H,1.4711220356,2.7463617083,3.4873948697\H,2.59
67805727,1.7574252128,4.4794198271\H,5.039677521,-1.6405661574,1.23246
17015\H,3.7980363606,-2.7144123524,0.5000888851\H,3.5517697441,-2.0387
854772,2.1226164824\Version=EM64L-G09RevA.02\State=2-A\HF=-803.238746
5\S2=0.753264\S2-1=0.\S2A=0.750007\RMSD=9.213e-09\RMSF=5.228e-06\Dipol
e=0.0443405,0.5219612,0.2045441\Quadrupole=-1.0529114,1.8340709,-0.781
1595,-4.8327058,-4.0792363,0.8461681\PG=C01 [X(C9H15O6)]\@

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PVA_4OOH

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1\I\GINC-V1289\FOpt\RB3LYP\Gen\C9H16O6\GXG501\27-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pva2oo.h.freq\0,1\C,-0.078370883,-0.0019454567,-0.0584218143\C,-0.0
839574146,0.013045816,1.4825828502\C,1.3206195768,-0.0292437998,-0.696
1042903\C,-1.4677841302,0.263808368,2.0626748224\C,1.2904397188,-0.061
7557474,-2.2189531715\O,0.8019841322,1.0884743414,1.8953066619\C,1.825
6264489,0.7762047071,2.7339256494\O,2.0250230301,-0.3336795428,3.18007
13759\O,2.0065983534,-1.2250145249,-0.2153983528\C,3.2718765915,-1.074
8279104,0.2741584945\O,3.8710591507,-0.023042631,0.2580581525\H,0.7960
801383,0.8366994192,-2.605007996\H,0.7426265809,-0.9341121229,-2.58609
46747\H,2.3107763652,-0.0852955408,-2.6128188733\H,-0.5745577918,0.906
152382,-0.4282412747\H,0.3230585324,-0.9240957839,1.8561909598\H,1.885
6156275,0.8364028797,-0.3486815159\H,-1.4307219374,0.2308568741,3.1559
26717\H,-1.8493180596,1.2448102713,1.7573447817\H,-2.1604244291,-0.506
2467863,1.7126672186\O,-0.9288138016,-1.0333384199,-0.5722259697\O,-0.
5890867796,-2.3103368478,0.0434324695\H,0.3045131487,-2.4732048326,-0.
3188569125\C,3.7791396758,-2.3622120406,0.8680685009\C,2.6995069516,1.
978328482,2.9876639078\H,3.1947532844,1.8703766255,3.9542829584\H,2.12
77174365,2.9079589666,2.9470110484\H,3.4672721246,2.0054872001,2.20532
70357\H,4.8690839273,-2.339106769,0.9097461861\H,3.4344501206,-3.23118
93517,0.3021760977\H,3.3868996005,-2.4347364923,1.8892372684\Version=
EM64L-G09RevA.02\State=1-A\HF=-803.8727976\RMSD=3.879e-09\RMSF=4.328e-
06\Dipole=0.3090518,0.4013207,-0.3429207\Quadrupole=-4.4720393,3.94766
5,0.5243743,-5.9591488,-1.4924173,2.1308727\PG=C01 [X(C9H16O6)]\@

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PVA_4R

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1\I\GINC-V1368\FOpt\UB3LYP\Gen\C9H15O4(2)\GXG501\27-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\pva2r.freq\0,2\C,0.0449487033,0.1238719544,-0.0239656311\C,-0.0
597679882,0.0931769826,1.4634180958\C,1.3618411337,0.007583771,-0.7195
075401\C,-1.4750034651,0.3066490744,1.9851684996\C,1.2417091123,-0.286
5609887,-2.2123313712\O,0.790145055,1.1759409035,1.9936052089\C,1.7419
710105,0.8436103856,2.8976059437\O,1.9007803618,-0.2743931026,3.345359
0261\O,2.1129089873,-1.0852822782,-0.1004521211\C,3.3235452569,-0.7962
021025,0.437799826\O,3.8391082767,0.3026784573,0.4079881063\H,0.675942
8198,0.5101741634,-2.7082172657\H,0.7250194027,-1.2369339524,-2.381265
5279\H,2.2331587675,-0.3398913765,-2.6717788249\H,-0.8272692178,0.3928
125294,-0.6140601569\H,0.3564243243,-0.8376733972,1.8603284185\H,1.958

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9391973,0.9157551149,-0.56556508\H,-1.4913094703,0.2639282244,3.078187
 3631\H,-1.864809746,1.2799092194,1.668023709\H,-2.1384613374,-0.475733
 3705,1.5998412588\C,3.9117026295,-2.0068786425,1.1179755722\C,2.606766
 1009,2.0345245672,3.230159657\H,4.9970814149,-1.9047654916,1.169439279
 8\H,3.51103416,-2.0420925126,2.1376272703\H,3.6330158231,-2.9296584248
 ,0.6040521652\H,3.0711613866,1.8874711561,4.2067801588\H,2.0333135003,
 2.9640952408,3.2095682501\H,3.3938338002,2.0962668957,2.4695787097\\Ve
 rsion=EM64L-G09RevA.02\State=2-A\HF=-652.8676082\S2=0.753934\S2-1=0.\S
 2A=0.750011\RMSD=3.650e-09\RMSF=9.027e-06\Dipole=-0.6909622,0.0381795,
 -0.495193\Quadrupole=0.4042821,0.1230172,-0.5272992,-2.0831323,1.65528
 49,2.6246595\PG=C01 [X(C9H15O4)]\\@

PMVC_1

1\1\GINC-V1431\FOpt\RB3LYP\6-31G(d)\C8H16O3\GXG501\07-Jun-2010\0\#B3L
 YP\6-31G* OPT Freq=norman maxdisk=268435456\pval.freq\0,1\C,-0.0776
 098018,0.0134279381,0.0252676968\C,-0.0455677077,-0.0693772481,1.55688
 31297\C,1.3756764565,0.0204558874,2.1221664664\C,-1.4671253064,-0.1544
 647083,-0.5916899591\C,-1.459331621,-0.0926875644,-2.1202284612\C,-2.8
 376740305,-0.2919225267,-2.7572223833\O,-2.3149333418,0.9347933146,-0.
 1168844388\C,-3.3371013072,0.6205573269,0.6900980252\O,-3.6437976514,-
 0.4821267357,1.0912082016\O,-3.9820817494,1.7618761947,0.9880235567\C,
 -5.1134776881,1.5982798378,1.8555572605\H,-3.5297844065,0.4993009271,-
 2.451701573\H,-2.7675940054,-0.2710025264,-3.8502202408\H,-3.275572218
 3,-1.2544579904,-2.4672200238\H,-1.0373497022,0.8719301211,-2.43199774
 88\H,-0.7682946944,-0.8676971366,-2.4776350967\H,-1.9207585693,-1.0901
 565511,-0.2515245748\H,0.3441800139,0.9734717405,-0.3037485363\H,0.566
 173911,-0.7714402419,-0.3967268845\H,-0.515609057,-1.0072749061,1.8818
 284922\H,-0.654872597,0.7413493748,1.9751694201\H,1.8580588929,0.96355
 29211,1.8371048417\H,2.0047375889,-0.79809908,1.7507817312\H,1.3717339
 607,-0.0333006514,3.2165992978\H,-4.8072976128,1.1720040957,2.81470046
 75\H,-5.8611686919,0.945193821,1.3975464031\H,-5.5165754794,2.60191104
 86,1.9947532341\\Version=EM64L-G09RevA.02\State=1-A\HF=-540.1858614\RM
 SD=3.547e-09\RMSF=6.321e-07\Dipole=0.1041953,0.125205,-0.0852598\Quadr
 upole=2.5283777,-3.4102564,0.8818787,-3.4571947,-2.2153014,2.8408578\PG
 G=C01 [X(C8H16O3)]\\@

PMVC_100

1\1\GINC-V1424\FOpt\UB3LYP\6-31G(d)\C8H15O5(2)\GXG501\07-Jun-2010\0\#
 B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pvaloo.freq\0,2\C,-0
 .1917377172,0.069138031,0.1176104\C,-0.1420820596,-0.0213488321,1.6498
 998527\C,1.306228377,0.0108870237,2.1521382445\C,-1.5315744941,-0.1091
 778005,-0.6061837055\C,-1.3499148494,-0.1592278318,-2.1296669132\C,-2.
 6486257146,-0.3088388875,-2.9266683754\O,-2.476914086,0.932210226,-0.3
 733283878\C,-3.1877906084,1.0557580916,0.7741872645\O,-3.1287030972,0.
 3706497465,1.7647000625\O,-3.996463931,2.1106969373,0.5951446824\C,-4.
 848266054,2.4031655535,1.7155240712\H,-3.3217345255,0.5346821348,-2.75
 11337089\H,-2.4237723551,-0.3496654738,-3.9975509074\H,-3.1748589107,-
 1.2299573321,-2.6580017063\H,-0.8256330023,0.7572101836,-2.4247881504\
 H,-0.6784500243,-0.9990838816,-2.3345016974\H,0.2043643985,1.038213548
 4,-0.212658335\H,0.4715659086,-0.6969044103,-0.2991180251\H,-0.6314010
 271,-0.9427589949,1.9802023736\H,-0.7054681774,0.7997766038,2.10107589
 7\H,1.8171200344,0.9333959162,1.8481271144\H,1.8850876362,-0.833559565
 ,1.7581673775\H,1.3414825602,-0.0429239423,3.2457078218\H,-4.251837248
 9,2.6244831752,2.6043923834\H,-5.507887271,1.5576851698,1.9267388006\H
 ,-5.4272335294,3.2762444695,1.4142971128\O,-2.2166266098,-1.3530784603
 ,-0.1827268947\O,-1.4436403667,-2.40968603,-0.3542674213\\Version=EM64
 L-G09RevA.02\State=2-A\HF=-689.8868264\S2=0.753309\S2-1=0.\S2A=0.75000
 7\RMSD=2.193e-09\RMSF=3.959e-06\Dipole=0.0627302,1.0892382,-0.2361804\
 Quadrupole=3.8586639,-4.1583085,0.2996446,-2.9408538,-2.4498595,3.3305
 499\PG=C01 [X(C8H15O5)]\\@

PMVC_100H

1\1\GINC-V1385\FOpt\RB3LYP\6-31G(d)\C8H16O5\GXG501\07-Jun-2010\0\#\B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\pva100h.freq\0,1\C,-0.0980139015,0.180369175,0.0033235966\C,0.1492428424,-0.555241937,1.3298099619\C,1.2933322395,0.0837908685,2.1243320461\C,-1.3882807663,-0.1605276812,-0.792987369\C,-1.1000691922,-0.3292290297,-2.2904282232\C,-2.3276935715,-0.6341415897,-3.1511485631\O,-2.3752470762,0.8877111666,-0.7355436291\C,-2.8533509346,1.3396807501,0.4411393989\O,-2.489403183,1.0450436719,1.555913711\O,-3.8218540217,2.2203539191,0.1466375403\C,-4.4448807167,2.8274976739,1.289356486\H,-3.0650841394,0.1710853765,-3.0902923395\H,-2.0308434773,0.7481581189,-4.1994742912\H,-2.8081074418,-1.56258802,-2.8298576535\H,-0.6111675838,0.5938020204,-2.6272265028\H,-0.3630089422,-1.1329445995,-2.3826551994\H,-0.112379816,1.2600422491,0.1908638107\H,0.7578528725,0.0044067404,-0.6598344355\H,0.4073721097,-1.6017376048,1.1221286182\H,-0.7645708017,-0.5462149486,1.9277278101\H,1.047355419,1.1161331328,2.3999916529\H,2.2256925232,0.1048056561,1.5460485317\H,1.4884764491,-0.4701120894,3.0494961278\H,-3.7107278557,3.3812064275,1.8806676673\H,-4.9142729737,2.0681111096,1.9200731969\H,-5.1959612986,3.5037013768,0.8805224785\O,-2.1322922955,-1.2811188076,-0.2759943341\O,-1.3664152128,-2.488304568,-0.5377082595\H,-1.1591206694,-2.7490110645,0.377537092\Version=EM64L-G09RevA.02\State=1-A\HF=-690.517975\RMSD=6.274e-09\RMSF=3.351e-06\Dipole=0.2950941,0.3457451,0.2837119\Quadrupole=1.4378638,1.6421245,-3.0799883,-4.6572919,-2.7984902,-0.3105166\PG=C01 [X(C8H16O5)]\@

PMVC_1R

1\1\GINC-V1419\FOpt\UB3LYP\6-31G(d)\C8H15O3(2)\GXG501\07-Jun-2010\0\#\B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\pva1r.freq\0,2\C,-0.2734346377,-0.0320706651,0.013477552\C,0.0096799941,-0.192891748,1.5291969811\C,1.5067344336,-0.2969034217,1.8345292962\C,-1.7282294658,0.0446964892,-0.3309864308\C,-2.557422755,1.2766651144,-0.1461606977\C,-3.7484645086,1.3776547645,-1.1138307282\O,-2.4986541606,-1.1172836747,-0.131346925\C,-2.2072207031,-2.2359140006,-0.8271773706\O,-1.360747837,-2.3653926447,-1.681289754\O,-3.0447419502,-3.1941293988,-0.3986086679\C,-2.88302507,-4.4612679315,-1.0538132789\H,-4.4203803508,0.5224094758,-0.9927613138\H,-4.3235030151,2.2907377444,-0.924794566\H,-3.4074451614,1.3961828694,-2.1547101461\H,-2.9402501044,1.3240567161,0.8896542625\H,-1.900542898,2.146581812,-0.2674504831\H,0.2086626528,0.8868203622,-0.3450953787\H,0.1893374765,-0.8644454125,-0.5288469249\H,-0.5086200556,-1.0884025856,1.8952162726\H,-0.4212265599,0.6579102378,2.0736701692\H,2.0433814616,0.5998516464,1.5009883271\H,1.9552779319,-1.1587408761,1.3257515641\H,1.6864675924,-0.4122866345,2.9095425835\H,-1.8750241445,-4.8530373501,-0.8933922907\H,-3.0625993081,-4.3660073275,-2.1280354494\H,-3.6255441727,-5.1170159881,-0.5984291636\Version=EM64L-G09RevA.02\State=2-A\HF=-539.5218942\S2=0.753517\S2-1=0.\S2A=0.750009\RMSD=6.011e-09\RMSF=3.617e-06\Dipole=-0.104762,-0.0795343,0.3038681\Quadrupole=-2.1283959,6.0601306,-3.9317348,2.1783374,2.6344282,0.8063097\PG=C01 [X(C8H15O3)]\@

PMVC_200

1\1\GINC-V1279\FOpt\UB3LYP\6-31G(d)\C8H15O5(2)\GXG501\07-Jun-2010\0\#\B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\pva300.freq\0,2\C,-0.1597607003,-0.0585159935,-0.095744985\C,-0.0351222815,0.0298235509,1.424650451\C,1.356249743,0.481882929,1.881196611\C,-1.5962467764,-0.2668361769,-0.605521172\C,-2.26111982,-1.5716696618,-0.1679235979\C,-3.7084417979,-1.7009675717,-0.6534460317\O,-1.5974484667,-0.2796469529,-2.0535846296\C,-1.4958585713,0.9131442171,-2.662423033\O,-1.4090198752,1.9925874724,-2.1146008687\O,-1.5188981841,0.7028327252,-3.9833685704\C,-1.4008829637,1.8911574053,-4.7818842342\H,-3.7585989714,-1.6879725585,-1.7459086682\H,-4.1487680455,-2.6408141584,-0.3040537119\H,-4.3301036099,-0.8797682082,-0.2754959199\H,-1.6602191441,-2.4116338081,-0.5339395432\H,-2.2355041413,-1.6152346657,0.9274355918\H,-2.1826495336,0.5

982199791,-0.274510208\H,0.2578821751,0.828703908,-0.5762344705\H,-0.2
72040903,-0.9468010134,1.8634649276\H,-0.7970995867,0.7316040226,1.788
1993737\H,1.5904138443,1.4837061317,1.5030416911\H,2.1289318445,-0.204
0635878,1.5198291444\H,1.414782133,0.512588824,2.9742172409\H,-0.45428
17752,2.3982059252,-4.5779554129\H,-2.2276087705,2.5765815925,-4.57765
24454\H,-1.4352057295,1.5462137991,-5.8153917065\O,0.675284601,-1.1845
350656,-0.5266406746\O,1.2699276879,-0.9482997701,-1.6869948861\\Versi
on=EM64L-G09RevA.02\State=2-A\HF=-689.8916955\S2=0.75309\S2-1=0.\S2A=0
.750006\RMSD=9.862e-09\RMSF=3.063e-06\Dipole=-0.6555912,0.3768755,0.50
46622\Quadrupole=-3.281385,-3.9183621,7.1997471,2.8373639,1.3033769,-4
.6404871\PG=C01 [X(C8H15O5)]\\@

PMVC_200H

1\1\GINC-V1386\FOpt\RB3LYP\6-31G(d)\C8H16O5\GXG501\07-Jun-2010\0\#B3L
YP\6-31G* OPT Freq=noraman maxdisk=268435456\pva3ooh.freq\0,1\C,0.06
03584767,0.0284692074,0.0334215861\C,0.0305096465,-0.0184476652,1.5657
982493\C,1.4317411808,0.021654752,2.1832906\C,-1.3211292895,0.28585197
9,-0.6000987225\C,-2.3764132369,-0.7761683672,-0.301654281\C,-3.726942
434,-0.5045036983,-0.9720951774\O,-1.1571324768,0.3005480641,-2.054711
1159\C,-0.7660191695,1.4644964347,-2.605451096\O,-0.6229241658,2.52120
11595,-2.0317906532\O,-0.564687527,1.2434011899,-3.9123999383\C,-0.139
9746681,2.3978198299,-4.6571512152\H,-3.6318120946,-0.4916021757,-2.06
18308454\H,-4.4524965906,-1.280145371,-0.7047567547\H,-4.1404749804,0.
4618307903,-0.6580288729\H,-1.9854460215,-1.7545004531,-0.6039316548\H
,-2.5087374978,-0.8148119534,0.7862200862\H,-1.6688390195,1.2795152583
,-0.2999847215\H,0.7446550704,0.8179361202,-0.2974576908\H,-0.48915784
27,-0.9301655416,1.8847147224\H,-0.5679929788,0.8285060654,1.927310234
4\H,1.9451104092,0.9587823742,1.9378833213\H,2.0407724284,-0.805678727
4,1.8077954666\H,1.3792744237,-0.0569475663,3.2745763463\H,0.806593945
7,2.7790814162,-4.2659807851\H,-0.8950196871,3.1863866759,-4.606069071
7\H,-0.0189213255,2.0487712196,-5.6826761905\O,0.5970391701,-1.2312147
593,-0.3963721023\O,1.2625893213,-1.0510742534,-1.6749171009\H,0.49939
26485,-1.0826657663,-2.2837172498\\Version=EM64L-G09RevA.02\State=1-A\
HF=-690.5264263\RMSD=5.480e-09\RMSF=2.914e-06\Dipole=-0.6960938,0.4005
734,-0.1956199\Quadrupole=-3.1388885,-4.6619198,7.8008083,3.5512123,-1
.9683626,-3.2835349\PG=C01 [X(C8H16O5)]\\@

PMVC_2R

1\1\GINC-V1419\FOpt\UB3LYP\6-31G(d)\C8H15O3(2)\GXG501\07-Jun-2010\0\#
B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\pva3r.freq\0,2\C,1.1
382970232,-0.7848712868,0.6246784769\C,0.0499184921,-0.0441018785,1.33
15841564\C,0.3346200832,0.1720890459,2.8330882516\C,1.9359039462,-0.24
0468215,-0.5089852613\C,2.0034799553,-1.1792686028,-1.7187065763\C,2.7
854508022,-0.6085997555,-2.9058943905\O,3.3472925558,-0.0472728359,-0.
1044558731\C,3.5977332414,1.0285073139,0.6475537184\O,2.7985924512,1.8
701990443,1.0053483589\O,4.90961471,1.0300862964,0.943107563\C,5.33967
52565,2.1396239745,1.744862156\H,3.8254989705,-0.4094850601,-2.6317565
701\H,2.782738422,-1.3123939481,-3.7454602945\H,2.3420880279,0.3312868
702,-3.2572646885\H,2.4441511744,-2.1313150919,-1.3958711187\H,0.97044
71814,-1.3976208769,-2.0178686051\H,1.553967643,0.741450578,-0.8059065
477\H,1.4128232978,-1.7762519296,0.9856070823\H,-0.10918241,0.92864384
73,0.852057889\H,-0.8980124756,-0.6008243112,1.2383744765\H,1.22271105
81,0.7970021327,2.9634332599\H,0.5041862396,-0.7829540146,3.3444863526
\H,-0.5130874877,0.6686706108,3.3195060226\H,4.8206079285,2.145910934,
2.7072108208\H,5.1491357595,3.0856561242,1.2309623376\H,6.4104251421,1
.9922825074,1.8895587083\\Version=EM64L-G09RevA.02\State=2-A\HF=-539.5
202093\S2=0.753988\S2-1=0.\S2A=0.750011\RMSD=7.211e-09\RMSF=3.319e-06\
Dipole=-0.0059522,-0.124632,-0.0235982\Quadrupole=1.1634227,-1.4262065
,0.2627838,4.216045,2.7683186,0.7265394\PG=C01 [X(C8H15O3)]\\@

PMVC_300

1\1\GINC-V1423\FOpt\UB3LYP\6-31G(d)\C8H15O5(2)\GXG501\07-Jun-2010\0\#\nB3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pva400.freq\0,2\C,0.0391757289,0.0527249405,0.0092893078\C,0.1258363097,-0.0088736912,1.5396616977\C,1.5655206918,0.0923685583,2.053793753\C,-1.3731433592,-0.1074684078,-0.5516879903\C,-1.4284764953,-0.0872098568,-2.0797944055\C,-2.8366960206,-0.2507602617,-2.6599571769\O,-2.170627585,1.0212331195,-0.0593063025\C,-3.2778371524,0.747762793,0.6210051097\O,-3.7329968241,-0.3340683054,0.9099161489\O,-3.8334661653,1.9476364822,0.9702119162\C,-5.0732362041,1.8752400503,1.6245179326\H,-3.4836852632,0.5851484275,-2.3749080701\H,-2.8010366979,-0.2825937195,-3.7541006155\H,-3.308568506,-1.1764095811,-2.3109920654\H,-0.9804174472,0.849510977,-2.4365173956\H,-0.7824294521,-0.8999453044,-2.4375705632\H,-1.8373998026,-1.0200283131,-0.1667281074\H,0.4591546064,1.0021409017,-0.3505022236\H,0.6559655291,-0.746225101,-0.4254671459\H,-0.326744805,-0.9460334385,1.892456778\H,-0.4721128216,0.8050031275,1.9681872336\H,2.0329875924,1.0343812072,1.7421283795\H,2.1844533807,-0.7276584836,1.6693216498\H,1.5996234372,0.0503758379,3.1480583346\H,-5.1890654231,2.7970555122,2.1911354218\H,-5.1627154764,0.9665406685,2.219551755\O,-6.1503172942,1.794972897,0.6652787543\O,-6.4272950745,2.9949006138,0.166369254\Version=EM64L-G09RevA.02\State=2-A\HF=-689.8923515\S2=0.752859\S2-1=0.\S2A=0.750006\RMSD=3.235e-09\RMSF=1.623e-06\Dipole=1.1004918,-0.3268642,0.3187272\Quadrupole=-3.0453869,-2.3396384,5.3850253,-0.3596834,-4.5441903,3.6498809\PG=C01 [X(C8H15O5)]\@

PMVC_300H

1\1\GINC-V1386\FOpt\RB3LYP\6-31G(d)\C8H16O5\GXG501\07-Jun-2010\0\#\nB3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pva400h.freq\0,1\C,-0.1865882075,-0.0245596227,-0.0021657317\C,-0.3187303585,-0.0157811127,1.5263945378\C,1.0374808912,-0.100248211,2.234061996\C,-1.5147957024,-0.0119052602,-0.7589422083\C,-1.3489367512,-0.0572889236,-2.2781382542\C,-2.6713955063,-0.0774306828,-3.0504247496\O,-2.2082867936,1.239907131,-0.4386982769\C,-3.3363298508,1.1782738002,0.2610187921\O,-3.8467378689,0.1646950676,0.7138058123\O,-3.8177025413,2.422487964,0.3825679179\C,-4.9847926048,2.6313966086,1.2247893821\H,-3.248684626,0.8353895211,-2.8715882093\H,-2.4891430582,-0.1498150553,-4.127901945\H,-3.2917571651,-0.9329951812,-2.7578482367\H,-0.7416821597,0.8015807146,-2.59237871\H,-0.7657477781,-0.9569478531,-2.5148605538\H,-2.1542535712,-0.8314325628,-0.4191825462\H,0.4160714384,0.8339560809,-0.3295114596\H,0.3583436845,-0.9259393884,-0.3160496397\H,-0.9551693045,-0.853043908,1.8426759003\H,-0.8350471711,0.9000183012,1.8405466302\H,1.683344351,0.7420103893,1.9570902625\H,1.5672401421,-1.0240781505,1.9709846315\H,0.9179413185,-0.0838055021,3.3229593508\H,-5.1292146038,3.7107461377,1.1550462812\H,-4.7663167386,2.304183718,2.2436120188\O,-6.1391912895,2.027695094,0.7561647867\O,-6.3733736834,0.7892486769,1.4804299229\H,-5.6196442481,0.24909044,1.1452106959\Version=EM64L-G09RevA.02\State=1-A\HF=-690.5346174\RMSD=6.392e-09\RMSF=1.788e-06\Dipole=1.4347677,-0.0819405,-0.2000669\Quadrupole=-7.4259849,3.9720424,3.4539426,-2.397754,0.7583817,3.372095\PG=C01 [X(C8H16O5)]\@

PMVC_3R

1\1\GINC-V1279\FOpt\UB3LYP\6-31G(d)\C8H15O3(2)\GXG501\07-Jun-2010\0\#\nB3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pva4r.freq\0,2\C,0.0059323754,-0.0118173839,-0.0077509569\C,0.0030369623,-0.0807361857,1.5249243525\C,1.4168441354,-0.0781530002,2.1156241449\C,-1.3772300064,-0.1024599453,-0.65431031\C,-1.3356660366,-0.0434531359,-2.181655289\C,-2.7086860686,-0.1731239857,-2.8477677537\O,-2.17285717,1.038593751,-0.2006541947\C,-3.198031165,0.791473511,0.6168755797\O,-3.5666957419,-0.2759974259,1.0493370815\O,-3.7813832773,1.9905511272,0.8882245888\C,-4.8446549991,1.9912253578,1.7572876041\H,-3.3675569635,0.6510131866,-2.5560756184\H,-2.614099928,-0.1548980684,-3.9388362563\H,-3.1998356693,-1.1132360334,-2.5695918775\H,-0.8573994819,0.897181408,-2.4848193111\H,-0.6780073687,-0.8538276521,-2.5228282598\H,-1.8927140996,-1.0080861

878,-0.3212455683\H,0.4921180542,0.9168977661,-0.337590505\H,0.6083429
296,-0.8389782324,-0.4094042493\H,-0.5334915228,-0.9821735623,1.849460
9846\H,-0.5584094098,0.7724771248,1.9252486123\H,1.96555353,0.82767461
1,1.8296495115\H,1.9969785579,-0.9408110986,1.7650342614\H,1.389200347
5,-0.1183160201,3.2101591288\H,-5.3580209638,2.9411693039,1.7837608482
\H,-5.288604093,1.0402344002,2.0160368459\\Version=EM64L-G09RevA.02\St
ate=2-A\HF=-539.51719\S2=0.753158\S2-1=0.\S2A=0.750006\RMSD=6.707e-09\
RMSF=5.363e-06\Dipole=0.3411695,0.0002617,-0.3731676\Quadrupole=1.7081
597,-1.7552356,0.0470759,-3.1759491,-0.8187132,2.0883259\PG=C01 [X(C8H
15O3)]\@

PMVC_4

1\1\GINC-V1285\FOpt\RB3LYP\6-31G(d)\C9H16O6\GXG501\10-Jun-2010\0\#B3L
YP/6-31G* OPT=rfo Freq=noraman maxdisk=268435456\pva2.freq\0,1\C,0.0
000355147,-0.0000337636,0.0000428672\C,0.000008767,0.0000037182,1.5304
229922\C,1.3951400193,-0.0000126224,-0.6289641629\C,-1.3983642063,0.06
76776588,2.1313667002\C,1.3683559008,-0.0697188498,-2.1506759301\O,0.7
36160692,1.1796021426,1.9638975588\C,1.7685929854,0.9878315234,2.80127
51721\O,2.1263064735,-0.0672884723,3.2833549391\O,2.338020544,2.179410
5707,3.0199442662\C,3.5433665059,2.1306031107,3.7992187363\O,2.0933737
941,-1.1788985871,-0.1347292047\C,3.2800359849,-0.985775833,0.46375333
21\O,3.7140335631,-2.17683598,0.8938608054\C,4.9189328902,-2.126753499
5,1.6738117032\O,3.8653667824,0.069965779,0.5920496191\H,0.8329964443,
0.7937098942,-2.5611932447\H,0.8681866273,-0.982731497,-2.4918106317\H
,2.3867122817,-0.0619770345,-2.551738005\H,-0.5545845877,-0.883850785,
-0.3412785951\H,-0.5391565541,0.8835783189,-0.3656058027\H,0.530557760
7,-0.8775421458,1.9039258196\H,1.9536030686,0.878012806,-0.3000166529\
H,5.7311489083,-1.6680191581,1.1041689561\H,4.7456856188,-1.5574539084
,2.59061605\H,5.153008354,-3.1658611788,1.9071505697\H,3.8501690465,3.
1701267331,3.9186570244\H,4.3097397358,1.5636591835,3.2644652967\H,-1.
3454440543,0.0610567298,3.2245566435\H,-1.9167397881,0.9793378231,1.81
4623547\H,-1.9907285916,-0.7972671094,1.8125600028\H,3.3576554397,1.66
99702862,4.7728321626\\Version=EM64L-G09RevA.02\State=1-A\HF=-803.9751
938\RMSD=4.411e-09\RMSF=4.236e-05\Dipole=-0.1496093,-0.0001441,-0.0969
402\Quadrupole=4.652536,-4.9414213,0.2888853,-0.6627335,4.8536776,1.03
63038\PG=C01 [X(C9H16O6)]\@

PMVC_400

1\1\GINC-V1295\FOpt\UB3LYP\6-31G(d)\C9H15O8(2)\GXG501\04-Jun-2010\0\#
B3LYP/6-31G* OPT=rfo Freq=noraman maxdisk=268435456\pva2oo.freq\0,2\C,0.
0193014003,0.0301809586,-0.0324178507\C,-0.0018268802,-0.0061447173,1.
5060068721\C,1.4222713567,-0.0066882566,-0.6512034497\C,-1.4030283839,
0.0889396701,2.0933080565\C,1.4228201606,-0.0934400239,-2.1721629969\O
,0.7583940894,1.1525304266,1.9252133022\C,1.7808425419,0.9449898632,2.
7804891883\O,2.1097125054,-0.1178060664,3.2624126551\O,2.3585825793,2.
1269459658,3.004425014\C,3.5548913959,2.0695084062,3.8000486661\O,2.11
06530501,-1.1656735087,-0.1210449433\C,3.2943479111,-0.9512636276,0.48
41310462\O,3.7439325539,-2.1307647252,0.9172040282\C,4.9454761644,-2.0
654288832,1.7034325989\O,3.8549549408,0.1181512907,0.6086207579\H,0.87
34567739,0.749665849,-2.6040094282\H,0.9572938197,-1.021429805,-2.5138
991221\H,2.4527030656,-0.0597543388,-2.539804394\H,-0.5117412002,0.910
1280895,-0.4055483881\H,0.5070029881,-0.905100042,1.85827179\H,1.95302
19539,0.8888342957,-0.3200994578\H,5.7487669576,-1.5812411262,1.142769
2051\H,4.7539911856,-1.5137392642,2.6271781739\H,5.2001280423,-3.10236
37163,1.9229807171\H,3.8607620763,3.1074664229,3.9317955015\H,4.325576
9662,1.5066052682,3.2678256906\H,-1.348590757,0.0665766846,3.185889826
6\H,-1.893115128,1.0197004526,1.7880370286\H,-2.0131771163,-0.75537951
02,1.7599690881\H,3.3539523181,1.6006015292,4.7663121483\O,-0.74805404
9,-1.1347687097,-0.4730633449\O,-1.5752326037,-0.8394763504,-1.4652357
556\\Version=EM64L-G09RevA.02\State=2-A\HF=-953.6765386\S2=0.753257\S2
-1=0.\S2A=0.750007\RMSD=8.433e-09\RMSF=4.945e-06\Dipole=0.7437619,0.51
67278,0.5785704\Quadrupole=2.3207517,-3.1940726,0.873321,-3.7828037,-0
.110791,-0.4669993\PG=C01 [X(C9H15O8)]\@

PMVC_400H

1\1\GINC-V1436\FOpt\RB3LYP\6-31G(d)\C9H16O8\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pva2ooh.freq\0,1\C,-0.0137824819,-0.09674998,0.0511690568\C,-0.0488507091,-0.0293066584,1.5910893875\C,1.3933257584,0.0008739115,-0.5638237468\C,-1.4627927848,0.0137316117,2.1487538884\C,1.3849164678,-0.0024984053,-2.0865490294\O,0.636028288,1.1991919837,1.9565022285\C,1.7095039597,1.0862242406,2.7606568219\O,2.1417195837,0.0645787888,3.2517550095\O,2.2202279857,2.3113161889,2.9236213655\C,3.4502303152,2.3518436365,3.6662950806\O,2.1502991246,-1.1607681047,-0.1072252454\C,3.3439711143,-0.9331056177,0.4799994888\O,3.8188847881,-2.1102182107,0.8932949324\C,5.0434123114,-2.0314472664,1.6447344803\O,3.8862373389,0.1434561692,0.5988923688\H,0.8472883097,0.8757940254,-2.4606416903\H,0.8906221447,-0.8976555518,-2.4738892725\H,2.4095730576,0.03646724,-2.4678899231\H,-0.5935669282,0.7455721129,-0.3504025602\H,0.5040278103,-0.8675166995,2.0106461026\H,1.8920870918,0.8943046785,-0.1859324666\H,5.8310751427,-1.5641323222,1.0486624092\H,4.8813709939,-1.4554949717,2.5590040946\H,5.30057379,-3.0639150331,1.8810994187\H,3.7128911352,3.4082134079,3.7272715748\H,4.2244517485,1.7927014049,3.135040432\H,-1.4343153263,0.0480508189,3.2422165347\H,-1.999806521,0.8978567436,1.7875946436\H,-2.0086500561,-0.8808689206,1.839184588\H,3.312607348,1.9313274436,4.6656121933\O,-0.7361591673,-1.2284095611,-0.443970569\O,-0.3123354137,-2.434443531,0.2569833992\H,0.5993506516,-2.5494438316,-0.079098712\Version=EM64L-G09RevA.02\State=1-A\HF=-954.312314\RMSD=5.185e-09\RMSF=3.044e-06\Dipole=0.9552601,0.3899614,0.0256322\Quadrupole=1.3213549,-2.9251975,1.6038426,-5.346578,1.956028,0.579155\PG=C01 [X(C9H16O8)]\@

PMVC_4R

1\1\GINC-V1469\FOpt\UB3LYP\6-31G(d)\C9H15O6(2)\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pva2r.freq\0,2\C,0.1121386533,0.1664626342,0.0303876704\C,0.0304224471,0.0847083852,1.5181165366\C,1.4100237895,0.0184073039,-0.6973301073\C,-1.3914090495,0.1528297487,2.057434339\C,1.2448793543,-0.1964260023,-2.1991091109\O,0.7703755024,1.2385336351,2.0682401141\C,1.8186560353,0.9711187918,2.8613856839\O,2.1940132897,-0.1245627035,3.2288903607\O,2.3843936686,2.1389480364,3.1928547888\C,3.5908164861,2.0227437352,3.9627773861\O,2.1128902726,-1.1401854862,-0.1533742027\C,3.2950873761,-0.9141182269,0.4457783129\O,3.7451028532,-2.0875610739,0.9023580282\C,4.9396291689,-2.0037654359,1.6958381667\O,3.8619648406,0.1545032232,0.5499663156\H,0.7134952924,0.6527269242,-2.642915839\H,0.674618867,-1.108937233,-2.4001116331\H,2.228124598,-0.280813238,-2.681985166\H,-0.7428954054,0.5437632856,-0.5252854537\H,0.540483414,-0.8107035138,1.8822284313\H,2.0525809296,0.8896277188,-0.5127670097\H,5.746213625,-1.5267214914,1.1334196935\H,4.7386964765,-1.4365350351,2.6079963887\H,5.1970728496,-3.0357825517,1.9358786436\H,3.8907100123,3.0477917807,4.1827175452\H,4.3616094599,1.5159084155,3.3763599134\H,-1.3912771443,0.0937273908,3.1498375721\H,-1.8764048211,1.0886655119,1.7596411597\H,-1.9793893483,-0.6844212418,1.6654473379\H,3.4095248136,1.4683955954,4.8871976567\Version=EM64L-G09RevA.02\State=2-A\HF=-803.3055934\S2=0.753847\S2-1=0.\S2A=0.75001\RMSD=4.751e-09\RMSF=2.410e-06\Dipole=-0.1186729,0.0310409,-0.0874358\Quadrupole=4.7991549,-6.2100128,1.4108579,-1.0580633,5.1930611,0.6555217\PG=C01 [X(C9H15O6)]\@

PU_1

1\1\GINC-V1292\FOpt\RB3LYP\6-31G(d)\C7H15N1O2\GXG501\31-May-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pu1.freq\0,1\C,-0.0644257305,-0.4649967676,-0.5228029147\O,-0.1200182733,-0.364449762,0.6914364448\O,1.0590331307,-0.2680422301,-1.2700516047\C,2.2546838548,0.0525628473,-0.530698281\C,2.9677704129,-1.1997346519,-0.0304063612\C,4.2

842769373,-0.8607711988,0.6769466905\N,-1.1053438528,-0.8085229911,-1.3346014966\C,-2.4657714135,-0.9037547356,-0.8250219986\C,-3.2178778485,0.4341352162,-0.7960918043\C,-4.6449473804,0.2861838375,-0.2598595484\H,4.1137872727,-0.2132284078,1.5453625152\H,4.9797681196,-0.3420639621,0.0053192653\H,4.7825570944,-1.7685688977,1.0330619211\H,3.1548537686,-1.8658475112,-0.8823010754\H,2.8773930836,0.6035954749,-1.2422662873\H,1.9928675918,0.7099939636,0.3031446494\H,-2.3981893642,-1.3142270371,0.1863849756\H,-3.0069947763,-1.6321816455,-1.4414865936\H,-2.6504730822,1.1343527602,-0.1711348733\H,-4.6442652403,-0.1094404776,0.7629021503\H,-5.2369296483,-0.3982875039,-0.8804210678\H,-5.1634855681,1.2507913108,-0.2427421898\H,-3.2406929542,0.8594524606,-1.8091757101\H,2.2972541793,-1.7288246052,0.6558476\H,-0.9533294526,-0.718448875,-2.3293983354\Version=EM64L-G09RevA.02\State=1-A\HF=-481.0119603\RMSE=4.123e-09\RMSE=4.983e-06\Dipole=-0.1197273,0.011734,-0.8106797\Quadrupole=4.0879958,-1.7205273,-2.3674685,0.473888,1.8822712,0.0186944\PG=C01 [X(C7H15N1O2)]\@

PU_100

1\1\GINC-V1293\FOpt\UB3LYP\6-31G(d)\C7H14N1O4(2)\GXG501\03-Jun-2010\0\B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pu100.freq\0,2\C,-0.1029901478,-0.0547495557,-0.3406402262\O,-0.1805058932,-0.643894415,0.7172484251\O,1.0870494001,0.1795190667,-1.0201811848\C,2.2661875257,0.0338793478,-0.281864477\C,3.3617318553,-0.5879657143,-1.1260417162\C,3.0547775835,-2.0415500021,-1.4992909012\N,-1.1335933656,0.4128278124,-1.0862394635\C,-2.5005521218,0.413337422,-0.5774937361\C,-2.8556689468,1.6671763032,0.2325336536\C,-4.2966976285,1.6307339902,0.750172306\H,2.1318140051,-2.1102051658,-2.0832586385\H,2.9374832349,-2.6670336716,-0.6069838793\H,3.8684735989,-2.4614212518,-2.0990832322\H,4.2966049,-0.5250552932,-0.5569021652\H,2.0585794564,-0.4971518013,0.6492057549\H,-2.6072212042,-0.4792606499,0.0448014233\H,-3.1781197468,0.3031811007,-1.4328509803\H,-2.1532025146,1.7479310209,1.0706468818\H,-4.4616891044,0.7637389047,1.4011151301\H,-5.0176568954,1.5696458324,-0.0746789024\H,-4.5302043157,2.5303477993,1.3292216951\H,-2.7049333492,2.5577148863,-0.3931668128\H,3.4899160143,0.0243269961,-2.0265493851\H,-0.8937447956,1.018688235,-1.8589600239\O,2.7568031646,1.3740009996,0.0842036176\O,1.8364310689,2.0606947574,0.7398538207\Version=EM64L-G09RevA.02\State=2-A\HF=-630.7242494\S2=0.752923\S2-1=0.\S2A=0.750006\RMSE=1.602e-09\RMSE=4.535e-06\Dipole=-0.369875,-0.2538996,-1.0654896\Quadrupole=5.3265938,-3.5796205,-1.7469733,-6.2199077,-0.1408449,-0.5778615\PG=C01 [X(C7H14N1O4)]\@

PU_100H

1\1\GINC-V1481\FOpt\RB3LYP\6-31G(d)\C7H15N1O4\GXG501\03-Jun-2010\0\B3LYP\6-31G* OPT Freq=norman maxdisk=268435456\pu100h.freq\0,1\C,0.0750394204,0.3074492985,0.3516805774\O,0.0799764091,0.9900336726,1.3738083996\O,1.1732599236,-0.0478175724,-0.3580015327\C,2.4927046904,0.2740778694,0.1773982956\C,3.4915272521,-0.357275296,-0.7836537788\C,3.3435776923,-1.8751438781,-0.9208086025\N,-1.0423565507,-0.2119745626,-0.2137324471\C,-2.3839504149,0.149108407,0.2283219059\C,-2.9988942238,1.3129661259,-0.559984341\C,-4.4130492036,1.6529002245,-0.0795698284\H,2.3633142007,-2.1433751828,-1.3250159876\H,3.4577255731,-2.3755392359,0.048392072\H,4.1105087469,-2.2739504877,-1.5929656213\H,4.488096122,-0.0996403981,-0.4094709141\H,2.5613042129,-0.1235698685,1.1935157645\H,-2.3082020756,0.4070023588,1.2876362357\H,-3.0183651412,-0.742440396,0.1499482584\H,-2.3444670968,2.1874479148,-0.4580669182\H,-4.4137421979,1.9410241863,0.9783989089\H,-5.0905233133,0.7973534131,-0.1920164625\H,-4.8333929241,2.4867253839,-0.6515001675\H,-3.0187138864,1.0571269213,-1.6284457559\H,3.378789133,0.133593942,-1.7577260875\H,-0.9222706726,-0.6929728204,-1.0941889418\O,2.7166520412,1.651171433,0.2056248679\O,2.5015816264,2.1626265944,1.5492420613\H,1.530219699,1.9996507579,1.6375727837\Version=EM64L-G09RevA.02\State=1-A\HF=-631.3660889\RMSE=4.043e-09\RMSE=4.253e-06\Dipole=-1.104451,-1.2530442,-0.8944246\Quadrupole=3.4394895,-2.2332228,-1.2062667,-4.9668928,-0.6995498,-0.5610955\PG=

C01 [X(C7H15N1O4)]\@

PU_1R

1\1\GINC-V1284\FOpt\UB3LYP\6-31G(d)\C7H14N1O2(2)\GXG501\01-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pulr.freq\0,2\C,-0.3798450478,0.0168274547,0.6406044116\O,-0.303663731,0.6781975541,1.6573181097\O,0.6909212961,-0.5905833295,0.0208676459\C,1.9486430393,-0.3793427158,0.5583554104\C,2.9919440791,-1.3165845378,0.0606906734\C,2.8395580564,-2.7659504144,0.5773180027\N,-1.5159245007,-0.2672495637,-0.0529342912\C,-2.7863225673,0.3654327885,0.2738470629\C,-3.0152872511,1.7042662037,-0.4411867547\C,-4.3662180019,2.3295819455,-0.0809264298\H,1.8688285107,-3.1792843792,0.2842272317\H,2.9058063898,-2.8027663499,1.6703673497\H,3.624903572,-3.4110168203,0.165935982\H,3.9715049334,-0.9230546879,0.3594100334\H,1.957220394,0.0774926017,1.5413379575\H,-2.797095566,0.5132397607,1.3572088661\H,-3.5892159795,-0.340700718,0.0286613748\H,-2.1994176915,2.3852487077,-0.1698336756\H,-4.4406452455,2.5171971575,0.9969363942\H,-5.1991456965,1.6732808167,-0.3625505778\H,-4.5086264045,3.2858851926,-0.5953343632\H,-2.9516013313,1.5507089252,-1.527480996\H,2.9782310199,-1.3280845987,-1.0385013822\H,-1.4017555654,-0.7202760782,-0.9488145859\Version=EM64L-G09RevA.02\State=2-A\HF=-480.3485342\S2=0.753219\S2-1=0.\S2A=0.750007\RMSD=4.368e-09\RMSF=4.169e-06\Dipole=-0.4355046,-0.4041091,-0.8443284\Quadrupole=4.1400163,-1.7361771,-2.4038392,-1.6602349,1.5141818,-0.6889037\PG=C01 [X(C7H14N1O2)]\@

PU_200

1\1\GINC-V1380\FOpt\UB3LYP\6-31G(d)\C7H14N1O4(2)\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\puloo.freq\0,2\C,-0.0273582065,0.1443690272,0.2978814851\O,-0.1624263705,-0.5311234808,1.2990591097\O,1.151123612,0.5206842672,-0.2477646201\C,2.3414463339,0.0438383375,0.4224120299\C,2.7376404095,-1.3486092592,-0.055712737\C,4.0487466511,-1.8163142925,0.5855390128\N,-1.064728801,0.615477772,-0.4839086691\C,-2.3983225199,0.6211579908,0.0034682144\C,-3.4392070319,0.4883360544,-1.1020056318\C,-4.8799770314,0.453161168,-0.5840564314\H,3.9640901141,-1.8627236244,1.6777458122\H,4.878196057,-1.1407679929,0.3427365035\H,4.3208573833,-2.8160273472,0.231465164\H,2.8338156375,-1.334318542,-1.148689216\H,3.1068723779,0.7834383766,0.1710614085\H,2.1678200287,0.0558632298,1.5016814531\H,-2.4913560879,-0.1435987384,0.7754357655\H,-3.3058183874,1.3256427546,-1.7986460152\H,-5.1358186452,1.3779351712,-0.0586061678\H,-5.0335823402,-0.3827808758,0.1086250943\H,-5.5811756055,0.3305721212,-1.415757388\H,-3.2071776855,-0.4305235037,-1.6530117944\H,1.9291610547,-2.0461501781,0.1908975944\H,-0.8278869492,1.3111236364,-1.1801930889\O,-2.6720725511,1.8784628276,0.7778259181\O,-2.4027744219,2.9431170097,0.0436108518\Version=EM64L-G09RevA.02\State=2-A\HF=-630.7257329\S2=0.75317\S2-1=0.\S2A=0.750007\RMSD=7.825e-09\RMSF=2.668e-06\Dipole=0.323275,-0.5407699,-0.8852655\Quadrupole=7.1851198,-5.3435022,-1.8416177,2.2310669,2.5964199,-0.2543748\PG=C01 [X(C7H14N1O4)]\@

PU_200H

1\1\GINC-V1487\FOpt\RB3LYP\6-31G(d)\C7H15N1O4\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\puloooh.freq\0,1\C,0.0371662087,0.0606038124,-0.0304443227\O,0.0626005736,0.1351332969,1.1836919244\O,1.1317472691,-0.0159128468,-0.8331789482\C,2.4066770617,-0.0623282276,-0.155600586\C,2.7774737108,-1.483060375,0.2563893747\C,4.1702713041,-1.5459631114,0.8926528216\N,-1.0981042972,0.0148599557,-0.7991022704\C,-2.3994958811,0.2999568394,-0.2557520157\C,-3.4854447161,-0.5219334007,-0.9541242049\C,-4.8863748137,-0.2572512992,-0.3974358464\H,4.2251744961,-0.9241697644,1.7941558116\H,4.9454962488,-1.1978992932,0.1987893409\H,4.421159697,-2.5717540766,1.1821824309\H,2.7348732615

, -2.1313350689, -0.6280427185\H, 3.1174388902, 0.3363641146, -0.8855984504
 \H, 2.3709976152, 0.6007846553, 0.7130660955\H, -2.3612123119, 0.0840421116
 , 0.8162203449\H, -3.4617502129, -0.2994037566, -2.0279055484\H, -5.1656098
 061, 0.7921626487, -0.5251605875\H, -4.9401541978, -0.4922464947, 0.6724939
 566\H, -5.6283070682, -0.8764353336, -0.9128238685\H, -3.2193905485, -1.579
 7931406, -0.8406135376\H, 2.024597043, -1.8480686652, 0.9640346393\H, -0.98
 13154468, 0.050463515, -1.8024196675\O, -2.6973181955, 1.7032621934, -0.246
 0728894\O, -2.7366543499, 2.1484854914, -1.637430762\H, -1.996263212, 2.780
 2451448, -1.6179997178\Version=EM64L-G09RevA.02\State=1-A\HF=-631.3578
 526\RMSD=7.832e-09\RMSF=3.134e-06\Dipole=0.587888, -0.2465306, -0.840946
 7\Quadrupole=1.6741921, 0.9119759, -2.586168, 2.7916525, -0.427302, -1.8608
 334\PG=C01 [X(C7H15N1O4)]\@

PU_2R

1\1\GINC-V1301\FOpt\UB3LYP\6-31G(d)\C7H14N1O2(2)\GXG501\01-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pul1r.freq\0,2\C,0
 .0052503458, -0.0382513629, -0.1138094809\O, 0.0622314546, 0.3525105336, 1.
 0381262598\O, 1.0739758728, -0.338951141, -0.9036899694\C, 2.3693442769, -0
 .1855621231, -0.2868222818\C, 2.775922964, -1.4301383457, 0.4957646014\C, 4
 .1899886545, -1.3022011444, 1.0724537197\N, -1.1531228754, -0.2380233239, -
 0.8242805517\C, -2.4283853988, -0.0957456777, -0.2875038831\C, -3.60417183
 01, -0.0469024699, -1.2057785752\C, -4.9279081199, -0.3065964081, -0.474597
 7614\H, 4.2655211252, -0.4481025434, 1.7559905624\H, 4.9362018351, -1.16309
 77784, 0.2803066185\H, 4.465980501, -2.201064907, 1.6336345395\H, 2.7144196
 419, -2.3021735207, -0.16774132\H, 3.0510297225, -0.0040815237, -1.12326899
 59\H, 2.3519249228, 0.6949359872, 0.3614983576\H, -2.4518561806, 0.33041130
 7, 0.7076609696\H, -3.6665652851, 0.9309113137, -1.7208388332\H, -5.0869496
 696, 0.4314957098, 0.3202426373\H, -4.9337114352, -1.2999170149, -0.0133384
 58\H, -5.7761818179, -0.2420590746, -1.1643028028\H, -3.4800464076, -0.7900
 253258, -2.0099291524\H, 2.0524372284, -1.5843551243, 1.304113683\H, -1.046
 9106179, -0.5868427612, -1.7682869944\Version=EM64L-G09RevA.02\State=2-
 A\HF=-480.3553802\S2=0.753676\S2=1=0\S2A=0.75001\RMSD=8.575e-09\RMSF=
 6.442e-06\Dipole=0.0328608, -0.3059424, -0.8627664\Quadrupole=4.5632103,
 -2.3001897, -2.2630206, -0.6542511, 1.6556048, -0.7747705\PG=C01 [X(C7H14N
 1O2)]\@

PES_1

1\1\GINC-V1414\FOpt\RB3LYP\6-31G(d)\C7H14O2\GXG501\01-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pes1.freq\0,1\C,1.02819
 34412, 0.4247355767, 0.4900046628\O, 1.7615294523, 1.0459965412, 1.22904168
 45\C, 1.4743778777, -0.4535253766, -0.6637036158\C, 2.9895658899, -0.444616
 8193, -0.8769586555\C, 3.4218108201, -1.3486533382, -2.0349663508\O, -0.320
 4079012, 0.4291180869, 0.599256373\C, -0.8683616217, 1.2270619293, 1.673899
 3617\C, -2.3830476641, 1.0892567638, 1.6355332863\C, -2.8786059945, -0.3366
 592685, 1.8966810742\H, -2.4866634469, -1.0302619084, 1.1461890803\H, -2.55
 68500002, -0.6920292105, 2.8834281353\H, -3.9724931023, -0.3846250851, 1.86
 46258059\H, -2.7459384525, 1.4421644601, 0.661752664\H, -2.7937126824, 1.77
 41672724, 2.3895089344\H, -0.4512115184, 0.8737715428, 2.6237170925\H, -0.5
 505845556, 2.2660768354, 1.5380248433\H, 0.9437880275, -0.1226033199, -1.56
 66279579\H, 1.1102394076, -1.4720044036, -0.4693769274\H, 4.5091389439, -1.
 3264765617, -2.1670445873\H, 3.12946767, -2.391349604, -1.858801916\H, 2.96
 5517514, -1.0333194546, -2.9815987352\H, 3.4831238312, -0.7568547481, 0.050
 6324074\H, 3.3199169985, 0.5849250307, -1.0588278548\Version=EM64L-G09Re
 vA.02\State=1-A\HF=-425.649578\RMSD=3.723e-09\RMSF=2.241e-06\Dipole=-0
 .605246, -0.2528837, -0.271223\Quadrupole=-0.3893627, -0.1275511, 0.516913
 9, -2.9743293, -3.376106, -0.2869849\PG=C01 [X(C7H14O2)]\@

PES_100

1\1\GINC-V1286\FOpt\UB3LYP\6-31G(d)\C7H13O4(2)\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\pes100.freq\0,2\C, -0

.1497228053,0.0407782485,0.0333066375\O,-0.2071364138,-0.2846635311,1.1924956846\C,1.0961989975,0.1246260005,-0.8163834719\C,2.3457494383,-0.4098329349,-0.1128532052\C,3.6001270094,-0.2834796304,-0.9819845626\O,-1.2555622789,0.3752842931,-0.7220493108\C,-2.4705097013,0.5869300171,-0.0461015964\C,-3.6308011943,-0.010263077,-0.8180702063\C,-3.5732253933,-1.5400884114,-0.8671293866\H,-2.660231196,-1.8834551204,-1.3636528968\H,-3.5956782035,-1.9742796652,0.1390495714\H,-4.4292780399,-1.9360420024,-1.4222681187\H,-3.6203968684,0.4105991545,-1.8303200701\H,-4.5573664521,0.325164751,-0.3375244601\H,-2.388938094,0.2399097788,0.9855963776\H,1.2210646513,1.1801584678,-1.0967062018\H,0.9046263407,-0.4061885041,-1.7582262044\H,4.4801828388,-0.6733524852,-0.459291506\H,3.4958418968,-0.8420976564,-1.9203749153\H,3.8031432226,0.7630318178,-1.2404870821\H,2.182894933,-1.4589093152,0.1624450624\H,2.4826542446,0.1310949005,0.8302405576\O,-2.7171754871,2.0332014279,-0.0009981888\O,-1.7186259596,2.6737660099,0.5838592163\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-575.3601261\\S2=0.752913\\S2-1=0.\\S2A=0.750006\\RMSD=7.443e-09\\RMSF=5.414e-06\\Dipole=-0.0917325,-0.8175093,-0.8113128\\Quadrupole=6.345177,-4.0026144,-2.3425626,3.0429754,-0.9345168,0.1788454\\PG=C01 [X(C7H13O4)]\\@

PES_10OH

1\1\GINC-V1438\FOpt\RB3LYP/6-31G(d)\C7H14O4\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pes10oh.freq\0,1\C,-0.1587254162,0.2714360943,-0.0175960933\O,-0.1241698203,1.025218766,0.9412838407\C,1.0684718248,-0.2188876999,-0.7574382748\C,2.3788561811,0.3690109163,-0.229195008\C,3.5977940868,-0.1436832814,-1.0014393184\O,-1.2824699697,-0.2307046215,-0.5560195255\C,-2.5848886386,0.0348491194,0.0693753913\C,-3.606513743,-0.7027674969,-0.7849067209\C,-3.3643168664,-2.2122019598,-0.8724899929\H,-2.4005553635,-2.432985208,-1.3398901998\H,-3.373659344,-2.6755903375,0.1215547852\H,-4.1494506878,-2.6892470834,-1.4680982169\H,-3.6007198722,-0.2500678478,-1.783587956\H,-4.5875408084,-0.4940954084,-0.3446098616\H,-2.5430607206,-0.3235399643,1.1013745436\H,0.9275080982,0.0145737064,-1.8213722731\H,1.0750259469,-1.3162628294,-0.7002654542\H,4.5224931943,0.291255813,-0.6072716921\H,3.6873580129,-1.2348258244,-0.9310190881\H,3.5358098173,0.1152688074,-2.0656218666\H,2.4776572623,0.1275495192,0.8354240855\H,2.3299963229,1.4627591664,-0.2859170897\O,-2.8957663578,1.3938192203,0.0636047212\O,-2.6288530769,1.9700195781,1.3700367617\H,-1.6435111338,1.9152341895,1.3794449626\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-576.0014124\\RMSD=9.505e-09\\RMSF=3.089e-06\\Dipole=0.6361919,-1.1873192,-0.598032\\Quadrupole=2.202809,-1.8315549,-0.3712542,4.4982874,0.6829787,-2.152287\\PG=C01 [X(C7H14O4)]\\@

PES_1R

1\1\GINC-V1337\FOpt\UB3LYP/6-31G(d)\C7H13O2(2)\GXG501\01-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pes1r.freq\0,2\C,0.2875709618,-0.4462395181,0.3132077242\O,0.370771224,-1.4943134164,0.9109765783\C,1.3941519352,0.2363005365,-0.4608134004\C,2.7323081002,-0.5005427648,-0.3712733947\C,3.8365172126,0.1976353767,-1.17012182\O,-0.8657349168,0.2930779289,0.2464080394\C,-2.0062163645,-0.1962386324,0.8517535301\C,-3.1119297196,0.789247019,0.9860504641\C,-2.858002674,1.880679697,2.0516194594\H,-2.7294062415,1.4384106483,3.0457114688\H,-1.9521101417,2.4479955684,1.8137671201\H,-3.6990217184,2.5823548234,2.0963323467\H,-3.28710264,1.2745246627,0.0156133597\H,-4.0283921638,0.2405171495,1.2359174658\H,-1.863223356,-1.0564103396,1.4949758285\H,1.4827334819,1.2675830373,-0.0928693352\H,1.0648669121,0.3284992229,-1.505492301\H,4.7829333979,-0.3484651517,-1.0923914653\H,3.5784043579,0.2658868003,-2.2342495333\H,4.0104952175,1.2178534486,-0.8061735806\H,2.5995062028,-1.5282097026,-0.7287346598\H,3.025446179,-0.5854513206,0.6818570407\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-424.9860296\\S2=0.753568\\S2-1=0.\\S2A=0.750009\\RMSD=7.666e-09\\RMSF=7.620e-06\\Dipole=-0.0742985,0.6839639,-0.2323209\\Quadrupole=3.2897572,-3.4004076,0.1106503,0.3647772,-2.0460619,1.251922\\PG=C01 [X(C7H13O2)]\\@

PES_200

1\1\GINC-V1308\FOpt\UB3LYP\6-31G(d)\C7H13O4(2)\GXG501\04-Jun-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pes11oo.freq\0,2\C,0
.1224107276,-0.2055824886,0.1658729825\O,-0.2685912109,0.532616942,1.0
430404635\C,1.3872992125,0.0722273499,-0.6580512668\C,2.4028628773,0.9
301276901,0.0898880292\C,3.5827758794,1.3651455187,-0.7830391706\O,-0.
5040877162,-1.3122459413,-0.2460513097\C,-1.7095280129,-1.6832827225,0
.4722848582\C,-2.0788348221,-3.0967531985,0.0497579064\C,-1.0347611117
,-4.1438191193,0.451236411\H,-0.0594027929,-3.9146519177,0.0109925217\H,
-0.9115389473,-4.1793087558,1.540619394\H,-1.3346202253,-5.142360397
4,0.1159021872\H,-2.2338978327,-3.1123442727,-1.0364567353\H,-3.048813
2801,-3.3318178846,0.5081096144\H,-1.5099288228,-1.6120982323,1.546007
1429\H,-2.4931280488,-0.9593491442,0.2241589617\H,1.0835705641,0.54980
47676,-1.5983337339\H,4.2820137568,1.9758118754,-0.2027072935\H,4.1327
537708,0.501681777,-1.1709130901\H,3.2482206691,1.9640543866,-1.639011
8495\H,2.750271126,0.3572801706,0.9566413678\H,1.8637411891,1.79813958
07,0.4817979919\O,1.9874248823,-1.1776565458,-1.1284972961\O,2.3363514
265,-1.9528002689,-0.112854605\Version=EM64L-G09RevA.02\State=2-A\HF=
-575.3507621\S2=0.753178\S2-1=0.\S2A=0.750007\RMSE=9.880e-09\RMSE=1.82
8e-06\Dipole=-0.4752314,0.2347219,-0.3307497\Quadrupole=2.1714863,-0.4
605751,-1.7109112,5.8674578,0.6673549,-3.699381\PG=C01 [X(C7H13O4)]\@

PES_200H

1\1\GINC-V1380\FOpt\RB3LYP\6-31G(d)\C7H14O4\GXG501\04-Jun-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\pes11ooh.freq\0,1\C,0.0
349534362,0.1763752474,-0.0675848424\O,-0.0149432306,0.4680938291,1.10
61945685\C,1.345902757,0.115035935,-0.8648864347\C,2.4194398448,-0.683
6377318,-0.1124037206\C,3.7867953055,-0.6105772298,-0.7943380962\O,-1.
054266976,-0.1045323899,-0.8194814879\C,-2.3321901299,-0.0266332034,-0
.1338763404\C,-3.4355937901,-0.2888438962,-1.1475033824\C,-3.416261639
6,-1.6967222239,-1.7514053089\H,-2.5058305683,-1.8727543679,-2.3347876
4\H,-3.4695360414,-2.4653059564,-0.9709763919\H,-4.2672755175,-1.84344
01339,-2.4246862532\H,-3.3759082229,0.4652231962,-1.9421875967\H,-4.38
99095211,-0.1225940422,-0.6304375356\H,-2.3359779643,-0.7639648066,0.6
764430593\H,-2.4198883985,0.9663612811,0.3162735686\H,1.6816486728,1.1
564627701,-0.9793160941\H,4.5239841462,-1.2038649972,-0.2428539429\H,3
.7350866756,-0.9953089203,-1.8171600591\H,4.1557940165,0.4217593247,-0
.8405387436\H,2.0870634814,-1.7247935366,-0.0420698136\H,2.4673033332,
-0.2892884799,0.9079666016\O,1.1664251517,-0.2848748917,-2.2175612495\O,
0.7286486658,-1.670979806,-2.2346052262\H,-0.2355307622,-1.530445319
3,-2.159221221\Version=EM64L-G09RevA.02\State=1-A\HF=-575.9866219\RMSE
D=6.668e-09\RMSE=2.866e-06\Dipole=-0.9567283,0.0636108,0.0776357\Quadr
upole=6.4546551,0.0792566,-6.5339117,1.5370595,2.0488577,-2.11631\PG=C
01 [X(C7H14O4)]\@

PES_2R

1\1\GINC-V1287\FOpt\UB3LYP\6-31G(d)\C7H13O2(2)\GXG501\01-Jun-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pes11r.freq\0,2\C,0.
0267274449,0.1079283193,0.0846368498\O,0.0696756108,-0.251499818,1.255
1980281\C,1.1710829611,0.5240198821,-0.7029091917\C,2.5464770137,0.551
920414,-0.1361805099\C,3.5477331493,-0.3035047589,-0.9396204941\O,-1.1
274175329,0.163106672,-0.6363598875\C,-2.3227262641,-0.2341727953,0.06
5232297\C,-3.4908791794,-0.1405656873,-0.9056085999\C,-3.3803365347,-1
.1002628202,-2.094627134\H,-2.4752521821,-0.8988417138,-2.6760419909\H
,-3.3373756764,-2.1431760071,-1.7570605503\H,-4.2428995263,-1.00003069
66,-2.7623841908\H,-3.572166525,0.8941209866,-1.2624933937\H,-4.407622
4021,-0.3491456129,-0.3379408156\H,-2.1905254831,-1.2542933787,0.44481
24869\H,-2.4609708905,0.4229043069,0.9311006033\H,0.9998123066,0.81216
93708,-1.7367749702\H,4.5509508471,-0.2235231535,-0.5070776471\H,3.256

7290209,-1.3591226276,-0.9313958138\H,3.6036907306,0.0231090235,-1.984
5197055\H,2.5061215716,0.2193211973,0.9055660081\H,2.9104273929,1.5926
824616,-0.1277927903\\Version=EM64L-G09RevA.02\State=2-A\HF=-424.99437
02\S2=0.756715\S2-I=0.\S2A=0.750029\RMSD=7.030e-09\RMSF=4.207e-06\Dipo
le=-0.0119205,0.1885746,-0.6746343\Quadrupole=5.1845616,-0.5717578,-4.
6128038,1.3158768,-1.6104955,0.315726\PG=C01 [X(C7H13O2)]\\@

PES_3

1\1\GINC-V1293\FOpt\RB3LYP\6-31G(d)\C5H8O4\GXG501\01-Jun-2010\0\#B3LY
P/6-31G* OPT Freq=noraman maxdisk=268435456\\pes3.freq\0,1\C,-0.00258
09028,0.4183643166,-0.1274658756\O,0.1281604996,0.5149619171,1.2843628
653\C,1.076011909,-0.2962707094,1.836482421\C,-0.7800309204,-0.8345145
004,-0.5171892744\O,1.831902906,-0.9738175278,1.180023614\O,-1.2604058
956,-1.6301401856,0.2534979029\C,1.0290983721,-0.216846015,3.340547082
1\O,-0.8627772958,-0.9121181703,-1.8593371141\C,-1.5755365953,-2.05420
83029,-2.3686434885\H,-1.5498596464,-1.9538721172,-3.453783014\H,-2.60
64442126,-2.0548840215,-2.0053109625\H,-1.0846210809,-2.9789182706,-2.
0550708604\H,0.9746778442,0.4034530235,-0.6172058923\H,-0.5531197046,1
.306379775,-0.4479802895\H,0.1217004484,-0.7178170575,3.6956032021\H,0
.9838144886,0.8242171257,3.6732061334\H,1.905404882,-0.7132073476,3.75
86995477\\Version=EM64L-G09RevA.02\State=1-A\HF=-496.2601231\RMSD=9.61
4e-09\RMSF=1.505e-05\Dipole=-0.4115844,0.5024074,-0.3954722\Quadrupole
=-4.3371202,-1.0980037,5.4351239,1.779905,3.6710661,2.8841001\PG=C01 [X
(C5H8O4)]\\@

PES_300

1\1\GINC-V1282\FOpt\UB3LYP\6-31G(d)\C5H7O6(2)\GXG501\04-Jun-2010\0\#B
3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\pes300.freq\0,2\C,0.2
38026161,0.4299152883,-0.0278778531\O,0.2468659533,0.4721446805,1.3684
128593\C,1.124085608,-0.3728377069,2.018029342\C,-1.2189877063,0.40368
19385,-0.5147472672\O,1.8422308894,-1.1502092739,1.4417316839\O,-2.157
5474155,0.1192236881,0.1860867204\C,1.0199270353,-0.168525421,3.503822
2416\O,-1.2659132351,0.6609464645,-1.8269631385\C,-2.5823816564,0.6368
575934,-2.4136180477\H,-2.4312937694,0.8542121117,-3.4704264751\H,-3.2
148013233,1.3967060672,-1.9484999826\H,-3.0397485991,-0.3465358873,-2.
2796149862\H,0.8046700851,-0.4284197836,-0.398046668\H,-0.0108341444,-
0.3386177683,3.8307105556\H,1.2748900338,0.8665262555,3.7540236274\H,1
.6965141739,-0.8545981188,4.0135788487\O,0.9573253434,1.5725124,-0.548
6993468\O,0.2734020412,2.6935202087,-0.3442703753\\Version=EM64L-G09Re
vA.02\State=2-A\HF=-645.959665\S2=0.752901\S2-I=0.\S2A=0.750006\RMSD=3
.518e-09\RMSF=3.730e-06\Dipole=-0.4754256,-0.2875854,-0.0327756\Quadru
pole=-3.0945815,-5.6621051,8.7566866,0.5291088,6.9761057,1.034865\PG=C
01 [X(C5H7O6)]\\@

PES_300H

1\1\GINC-V1487\FOpt\RB3LYP\6-31G(d)\C5H8O6\GXG501\04-Jun-2010\0\#B3LY
P/6-31G* OPT Freq=noraman maxdisk=268435456\\pes300h.freq\0,1\C,-0.09
4661376,0.4086746562,-0.1183062026\O,0.0408900414,0.4953534792,1.29852
24229\C,1.0224851453,-0.2770769919,1.8537487159\C,-0.9440763432,-0.832
9140715,-0.4626151425\O,1.802092731,-0.9229517906,1.1942178027\O,-1.34
32973148,-1.6332589059,0.3479102181\C,0.9732881362,-0.2004961427,3.356
7845058\O,-1.1306161233,-0.8979860061,-1.7853180248\C,-1.9197918218,-2
.0122356984,-2.2432312306\H,-1.9604846538,-1.9125141112,-3.3275732981\H
H,-2.9232265187,-1.9655274648,-1.8130475357\H,-1.4473518335,-2.9552942
133,-1.9570757553\H,0.8878747706,0.3417237388,-0.5946375779\H,0.074652
3557,-0.7173267668,3.7112763388\H,0.9120366147,0.8396475949,3.69038917
76\H,1.8585805045,-0.6815592044,3.7736627891\O,-0.6445904802,1.5963743
327,-0.5852676998\O,-2.0310367872,1.6445508499,-0.1437716023\H,-1.9182
833792,2.0104218512,0.7548309091\\Version=EM64L-G09RevA.02\State=1-A\H
F=-646.6001229\RMSD=5.453e-09\RMSF=2.918e-06\Dipole=-0.2919832,0.18841

31,0.3855589\Quadrupole=-3.8087716,-2.075711,5.8844826,2.5886103,1.895
3044,7.2013484\PG=C01 [X(C5H8O6)]\@

PES_3R

1\I\GINC-V1284\FOpt\UB3LYP\6-31G(d)\C5H7O4(2)\GXG501\02-Jun-2010\0\#B
3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\pes3r.freq\0,2\C,-0.1
465771045,0.1049081126,0.1680154561\O,0.0161519094,0.1061303841,1.5128
411272\C,1.2689913935,-0.2209479106,2.0204093087\C,-1.431657693,0.4388
956706,-0.3968605565\O,2.2035825493,-0.5019328515,1.3168079421\O,-1.62
79665252,0.4515435667,-1.6051705601\C,1.2390691544,-0.1614118597,3.521
9580672\O,-2.3743173484,0.7298771848,0.5332316081\C,-3.6614042631,1.06
54394784,-0.0036753778\H,-4.2933104593,1.269452889,0.861371241\H,-4.06
67572606,0.2338848532,-0.5872010667\H,-3.5951037151,1.9475793516,-0.64
68786657\H,0.6978044339,-0.1486234555,-0.4575508057\H,0.4874774924,-0.
8566687851,3.9103150681\H,0.9546163376,0.8431224058,3.8522404879\H,2.2
235125952,-0.4185932499,3.913358409\Version=EM64L-G09RevA.02\State=2-
A\HF=-495.6076063\S2=0.756648\S2-1=0\S2A=0.750026\RMSD=6.773e-09\RMSF
=2.448e-06\Dipole=-0.4074336,0.1583907,1.3554979\Quadrupole=0.5959697,
0.5985695,-1.1945392,0.0767193,1.9066668,-0.5871551\PG=C01 [X(C5H7O4)]
\@

PES_4

1\I\GINC-V1250\FOpt\RB3LYP\Gen\C6H10O4\GXG501\21-Jul-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pes6.freq\0,1\C,0.6002983126,0.6127439081,-0.1709888038\O,0.846797
0445,0.6210489794,1.2397280237\C,0.6090510459,-0.5519749932,1.88695193
75\C,-0.9087503254,0.5442919033,-0.4225086476\O,0.2874962643,-1.571048
5954,1.3190018225\O,-1.7673915959,0.7691673643,0.3972478465\C,0.794508
2711,-0.3872138708,3.3741074577\O,-1.1431770543,0.2344816974,-1.713034
746\C,-2.5308604708,0.1637123352,-2.0870356324\H,-2.5350385008,-0.0951
971629,-3.1459611624\H,-3.0217299645,1.1266113908,-1.9230348138\H,-3.0
424674862,-0.6032372824,-1.50029375\H,1.0593907431,-0.2729923254,-0.61
85293731\H,-0.0305958866,0.2140373013,3.7719571646\H,1.7256915349,0.14
31339198,3.5935180296\H,0.792071722,-1.3673983053,3.852155726\C,1.2042
264034,1.8934141065,-0.7419882414\H,2.2787101536,1.9203087236,-0.53869
12795\H,1.0475832688,1.9308395725,-1.8235615305\H,0.7408905024,2.77302
66052,-0.2842879183\Version=EM64L-G09RevA.02\State=1-A\HF=-535.578761
\RMSD=9.560e-09\RMSF=5.183e-06\Dipole=0.2992885,0.5465734,-0.4762978\Q
uadrupole=0.6778981,-5.3050195,4.6271214,1.3272827,4.5456138,-0.777571
\PG=C01 [X(C6H10O4)]\@

PES_400

1\I\GINC-V1259\FOpt\UB3LYP\Gen\C6H9O6(2)\GXG501\21-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\pes6oo.freq\0,2\C,0.1159617297,-0.0165761532,0.0122669563\O,0.05
8581506,-0.1758380567,1.4220474494\C,1.0555510843,0.3753239441,2.17453
05135\C,1.423372763,-0.5532259543,-0.6177256633\O,1.9529726872,1.03866
37888,1.7092210458\O,1.8100683361,-0.1776766105,-1.6998392338\C,0.8636
458163,0.0279434625,3.6273830041\O,2.0080638586,-1.4888477266,0.132873
0483\C,3.2183450685,-2.0457211607,-0.4165845472\H,3.5486098249,-2.7893
291352,0.3080563263\H,3.9698009147,-1.2621153194,-0.5396920583\H,3.014
8057606,-2.5099944794,-1.3842770059\H,0.9929283963,-1.0513024486,3.762
7074189\H,-0.1507675348,0.2797347958,3.9509291606\H,1.5977191812,0.565
8460914,4.2278776553\O,-0.9933360135,-0.8385647291,-0.4839682952\O,-0.
8435331906,-2.1250224755,-0.2100856328\C,-0.2209908774,1.3870366483,-0
.4509657083\H,-0.2531102402,1.4126275576,-1.5414096289\H,0.5451678023,
2.0799653454,-0.1010892868\H,-1.1945891027,1.6726518638,-0.0438167509\
\Version=EM64L-G09RevA.02\State=2-A\HF=-685.2785075\S2=0.753027\S2-1=0
\S2A=0.750006\RMSD=8.293e-09\RMSF=2.345e-05\Dipole=0.2899801,-0.04670
36,0.9350799\Quadrupole=-0.7299886,-0.4372381,1.1672268,-7.8904436,-1.

1622042,0.2837362\PG=C01 [X(C6H9O6)]\@

PES_400H

1\1\GINC-V1260\FOpt\RB3LYP\Gen\C6H10O6\GXG501\21-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pes60oh.freq\0,1\C,-0.0441932283,-0.0121179819,-0.0228185607\O,-0.0107644522,-0.023896414,1.4258720251\C,1.192027593,-0.004765037,2.0631734722\C,0.7405967992,-1.2034977696,-0.6277487547\O,2.255061235,0.084688973,1.4931245219\O,1.1390593081,-1.1911557607,-1.768535767\C,1.0003678317,-0.1155485154,3.5555466677\O,0.8748143978,-2.2294937103,0.2219798643\C,1.5773357564,-3.3687376511,-0.3088153207\H,1.5953537729,-4.1007375754,0.4985533204\H,2.5925540125,-3.0852437215,-0.5968984566\H,1.050619563,-3.7653190861,-1.1800145792\H,0.6244651322,-1.1148161973,3.8021465814\H,0.2612735418,0.6115501785,3.9051170198\H,1.9557742229,0.0465047619,4.0555587531\O,-1.407127518,-0.1065746203,-0.3547956321\O,-1.9194369478,-1.4043058866,0.0446007031\C,0.4016815976,1.3219166991,-0.6035892067\H,0.3021299696,1.2890446362,-1.6892903642\H,1.4443407756,1.5049311809,-0.3427968088\H,-0.2296324603,2.1158219354,-0.1962085321\H,-2.0068714753,-1.2715305168,1.0084854368\Version=EM64L-G09RevA.02\State=1-A\HF=-685.9183116\RMSD=3.829e-09\RMSF=1.698e-05\Dipole=-0.1030445,-0.3225095,1.4621414\Quadrupole=-5.4324366,5.384377,0.0480597,-2.4466879,-2.7061754,-0.2157412\PG=C01 [X(C6H10O6)]\@

PES_4R

1\1\GINC-V1306\FOpt\UB3LYP\Gen\C6H9O4(2)\GXG501\21-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pes6r.freq\0,2\C,-0.0658539672,-0.0275031219,0.0608930164\O,0.0447847072,-0.1528118921,1.4210863197\C,1.2282749248,0.0868451508,2.0920872556\C,-1.3578867351,0.4272386711,-0.4275097217\O,2.2145533348,0.5442085952,1.5742543474\O,-1.6369418241,0.4896742604,-1.6188570946\C,1.0661784836,-0.2937433872,3.5406590519\O,-2.2129102528,0.7813018511,0.5643175538\C,-3.4943625084,1.2388657609,0.1131203704\H,-4.0536385271,1.4770913609,1.0186901039\H,-4.005660735,0.4596012743,-0.459385979\H,-3.3896212497,2.1264511917,-0.5174748463\H,0.864739123,-1.3670077491,3.6258666675\H,0.210938969,0.2337230033,3.974572015\H,1.978064158,-0.0439089769,4.0835197564\C,1.0088575755,-0.468201213,-0.8676822298\H,1.3991482515,-1.4514947256,-0.5739398347\H,1.857731766,0.2246546106,-0.8644436836\H,0.5931345624,-0.5274602031,-1.8750555883\Version=EM64L-G09RevA.02\State=2-A\HF=-534.927309\S2=0.756248\S2-1=0.\S2A=0.750025\RMSD=5.988e-09\RMSF=4.687e-06\Dipole=-0.3230055,-0.3611255,1.0329432\Quadrupole=-0.3363391,1.0112052,-0.6748661,-3.6378886,-1.2056214,-0.515995\PG=C01 [X(C6H9O4)]\@

PET

1\1\GINC-V1297\FOpt\RB3LYP\Gen\C6H10O4\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pet1.freq\0,1\C,-0.4146787778,-0.0410738872,-0.2899656724\C,-0.4365292525,0.4209032091,1.1477757664\O,0.1118151319,1.4140112767,1.5722935573\O,-1.1658988022,-0.4363545804,1.9061522044\C,-1.2590851107,-0.1581462064,3.3177695924\C,-0.2205017079,-0.9518645364,4.0946488751\O,1.1150555492,-0.5560334728,3.7435659553\C,1.5758928256,0.5778309542,4.3409919422\O,0.9703871664,1.1665553411,5.2083615548\C,2.8989913148,0.9901868847,3.7506615663\H,3.3818700875,1.7167457315,4.4054351679\H,3.5472234235,0.1243086522,3.590917329\H,2.7049106242,1.4525193005,2.7760819437\H,-1.1430155884,0.9121976318,3.4933500828\H,-0.2786204423,-2.0130577654,3.8417687933\H,-0.3830475552,-0.8137470808,5.1675435854\H,0.1030208777,-1.0037623416,-0.361111991\H,0.1013305036,0.6994399041,-0.9018045255\H,-1.4344329071,-0.1903191678,-0.6581149273\H,-2.2623123711,-0.4770112825,3.6155618256\Version=EM64L-G09RevA.02\State=1-A\HF=-535.5828002\RMSD=7.440e-09\RMSF=9.583e-06\Dipole=-0.2051359,-0.9349158,-0.621207

8\Quadrupole=3.7457542,-3.13197,-0.6137842,1.0140646,-0.2953974,-1.868
3969\PG=C01 [X(C6H10O4)]\@

PETOO

1\1\GINC-V1439\FOpt\UB3LYP\Gen\C6H9O6(2)\GXG501\05-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\petloo.freq\0,2\C,0.0641005606,-0.3727681476,0.1551013918\C,-0.0
770537379,-0.1932105408,1.6428994493\O,0.8168145952,-0.2247703573,2.45
59062115\O,-1.3900004185,-0.0141859055,1.9840444324\C,-1.6653754767,0.
0336399176,3.3876115845\C,-1.7507362086,-1.3876148981,3.9314329204\O,-
2.8229076709,-2.0920958357,3.3330071752\C,-2.5116666875,-3.0400587628,
2.3947255765\O,-1.3915087463,-3.2360843443,1.9873737314\C,-3.757098776
3,-3.768651233,1.9628243712\H,-3.5037472463,-4.4915640262,1.1871076502
\H,-4.2030205753,-4.2815230183,2.821335332\H,-4.4977902211,-3.05604277
14,1.5861463331\H,-0.8871212226,0.5870841851,3.9174626703\H,-0.8193049
167,-1.9414544177,3.8218733575\H,-0.2411964317,-1.3951129371,-0.096177
3729\H,1.1066409286,-0.2299366954,-0.1315355417\H,-0.5847669206,0.3178
728335,-0.3897939504\H,-2.6305188655,0.5330048636,3.491529768\O,-2.064
4536604,-1.2596874983,5.3340018055\O,-1.9114796991,-2.4206039504,5.960
0784431\Version=EM64L-G09RevA.02\State=2-A\HF=-685.2879984\S2=0.75283
4\S2-1=0.\S2A=0.750006\RMSD=3.674e-09\RMSF=9.865e-06\Dipole=-1.0057053
,0.258146,-1.0636627\Quadrupole=-1.1769924,2.5758919,-1.3988996,2.3886
926,0.6046544,0.5479551\PG=C01 [X(C6H9O6)]\@

PETOOH

1\1\GINC-V1419\FOpt\RB3LYP\Gen\C6H10O6\GXG501\05-Jul-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\petlooh.freq\0,1\C,-0.0129430679,-0.063392801,0.0042365661\C,-0.03
96723408,-0.0330927935,1.5100035662\O,0.9256585644,0.0032218204,2.2380
256674\O,-1.3234719299,-0.0831268487,1.9701234055\C,-1.4768885727,-0.1
91973495,3.3927442699\C,-1.2938361457,-1.6449854269,3.8255863347\O,-2.
3089606742,-2.4618823056,3.2043473274\C,-1.9554160789,-3.1961604964,2.
1131903204\O,-0.8517802872,-3.1818367777,1.617435665\C,-3.1278458742,-
4.0091486448,1.6223594783\H,-2.8183618235,-4.6136757692,0.7694098269\H
, -3.5028768557,-4.6552899814,2.4225711548\H,-3.9453301599,-3.342445820
6,1.3282087524\H,-0.741174277,0.428597556,3.9083272163\H,-0.3045729424
, -2.0194048089,3.5529767824\H,-0.18630005,-1.0961612664,-0.3192814512\
H,0.9658211251,0.2629572003,-0.3496101365\H,-0.8041708515,0.5616522661
, -0.418118671\H,-2.4877294724,0.1462402749,3.6144051326\O,-1.363845097
4,-1.8311899398,5.2065037957\O,-2.6307018913,-1.2937472787,5.688433610
6\H,-3.19462006,-2.0852399563,5.6004480678\Version=EM64L-G09RevA.02\S
tate=1-A\HF=-685.9271512\RMSD=9.998e-09\RMSF=1.189e-05\Dipole=-1.51795
19,-0.4709916,-0.5576497\Quadrupole=-1.4938726,2.0352323,-0.5413597,3.
1173554,-1.5397413,-2.9621969\PG=C01 [X(C6H10O6)]\@

PETR

1\1\GINC-V1279\FOpt\UB3LYP\Gen\C6H9O4(2)\GXG501\04-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\petlr.freq\0,2\C,0.4422538877,1.0364907617,0.069270896\C,0.05070
53313,0.6690957224,1.4822693053\O,0.6842582668,0.9397431363,2.47953607
54\O,-1.1184411723,-0.0139597166,1.4938362153\C,-1.5995035583,-0.41523
87386,2.8257271395\C,-0.9264139526,-1.6148845683,3.3547071988\O,-1.409
0305062,-2.8131052426,2.892890656\C,-0.7236736208,-3.9658188218,3.2134
169431\O,0.2896063218,-3.9705057641,3.8675317481\C,-1.4291072613,-5.16
38208141,2.6339471312\H,-0.8653322513,-6.0654570763,2.8746802185\H,-2.
442165163,-5.2389363914,3.0435179162\H,-1.5231999956,-5.0601427312,1.5
479553538\H,-1.4529455622,0.4265021529,3.5052947663\H,0.0415915237,-1.
6225862675,3.8361802972\H,0.5881848529,0.128336309,-0.5251290282\H,1.3
647335373,1.6177251123,0.0881251433\H,-0.3558728362,1.6140914818,-0.40
78706182\H,-2.6639468888,-0.5982858159,2.6658291651\Version=EM64L-G09

RevA.02\State=2-A\HF=-534.9186506\S2=0.753662\S2-1=0.\S2A=0.75001\RMSD=8.567e-09\RMSF=8.592e-06\Dipole=-1.0185651,-0.3574761,-0.8207344\Quadrupole=-2.2266376,2.1445398,0.0820979,1.4943654,-4.4838575,-0.5596973\PG=C01 [X(C6H9O4)]\@

PA_1

1\1\GINC-V1285\FOpt\RB3LYP\Gen\C5H11N1O1\GXG501\03-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa1.freq\0,1\C,-0.542995061,-1.2983040595,0.196368134\N,0.013031361,-0.3730762001,1.1666310903\C,1.0552917417,0.4655104985,0.878839839\O,1.5799362163,0.5176506242,-0.2283279301\C,1.5457358865,1.3159421333,2.0525916372\C,2.0267288765,2.7031978493,1.6068668727\C,0.8980989581,3.6032351775,1.0949531297\H,1.2818756479,4.5874100509,0.8037057523\H,0.415011453,3.1621775016,0.216274631\H,0.13032682,3.7601560764,1.8636865349\H,2.3795681812,0.7696650075,2.5154838559\H,0.7652646018,1.4063776865,2.8209654461\H,2.7725916338,2.5647102904,0.8171058298\H,2.533919715,3.1864785714,2.4515819868\H,-0.3722608072,-0.359828277,2.0995803378\H,-0.0004567809,-1.1493997398,-0.7382636104\H,-0.4211550874,-2.3393535989,0.5199944963\H,-1.6090381874,-1.1041550665,0.0277287635\Version=EM64L-G09RevA.02\State=1-A\HF=-327.1518846\RMSD=7.035e-09\RMSF=5.602e-06\Dipole=-0.7560688,-0.3411254,1.0649213\Quadrupole=0.1519234,1.4326648,-1.5845882,2.6279649,1.1681896,-0.7213313\PG=C01 [X(C5H11N1O1)]\@

PA_100

1\1\GINC-V1300\FOpt\UB3LYP\Gen\C5H10N1O3(2)\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa100.freq\0,2\C,0.3365094533,0.3407579692,-0.1086164367\N,0.1548959442,0.4781685373,1.326503236\C,0.6720639927,-0.4093735474,2.2111405507\O,1.2974240654,-1.4184103581,1.9066778054\C,0.4378343138,-0.1109801379,3.7051584828\C,-0.2568813833,-1.2737225257,4.4110697573\C,-0.3018464032,-1.1208655937,5.9336451368\H,-0.8060502163,-1.9788344506,6.3904117492\H,0.7088166326,-1.0634461918,6.3552188806\H,-0.8422110869,-0.2157797955,6.2295109971\H,1.4073364766,0.1176138987,4.1572454221\H,0.2878014013,-2.177863536,4.121918217\H,-1.2718248401,-1.3715763171,4.0041310702\H,-0.3089921915,1.2998507711,1.6850701609\H,0.8193933134,-0.6200638326,-0.2905171472\H,-0.6298433626,0.3648361782,-0.6239646898\H,0.9709865256,1.14160661,-0.506312249\O,-0.3950007602,1.0776776713,3.8972231178\O,0.3215102796,2.1963228005,3.8982159247\Version=EM64L-G09RevA.02\State=2-A\HF=-476.8596149\S2=0.753351\S2-1=0.\S2A=0.750007\RMSD=4.121e-09\RMSF=1.039e-05\Dipole=-0.5183551,0.1452374,-0.2072133\Quadrupole=-0.9263331,-4.2262715,5.1526046,2.1152117,1.9771116,-5.5202782\PG=C01 [X(C5H10N1O3)]\@

PA_100H

1\1\GINC-V1292\FOpt\RB3LYP\Gen\C5H11N1O3\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa100h.freq\0,1\C,-0.0054612065,-0.0946525803,0.0617918272\N,0.0445058151,-0.0762282944,1.5110801777\C,1.1932931637,0.1368232306,2.2006227\O,2.3042987457,0.2648344522,1.6956759342\C,1.0465634661,0.1467771412,3.731649492\C,1.6441516621,-1.130524648,4.3382641968\C,1.742776408,-1.0966966463,5.8656082266\H,2.1865154227,-2.0237812595,6.2441937449\H,2.3729652596,-0.2642327822,6.2016211163\H,0.7563570368,-0.981788444,6.3256749611\H,1.5811122697,1.02826737,4.1048903119\H,2.6347640402,-1.2498362629,3.886872755\H,1.0395543832,-1.9866077591,4.0118659909\H,-0.8134181019,-0.1011405984,2.0448426789\H,1.0218866894,-0.0470566365,-0.3027744415\H,-0.4755369486,-1.0156657258,-0.3017188617\H,-0.5637153351,0.7645007244,-0.330149538\O,-0.3158437075,0.199818329,4.1720142365\O,-0.81726997,1.544802865,3.9023169112\H,-0.9247531553,1.8659492042,4.8161747806\Version=EM64L-G09RevA.02\State=1-A\HF=-477.4938896\RMSD=5.074e-09\RMSF=2.492e-05\Dipole=-0.9206031,-0.0338207,0.7012741\Quadrupol

e=-3.7042406,0.5089771,3.1952635,-1.6833356,3.772098,3.0078326\PG=C01
[X(C5H11N1O3)]\@

PA_1R

1\1\GINC-V1297\FOpt\UB3LYP\Gen\C5H10N1O1(2)\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa1r.freq\0,2\C,-0.0079010964,0.2131728584,0.0609745087\N,0.060884919,0.0714090253,1.500761318\C,1.2230436137,-0.2724704643,2.1587444435\O,2.2843455482,-0.4792499754,1.5592043248\C,1.1070895538,-0.373011032,3.6123863067\C,2.2745293273,-0.7293896356,4.4634477289\C,2.6233819326,0.3570759494,5.5017627629\H,3.4668989618,0.0361125005,6.1230554873\H,2.901865751,1.2942534834,5.0084279316\H,1.7759695719,0.5640564748,6.1662529709\H,0.1494457617,-0.1646957857,4.0895766199\H,3.1298585457,-0.9208798798,3.8086357604\H,2.0604216624,-1.6669026224,5.0025227326\H,-0.7759592609,0.2245102015,2.0441351115\H,0.988058567,0.0025216567,-0.3312450564\H,-0.7227389842,-0.4940860508,-0.3787099939\H,-0.2989197444,1.2308674328,-0.2291188064\Version=EM64L-G09RevA.02\State=2-A\HF=-326.4956849\S2=0.755495\S2-1=0.\S2A=0.750022\RMSD=7.610e-09\RMSF=2.101e-06\Dipole=-1.2324379,0.2711683,0.5056758\Quadrupole=0.7942009,-1.65383,0.8596291,-0.3318874,3.3221828,-1.3284936\PG=C01 [X(C5H10N1O1)]\@

PA_2

1\1\GINC-V1351\FOpt\RB3LYP\Gen\C5H11N1O1\GXG501\03-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa2.freq\0,1\C,0.016130082,0.0564845145,-0.0943635444\C,-0.057181521,0.0911744187,1.4351094122\C,1.3212044723,-0.0829405405,2.0878705722\N,1.2863156198,-0.0470774365,3.5435931657\C,1.1698574474,-1.1826673236,4.2993356252\O,1.163978887,-2.3061262939,3.8107268103\C,1.0615042257,-0.9603031123,5.8022010044\H,1.8460639916,-1.5384326623,6.2992418448\H,0.0998548295,-1.3514880606,6.1496548638\H,1.147275119,0.088607707,6.1042454085\H,1.197489025,0.8496552497,3.9993361221\H,2.0094355372,0.6971919083,1.7379056054\H,1.7445367753,-1.0523198071,1.8114530543\H,0.4259397394,-0.8968186913,-0.4489796331\H,0.656476739,0.8584673596,-0.4826866966\H,-0.7144281732,-0.7073389963,1.7999950395\H,-0.4998269371,1.0414162413,1.7659575173\H,-0.9764018138,0.1784471352,-0.5413642193\Version=EM64L-G09RevA.02\State=1-A\HF=-327.1541734\RMSD=4.431e-09\RMSF=1.383e-05\Dipole=-0.0902412,1.3773293,0.1882437\Quadrupole=-0.2985177,-3.0598939,3.3584117,0.9021076,0.0144244,1.6872453\PG=C01 [X(C5H11N1O1)]\@

PA_200

1\1\GINC-V1375\FOpt\UB3LYP\Gen\C5H10N1O3(2)\GXG501\05-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa2oo.freq\0,2\C,-0.0103380362,-0.1230495437,-0.0789063917\C,-0.0155200139,-0.0700594001,1.4518379751\C,1.3796842753,-0.0735626023,2.0658525674\N,1.3735161024,-0.0672638859,3.4884301829\C,2.3407054979,-0.7342486649,4.2259170417\O,3.1161988823,-1.5259749284,3.7175951544\C,2.3421155398,-0.4027254586,5.7077942054\H,2.9335712046,0.5052633972,5.8780401996\H,2.8103148774,-1.2241427343,6.2522777564\H,1.3334451379,-0.2291971554,6.0973108268\H,0.8628863798,0.688040433,3.9276362823\H,1.9963259707,-0.908431878,1.7307019685\H,0.5022340337,-1.0209826487,-0.4435134123\H,0.4937939018,0.7494632718,-0.5048703682\H,-0.5494018969,-0.9350848104,1.862682569\H,-0.5399911762,0.8290743298,1.7997037659\H,-1.0350543904,-0.143999447,-0.463617327\O,2.1392388203,1.1105347171,1.5468256332\O,1.6516737126,2.2313907916,2.048128689\Version=EM64L-G09RevA.02\State=2-A\HF=-476.8676303\S2=0.753179\S2-1=0.\S2A=0.750007\RMSD=4.564e-09\RMSF=3.336e-05\Dipole=-1.1702351,0.0168054,0.5345861\Quadrupole=-0.9906193,-5.0947551,6.0853744,1.8862225,0.7928953,3.2142348\PG=C01 [X(C5H10N1O3)]\@

PA_2OOH

1\1\GINC-V1418\FOpt\RB3LYP\Gen\C5H11NO3\GXG501\06-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435 456\pa2ooh.freq\0,1\C,-0.4437969289,-0.0033548498,-0.0022404395\C,-0.2196486037,0.0555741307,1.5097951849\C,1.2578369495,-0.0638546524,1.890608583\N,1.3699690979,-0.1706487783,3.3506319438\C,2.5544286777,-0.2552178213,4.0160717319\O,3.6472005816,-0.2746845795,3.4447332092\C,2.4686483086,-0.3390223414,5.5296316566\H,2.9783083381,0.5283479831,5.9608872908\H,3.0086312794,-1.2313317567,5.8596700884\H,1.4448404055,-0.3796335079,5.9130976012\H,0.5297218095,-0.0229634495,3.8929762824\H,1.7197687819,-0.9448106711,1.4345938413\H,-0.122315574,-0.9676772106,-0.4124647554\H,0.1244966914,0.7839319095,-0.5043173639\H,-0.7728863277,-0.7509401772,2.0092896488\H,-0.5993079333,1.0058489083,1.9098701429\H,-1.5045871344,0.1266923365,-0.2404578829\O,1.935014816,1.0773500565,1.3898181612\O,3.2506634146,0.682193123,0.9172357053\H,3.6700562609,0.4297736967,1.777321212\Version=EM64L-G09RevA.02\State=1-A\HF=-477.504616\RMSD=4.261e-09\RMSF=1.711e-05\Dipole=-1.5020837,-0.5614735,1.2801065\Quadrupole=-1.2701163,-1.4740696,2.7441859,-0.2167747,1.0463879,1.6648566\PG=C01 [X(C5H11NO3)]\@

PA_2R

1\1\GINC-V1291\FOpt\UB3LYP\Gen\C5H10NO1(2)\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pa2r.freq\0,2\C,0.2018725893,0.1796801144,-0.0639216102\C,-0.1665456796,0.0831542104,1.4231770113\C,0.8637043051,-0.6447334525,2.2199746136\N,0.9402948784,-0.4636516997,3.5895296658\C,1.7140048929,-1.240829432,4.4340665283\O,2.3655027088,-2.1922437605,4.0211655264\C,1.7008314046,-0.8257670884,5.8953752928\H,2.7136823594,-0.5359851382,6.1954939637\H,1.4169944411,-1.6880891099,6.5067370954\H,1.0197321301,0.0030516181,6.1158693313\H,0.4378283803,0.3172136972,3.9919739258\H,1.389725379,-1.5143473751,1.8483171676\H,0.332643773,-0.8179972772,-0.4986575041\H,1.1390437628,0.729255637,-0.2020262404\H,-1.1554548645,-0.4057054466,1.5116738354\H,-0.3076590827,1.0973087334,1.8306955831\H,-0.584163733,0.6904809604,-0.6303013137\Version=EM64L-G09RevA.02\State=2-A\HF=-326.4986606\S2=0.75538\S2-1=0\S2A=0.750019\RMSD=5.780e-09\RMSF=3.797e-06\Dipole=-0.9070361,1.1466495,0.2277018\Quadrupole=-1.7257122,-2.2399699,3.9656821,1.8222516,-0.3434767,2.0282183\PG=C01 [X(C5H10NO1)]\@

GLY

1\1\GINC-V1308\FOpt\RB3LYP\Gen\C4H8N2O2\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\gly.freq\0,1\C,-0.2507911799,0.1193289623,-0.2154255331\C,-0.0488719376,-0.1718472652,1.2609989537\O,1.0233480747,-0.5965519222,1.696309566\N,-1.120805693,0.0523373234,2.0696624985\C,-1.0900906007,-0.2146792479,3.5050858221\C,-0.4242296911,0.9079477256,4.3278731189\N,0.9189335781,1.0005732779,4.1366318339\O,-1.067844377,1.6224722758,5.0833646056\H,1.4116038563,1.7668835137,4.5740034405\H,-1.9429302841,0.4963107187,1.6871947609\H,-0.5560560712,-1.1577062333,3.6599065542\H,-2.1151790098,-0.3160717711,3.863190251\H,0.4783527853,0.8716214415,-0.5317589657\H,-0.0438493459,-0.7933244771,-0.7825682803\H,-1.2571552639,0.4705100722,-0.4626072579\H,1.369009056,0.4474034877,3.4123776793\Version=EM64L-G09RevA.02\State=1-A\HF=-417.2263344\RMSD=3.632e-09\RMSF=1.941e-05\Dipole=-0.3326713,-0.09901,-1.2904016\Quadrupole=2.0786789,-1.0950866,-0.9835923,4.573123,5.764449,-3.9221163\PG=C01 [X(C4H8N2O2)]\@

GLYOO

1\1\GINC-V1455\FOpt\UB3LYP\Gen\C4H7N2O4(2)\GXG501\05-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684

35456\glyoo.freq\0,2\C,-0.2316971657,-0.1779202543,-0.1367463538\C,-0.0988542963,-0.467963697,1.3458876878\O,0.6006747277,-1.3536822125,1.8050066927\N,-0.8683685684,0.3484515261,2.1616216414\C,-0.819846544,0.25425297,3.5577572745\C,-1.1776629535,1.6214987029,4.1830141072\N,-1.0663075375,1.6642652595,5.5309767213\O,-1.5041212602,2.5624031012,3.4717827633\H,-1.4278353273,2.4834345028,6.0022145906\H,-1.3354318348,1.1747231349,1.8017444679\H,0.1241448732,-0.1638014649,3.9105460867\H,0.5838481443,-0.6721041075,-0.6661459333\H,-1.1840881056,-0.575337553,-0.5075385624\H,-0.2116928905,0.8968705212,-0.3479273516\H,-1.0120431241,0.7917705747,6.0442653802\O,-1.859221993,-0.747802565,3.9979829516\O,-1.6968810004,-1.0923769785,5.259624629\Version=EM64L-G09RevA.02\State=2-A\HF=-566.9356091\S2=0.753304\S2-1=0.\S2A=0.750008\RMSD=5.720e-09\RM SF=8.981e-06\Dipole=-0.1347633,0.8913021,0.0684062\Quadrupole=-3.2657467,-7.6258483,10.891595,1.6340387,1.0005944,3.1310867\PG=C01 [X(C4H7N2O4)]\@

GLYOOH

1\1\GINC-V1380\FOpt\RB3LYP\Gen\C4H8N2O4\GXG501\06-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\glyooH.freq\0,1\C,-0.1228477074,-0.1571635094,-0.0811636078\C,-0.1866414761,-0.4423639079,1.4065874313\O,0.6579783848,-1.1621197872,1.9506807222\N,-1.2170825141,0.128322737,2.0796970464\C,-1.3956446861,0.0468652502,3.5145833562\C,-2.719463109,0.7821376797,3.8380507277\N,-3.2339623023,0.4600841721,5.044272962\O,-3.1903757936,1.6037081428,3.0614038137\H,-4.1299045545,0.8486082709,5.3037686718\H,-1.8901857453,0.72686317,1.6118869018\H,-0.5672412751,0.536284089,4.0423380846\H,0.8461737371,0.2976939032,-0.3082413916\H,-0.1734610934,-1.1055149356,-0.6247302278\H,-0.9203038107,0.5022687351,-0.4343889314\H,-2.8889131156,-0.3623194522,5.5207591094\O,-1.4879024716,-1.2746997048,4.0128910475\O,-0.1730951954,-1.6988152384,4.4650459331\H,0.296673391,-1.7285876515,3.5891749641\Version=EM64L-G09RevA.02\State=1-A\HF=-567.5780022\RMSD=3.645e-09\RM SF=1.608e-05\Dipole=-0.6496795,0.5436467,-0.2052305\Quadrupole=-1.092545,-6.171054,7.263599,4.0282692,-5.9231892,1.6955692\PG=C01 [X(C4H8N2O4)]\@

GLYR

1\1\GINC-V1287\FOpt\UB3LYP\Gen\C4H7N2O2(2)\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\glyr.freq\0,2\C,0.3142339011,-0.3309728541,0.0639576693\C,-0.0961884887,0.3449212307,1.3576116155\O,0.5754934326,1.2036256954,1.9091207245\N,-1.3085968113,-0.0764499854,1.8865848179\C,-1.8645389382,0.410807045,3.0326611876\C,-3.1389708675,-0.1708699213,3.4110381166\N,-3.7340941904,0.3302652452,4.5482184926\O,-3.6720992076,-1.0474987143,2.7164828487\H,-4.5200719631,-0.1989857677,4.9004789829\H,-1.8697111046,-0.79205253,1.4293433923\H,-1.327569301,1.1883437248,3.5580657576\H,0.398646178,0.4267687367,-0.7219706725\H,1.3060347945,-0.7747369089,0.1949471939\H,-0.3834968689,-1.1065482095,-0.2652828416\H,-3.1816797151,0.827036813,5.2330183819\Version=EM64L-G09RevA.02\State=2-A\HF=-416.5864561\S2=0.754919\S2-1=0.\S2A=0.750019\RMSD=6.469e-09\RM SF=2.162e-05\Dipole=-0.1032097,-0.1718463,0.3961793\Quadrupole=-6.06406,-3.7020662,9.7661262,-5.4007761,-5.5060026,2.3130012\PG=C01 [X(C4H7N2O2)]\@

ALA

1\1\GINC-V1296\FOpt\RB3LYP\Gen\C5H10N2O2\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\ala.freq\0,1\C,-0.0149117154,-0.0036191666,-0.0691580055\C,-0.1361756415,-0.4083832177,1.3897179453\O,0.5155190686,-1.3469668197,1.8542773149\N,-1.0079907556,0.3157663517,2.1423660215\C,-1.2816971839,0.0257344543,3.5554535406\C,-0.179953114,0.6432081168,4.4571790909\N,0.9975255169,-0.0378222858,4.4149403379\O,-0.3754810956,1.6396355627,5.1397

091348\H,1.7962253625,0.3807399135,4.8726214772\H,-1.4491759619,1.1315
388991,1.7405182628\H,-1.2352002837,-1.0638668318,3.6547078466\H,1.025
4681127,0.2640679561,-0.2779672021\H,-0.2598819302,-0.8687317652,-0.69
2923032\H,-0.6625728163,0.8321745649,-0.3506974344\H,1.1439911357,-0.7
341922549,3.6876370532\C,-2.6625523466,0.5422980107,3.9418299658\H,-2.
8893825949,0.26923897,4.975704647\H,-3.4296603357,0.1143849858,3.28834
87159\H,-2.6971616769,1.6348066917,3.8847720811\Version=EM64L-G09RevA
.02\State=1-A\HF=-456.5442098\RMSD=4.256e-09\RMSF=1.631e-05\Dipole=-0.
3220159,0.1107231,-1.1718129\Quadrupole=4.3401532,-4.6114188,0.2712656
,1.2590366,2.0679123,-6.1361916\PG=C01 [X(C5H10N2O2)]\@

ALAOO

1\1\GINC-V1382\FOpt\UB3LYP\Gen\C5H9N2O4(2)\GXG501\06-Jul-2010\0\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\alao0.freq\0,2\C,-0.0295053962,-0.4047146993,-0.1475641522\C,-
0.0813788378,-0.5764033499,1.3624871896\O,0.705312722,-1.2797621514,1.
9745141582\N,-1.0834863525,0.1577398299,1.9697167128\C,-1.3185031862,0
.2712362895,3.3611459078\C,-2.5863368086,1.1663905001,3.5225689214\N,-
2.9221816745,1.4569810081,4.8013072523\O,-3.2193001505,1.5314969774,2.
5397832997\H,-3.6501094165,2.1478007217,4.93181167\H,-1.6970994005,0.7
440040185,1.4109366136\H,0.5369981467,0.5014655388,-0.3937462516\H,0.4
901435726,-1.2619892371,-0.5782345548\H,-1.0253624018,-0.3136888668,-0
.5938219681\H,-2.2159362846,1.3596278054,5.5224897836\C,-1.3876550983,
-1.0424884193,4.1316688576\H,-1.4673426777,-0.8566582669,5.2036535249\
H,-0.492210104,-1.6273061884,3.9214660545\H,-2.2707030834,-1.598491665
2,3.8022479701\O,-0.1384476572,1.0870790418,3.8895464342\O,-0.14589526
64,1.2493094248,5.195028539\Version=EM64L-G09RevA.02\State=2-A\HF=-60
6.2511912\S2=0.753467\S2-1=0.\S2A=0.750009\RMSD=3.911e-09\RMSF=1.728e-
05\Dipole=-0.9895334,0.2969746,0.0836212\Quadrupole=-5.9249937,-1.3316
421,7.2566358,1.4755531,-5.9083663,1.4625865\PG=C01 [X(C5H9N2O4)]\@

ALAOOH

1\1\GINC-V1303\FOpt\RB3LYP\Gen\C5H10N2O4\GXG501\06-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\alaooh.freq\0,1\C,-0.0287496844,-0.0411763281,-0.033537069\C,-0.
1120399698,0.3559170798,1.428881025\O,0.8134593994,0.9846876544,1.9583
859348\N,-1.2419996242,-0.0154651494,2.0756898347\C,-1.541304323,0.204
2379477,3.4933619663\C,-3.073819023,-0.0507555046,3.6157462228\N,-3.65
75221161,0.577192654,4.6592844101\O,-3.6432594058,-0.8138327387,2.8444
098293\H,-4.6596960448,0.4990259688,4.7633901025\H,-1.9800990827,-0.51
01366683,1.5846891777\H,0.0737136163,0.8649407178,-0.6385927608\H,0.87
73648579,-0.6363486633,-0.1822034488\H,-0.8938259716,-0.6108077389,-0.
3839631255\H,-3.164488685,1.3358202635,5.1105319171\C,-0.7865793585,-0
.7878152792,4.3878603082\H,-0.9986024661,-0.5861881229,5.4407172723\H,
0.2875938341,-0.7012410354,4.222469852\H,-1.1099411515,-1.8030326455,4
.1398286233\O,-1.3589244539,1.5607792606,3.8793039246\O,-0.0124366974,
1.8040880663,4.3633406507\H,0.4851326366,1.6963132282,3.5074877283\Ve
rsion=EM64L-G09RevA.02\State=1-A\HF=-606.8944686\RMSD=4.120e-09\RMSF=7
.841e-06\Dipole=-0.7142525,-0.4545545,-0.1360436\Quadrupole=-1.7890611
, -3.7212601,5.5103211,-6.2606124,-5.706367,0.2144732\PG=C01 [X(C5H10N2
O4)]\@

ALAR

1\1\GINC-V1419\FOpt\UB3LYP\Gen\C5H9N2O2(2)\GXG501\06-Jul-2010\0\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\alar.freq\0,2\C,-0.0332910855,-0.0149051222,-0.0949423936\C,0.
0655287174,-0.1454984311,1.4161414459\O,1.140358831,-0.1710247352,2.00
12851757\N,-1.1548034241,-0.2499527462,2.0596972788\C,-1.4327523816,-0
.4175866381,3.3987645033\C,-2.8731113608,-0.4063173888,3.6506063695\N,
-3.3043375657,-0.52731164,4.9579070448\O,-3.6820910218,-0.3341996939,2
.711628927\H,-4.2922723947,-0.3466328386,5.07954102\H,-2.0139985847,-0

.1983606707,1.5124600959\H,0.6385776599,0.7835306339,-0.4214266793\H,0.3159576017,-0.9451861728,-0.557156926\H,-1.0451514782,0.1945342798,-0.4543906373\H,-2.7115093554,-0.2095011401,5.7113991317\C,-0.3632581678,-0.5828672422,4.4290729031\H,0.4297769496,-1.2418789938,4.069143946\H,-0.7783780069,-1.0077406244,5.3475367895\H,0.1264213541,0.3702933111,4.6744823106\Version=EM64L-G09RevA.02\State=2-A\HF=-455.9037964\S2=0.755329\S2-1=0.\S2A=0.750022\RMSD=7.823e-09\RMSF=1.480e-05\Dipole=-0.2704177,0.254223,0.5638698\Quadrupole=-9.1219683,-1.0405099,10.1624782,-1.4602784,-3.7913199,1.0392826\PG=C01 [X(C5H9N2O2)]\@

PHE_1

1\1\GINC-V1361\FOpt\RB3LYP\Gen\C9H11N1O1\GXG501\04-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\phe.freq\0,1\C,0.1319824277,0.1681876209,0.2455769661\O,-0.2197022115,-0.7742873828,0.9195481303\C,1.219849464,0.0949567124,-0.8238964716\C,2.2656107171,1.2273822186,-0.6368957461\N,1.8578524002,-1.2078701657,-0.941627912\C,3.1329755089,1.0762189461,0.5965677517\C,4.7293669626,0.7562885065,2.8949441607\C,4.3094732229,0.3131824885,0.5533832645\C,2.7748563212,1.6798362362,1.8102871324\C,5.1004281706,0.1528054389,1.6922020734\C,3.5636408372,1.5220921584,2.9504357918\H,6.0096457488,-0.4402412604,1.6375194105\H,1.8737304633,2.2875043356,1.8622567865\H,5.3463313212,0.6349485455,3.7811915817\H,3.2694427978,2.0014858161,3.8803752776\H,4.6031561074,-0.1557659682,-0.382355124\H,1.1326340127,-1.9182073163,-1.0382470794\H,0.7031103831,0.311798215,-1.774383727\H,-0.3585722086,1.1641864529,0.3561482206\H,2.8910893256,1.2347032391,-1.5352622406\H,2.3153702663,-1.4228990348,-0.0553868591\H,1.7355068148,2.1877841468,-0.6038947936\Version=EM64L-G09RevA.02\State=1-A\HF=-479.5378149\RMSD=8.715e-09\RMSF=6.946e-06\Dipole=0.1952288,0.5820525,-0.1808241\Quadrupole=-0.6455752,-0.6978923,1.3434675,-4.3847411,4.7059084,0.3048982\PG=C01 [X(C9H11N1O1)]\@

PHE_100

1\1\GINC-V1461\FOpt\UB3LYP\Gen\C9H10N1O3(2)\GXG501\05-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pheoo.freq\0,2\C,0.1432676727,-0.1501705847,0.251923217\O,0.2011276319,-0.2201319731,1.4548840751\C,1.3523608775,0.1186374141,-0.654678641\C,2.6353983558,0.3990817656,0.1260804059\N,1.4424467251,-0.911130431,-1.6056712832\C,3.8744415271,0.5234737538,-0.7364207446\C,6.1701137277,0.7350264221,-2.3498298511\C,4.1782966642,1.7245414675,-1.3948906129\C,4.7382644273,-0.5686025039,-0.9011393662\C,5.3167283361,1.8298089263,-2.193553392\C,5.8779710717,-0.4653948578,-1.7017984378\H,5.5390499462,2.7693049078,-2.6924367229\H,4.5201247052,-1.5036414446,-0.3901081576\H,7.0585135687,0.8191967972,-2.9698295949\H,6.5384447726,-1.321263065,-1.8126111046\H,3.5173317221,2.5790115768,-1.2789138659\H,2.2979253755,-0.846714883,-2.1533659131\H,-0.8101769684,-0.2781600861,-0.3035767965\H,2.4687359968,1.3131706349,0.7053913585\H,0.6384364162,-0.8972704369,-2.2296645096\H,2.7491118154,-0.4105304968,0.8530500561\O,0.9757736467,1.4875201309,-1.2893536583\O,0.133679621,1.331030181,-2.288073498\Version=EM64L-G09RevA.02\State=2-A\HF=-629.2550446\S2=0.753593\S2-1=0.\S2A=0.750009\RMSD=7.387e-09\RMSF=1.567e-05\Dipole=0.7901337,-0.3422296,-0.6438279\Quadrupole=1.7266802,1.4744091,-3.2010893,1.3328208,0.2252321,2.0939782\PG=C01 [X(C9H10N1O3)]\@

PHE_100H

1\1\GINC-V1455\FOpt\RB3LYP\Gen\C9H11N1O3\GXG501\06-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pheooh.freq\0,1\C,-0.0099648335,-0.0322867358,0.0373986679\O,-0.8302170184,0.8513168848,0.1730300378\C,1.220878108,0.059838675,-0.8761728475\C,2.5037516522,0.0152265853,-0.0048765873\N,1.1608893916,-1.0577324701,-1.7737690011\C,3.7767335316,-0.0891300686,-0.8166338502\C,6.1

334795592,-0.2856130252,-2.3387672808\C,4.3147410341,1.0426960311,-1.4
 48576375\C,4.4337740813,-1.3187835456,-0.964333251\C,5.4845870384,0.94
 41012545,-2.200972711\C,5.6049679348,-1.4181092659,-1.7189102138\H,5.8
 91723773,1.8305925535,-2.6801247242\H,4.0286712978,-2.2029836017,-0.47
 70240511\H,7.046558337,-0.3589730104,-2.9235300254\H,6.1041449549,-2.3
 785860638,-1.8167871038\H,3.81085864,1.9989715608,-1.3454263637\H,2.03
 79875633,-1.1434522185,-2.2844113452\H,-0.1073907961,-0.9991310519,0.5
 72331804\H,2.5076781777,0.9283106532,0.5965887807\H,0.4100022937,-0.92
 76426186,-2.4494413096\H,2.4225719903,-0.8387870136,0.6770490961\O,1.1
 501116756,1.2497382797,-1.6810476676\O,1.1756050881,2.4318761792,-0.82
 59600436\H,0.2413624282,2.4286713578,-0.5304325612\\Version=EM64L-G09R
 evA.02\\State=1-A\\HF=-629.890163\\RMSD=5.264e-09\\RMSF=9.656e-06\\Dipole=0
 .3713562,-0.7880558,-0.0457705\\Quadrupole=-0.8090971,-0.4195162,1.2286
 133,1.4129774,-0.924872,0.3583158\\PG=C01 [X(C9H11N1O3)]\\@

PHE_1R

1\I\GINC-V1288\FOpt\UB3LYP\Gen\C9H10N1O1(2)\GXG501\05-Jul-2010\0\#B3L
 YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268
 435456\pher.freq\0,2\C,0.0039926926,-0.724177047,-0.4334265808\O,-0.
 1190886173,-1.4844860407,0.5467242963\C,1.0448419384,0.2480267876,-0.5
 237969103\C,1.212525623,1.1817515684,-1.6904478669\N,1.9546449499,0.27
 23457897,0.4861901128\C,1.3536494597,2.6423734333,-1.2854508187\C,1.61
 53730076,5.3303320178,-0.4979022679\C,2.5753038722,3.3119096481,-1.422
 3944604\C,0.2633393651,3.3384906752,-0.7431805124\C,2.7075625877,4.647
 4917614,-1.0317171651\C,0.3910131479,4.6710093046,-0.3553645519\H,3.66
 30667443,5.1518426703,-1.1494448138\H,-0.6900006717,2.8283664549,-0.62
 44798314\H,1.7143041652,6.3694519924,-0.196046155\H,-0.4655998852,5.19
 69460567,0.0579026916\H,3.4278361426,2.7874416982,-1.8491956208\H,1.71
 00464888,-0.3053002079,1.2847703844\H,-0.6980940902,-0.7671599675,-1.2
 882285119\H,2.0990505759,0.8875439444,-2.2717041571\H,2.4859166786,1.1
 146825729,0.6611584963\H,0.3486352085,1.053768008,-2.3543232689\\Versi
 on=EM64L-G09RevA.02\\State=2-A\\HF=-478.9218664\\S2=0.757231\\S2-1=0.\\S2A=
 0.750022\\RMSD=4.078e-09\\RMSF=2.415e-06\\Dipole=0.7654172,1.415326,-0.32
 51555\\Quadrupole=4.0889558,-6.5247437,2.4357878,-3.9186937,2.3105683,5
 .2594159\\PG=C01 [X(C9H10N1O1)]\\@

PHE_200

1\I\GINC-V1471\FOpt\UB3LYP\Gen\C9H10N1O3(2)\GXG501\06-Jul-2010\0\#B3L
 YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268
 435456\phe100.freq\0,2\C,0.15803866,0.0540594195,0.1890689898\O,0.20
 51407794,-0.0357715198,1.3958057599\C,1.3936676151,0.0443106529,-0.696
 2759689\C,1.2680487608,1.1617417465,-1.7649154888\N,2.6063688109,0.129
 8864304,0.0900992522\C,1.3192725713,2.5830874578,-1.2750370395\C,1.338
 9606818,5.2363891422,-0.3681717715\C,0.1780124596,3.3870857275,-1.3984
 592007\C,2.4797760075,3.1252527534,-0.7027294535\C,2.4850956565,4.4462
 638698,-0.2560084003\C,0.1826325305,4.7043427513,-0.9398400035\H,3.388
 6974252,4.8596895388,0.1837470005\H,3.3610330472,2.5041341719,-0.60226
 68039\H,1.3488641616,6.2643941429,-0.0158451506\H,-0.7111390165,5.3142
 924562,-1.0379440158\H,-0.7204895025,2.9809822201,-1.8583788921\H,3.27
 9826637,-0.5746345783,-0.1909859884\H,1.3276320077,-0.8900892637,-1.28
 26663835\H,-0.8134424562,0.1307821165,-0.3427323211\H,2.3744700594,-0.
 0101424473,1.0722547223\H,0.3522595241,0.9909440969,-2.3411475485\O,2.
 376356486,0.9884540763,-2.7332334633\O,2.2889722033,-0.1650146703,-3.3
 677528899\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-629.2421072\\S2=0.753
 227\\S2-1=0.\\S2A=0.750007\\RMSD=3.316e-09\\RMSF=1.479e-05\\Dipole=-0.41869
 57,0.1207331,0.1161616\\Quadrupole=3.0358118,5.8746213,-8.9104331,-1.02
 79915,6.3686501,0.3564192\\PG=C01 [X(C9H10N1O3)]\\@

PHE_200H

1\I\GINC-V1304\FOpt\RB3LYP\Gen\C9H11N1O3\GXG501\06-Jul-2010\0\#B3LYP/

gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\phe1ooh.freq\0,1\C,-0.0392872954,0.2140797535,-0.0233100002\O,0.
1016182319,0.2133963822,1.18003455\C,1.1020031977,-0.0515740624,-0.995
1272086\C,1.1391272727,0.9885543193,-2.1591631808\N,2.4125853935,-0.17
79541144,-0.3603957375\C,1.06547528,2.4338409112,-1.696633289\C,0.8786
313402,5.0744471867,-0.7587944405\C,-0.1648031731,3.1037765606,-1.6926
328955\C,2.2079846924,3.1106947197,-1.2456804539\C,2.112671198,4.42250
28696,-0.7797915716\C,-0.2605142161,4.4128304355,-1.2200536344\H,3.006
5458936,4.9376940287,-0.4386545061\H,3.1742795662,2.6195655601,-1.2977
172429\H,0.8066456747,6.0959076176,-0.3955366421\H,-1.2224857252,4.917
9852143,-1.2224633229\H,-1.0531983647,2.6018667964,-2.0695259162\H,2.3
131893052,-0.7689319007,0.4650624069\H,0.8701097951,-1.0178081441,-1.4
682122854\H,-1.0412341399,0.363140021,-0.4818223318\H,2.696451107,0.73
30906905,0.0008254303\H,0.2849228838,0.7722404634,-2.8175184564\O,2.36
23773646,0.8831330968,-2.8882691972\O,2.668401246,-0.5147261845,-3.124
2010846\H,3.0659038917,-0.719365235,-2.2434047913\Version=EM64L-G09Re
vA.02\State=1-A\HF=-629.8773796\RMSD=4.978e-09\RMSF=4.383e-06\Dipole=-
0.4882399,0.3398714,0.4659958\Quadrupole=3.4505971,6.1232495,-9.573846
6,0.7521225,7.1075212,-0.2993812\PG=C01 [X(C9H11N1O3)]\@

PHE_2R

1\1\GINC-V1379\FOpt\UB3LYP\Gen\C9H10N1O1(2)\GXG501\06-Jul-2010\0\#B3L
YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268
435456\phe1r.freq\0,2\C,0.4927551239,-0.7153531357,-0.2764018367\O,-
0.0072801245,-0.5097874215,0.8078657511\C,1.7060025282,0.0763732197,-0
.8083837999\C,1.193450093,0.8873019895,-1.965474686\N,2.3301762898,0.9
311245557,0.1977649401\C,1.0463474985,0.4521696025,-3.3033860762\C,0.7
210121843,-0.3239264889,-6.0140770947\C,1.4443338234,-0.8390809968,-3.
7597244954\C,0.4798429636,1.3353550525,-4.2706807011\C,0.3233812323,0.
9531218612,-5.5927246652\C,1.2816314729,-1.2112442007,-5.0864217191\H,
-0.1111883637,1.6485021633,-6.3060349667\H,0.1694105458,2.3269170395,-
3.9505500644\H,0.5967031683,-0.6223152234,-7.0509740976\H,1.5950070142
,-2.2015501536,-5.4065482254\H,1.8873694378,-1.5444668157,-3.062958487
2\H,2.7220118235,0.3375836362,0.928861233\H,2.4501912331,-0.6533366306
,-1.158083197\H,0.0688305285,-1.4669388741,-0.9772560494\H,1.589976207
7,1.4539981961,0.6684104725\H,0.8530112418,1.8894640808,-1.7139137666\
\Version=EM64L-G09RevA.02\State=2-A\HF=-478.889264\S2=0.780278\S2-1=0.
\S2A=0.750653\RMSD=6.057e-09\RMSF=1.973e-06\Dipole=0.1049133,-0.293097
7,-0.7313312\Quadrupole=-3.3627445,3.4982329,-0.1354884,-4.7247764,4.1
515248,0.3616643\PG=C01 [X(C9H10N1O1)]\@

CYS_1

1\1\GINC-V1478\FOpt\RB3LYP\Gen\C4H8N2O2S1\GXG501\06-Jul-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\cys1.freq\0,1\N,-0.2965612274,-0.8116648892,0.3703639186\C,-0.3
24795957,0.3665893436,1.0397956349\O,0.5044426155,1.2558034579,0.87419
80497\C,-1.4977375836,0.5481819283,2.0277407787\N,-1.4344044151,1.9208
602172,2.4880833833\C,-2.4982855159,2.5345363905,3.0647775654\O,-3.550
0742994,1.977955091,3.3480153453\C,-1.4437531428,-0.4210754076,3.23764
40553\S,-1.9550725389,-2.1578349706,2.8860281052\H,-0.8891135246,-1.58
43218404,0.6523863894\H,0.5135569075,-0.999720676,-0.2050591769\H,-3.2
756652921,-1.9037598249,2.7610264263\H,-0.4288911136,-0.4812292202,3.6
411845841\H,-2.1006827735,-0.0277017406,4.0136278021\H,-2.4489318107,0.
3888856176,1.50416287\H,-0.6192961865,2.4405806055,2.1750647321\H,-2.
3111877771,3.6062260853,3.26774576\Version=EM64L-G09RevA.02\State=1-A
\HF=-815.4033599\RMSD=9.455e-09\RMSF=1.339e-05\Dipole=0.4729412,-0.591
9913,-0.422561\Quadrupole=-3.8416592,2.7720378,1.0696215,0.774615,2.93
7296,3.9225159\PG=C01 [X(C4H8N2O2S1)]\@

CYS_100

1\1\GINC-V1363\FOpt\UB3LYP\Gen\C4H7N2O4S1(2)\GXG501\08-Jul-2010\0\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\cys1oo.freq\0,2\N,-0.5720907791,0.3533237369,-0.3976871926\C
,-0.1186625065,0.3987133223,0.8764036193\O,0.980115412,0.8184452944,1.
210801645\C,-1.1075233022,-0.1516137775,1.9523461419\N,-0.4752307327,0.
.0298675114,3.205369397\C,-0.8988171037,-0.4415845698,4.421525537\O,-1
.8808127988,-1.130699068,4.6230133924\C,-1.6621118532,-1.5564793375,1.
6730985229\S,-0.3651457432,-2.8430467665,1.5394693948\H,-1.5703853139,
0.2888268357,-0.559587691\H,-0.0053163293,0.8210392146,-1.0936949531\H
,-0.2007666373,-3.0229228288,2.8665940802\H,-2.3646992497,-1.815668198
5,2.4638345503\H,-2.1904833787,-1.5500089005,0.7198708759\H,0.38910621
41,0.5643368161,3.1459499332\H,-0.2164093063,-0.1215808347,5.231030623
8\O,-2.3049520307,0.7958925128,1.9842620753\O,-3.0434527311,0.749999001
29,0.8948328013\Version=EM64L-G09RevA.02\State=2-A\HF=-965.1069437\S2
=0.753499\S2-1=0.\S2A=0.750009\RMSD=9.316e-09\RMSF=1.319e-05\Dipole=0.
3910985,0.3582698,-0.6385538\Quadrupole=-5.0272682,-1.6825301,6.709798
4,0.6383712,5.6905277,-1.2826464\PG=C01 [X(C4H7N2O4S1)]\@

CYS_100H

1\1\GINC-V1289\FOpt\RB3LYP\Gen\C4H8N2O4S1\GXG501\08-Jul-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\cys10oh.freq\0,1\N,-0.0603043364,0.3024411302,0.1057257976\C,-0
.054890071,-0.0988664535,1.3976039326\O,0.9254002046,-0.5009012374,2.0
069032968\C,-1.4626659455,-0.0562714379,2.0746163608\N,-1.189471161,-0
.1751646187,3.5056589813\C,-2.0012578287,0.2026423551,4.5163387019\O,-
3.1317799253,0.6773654076,4.4130479769\C,-2.3858688727,-1.1870842693,1.
.565622904\S,-1.6865231186,-2.8799982538,1.6623881163\H,-0.8277652605,
0.8720519803,-0.2243426461\H,0.832640946,0.3747679782,-0.3631974386\H,
-1.6799106292,-2.971346632,3.0090925144\H,-3.3322942247,-1.1424354552,
2.1017868898\H,-2.5977111518,-1.0166730719,0.5079461673\H,-0.225911357
5,-0.4395108137,3.7034937596\H,-1.5450957904,0.0320099658,5.5060608899
\O,-1.9747632503,1.2242570965,1.715548614\O,-3.4242842523,1.2750593932
,1.8118094692\H,-3.5270425966,1.2481157986,2.8004483132\Version=EM64L
-G09RevA.02\State=1-A\HF=-965.748065\RMSD=4.234e-09\RMSF=1.488e-05\Dip
ole=0.5970516,0.0425487,-0.2068018\Quadrupole=-4.6173626,-4.1949737,8.
8123363,4.665895,-0.4737721,-5.0812939\PG=C01 [X(C4H8N2O4S1)]\@

CYS_1R

1\1\GINC-V1287\FOpt\UB3LYP\Gen\C4H7N2O2S1(2)\GXG501\08-Jul-2010\0\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\cys1r.freq\0,2\N,0.2863141297,0.6293059124,0.0020321135\C,-0
.2371499546,-0.41975683,0.7269308076\O,0.3583382325,-1.4968383949,0.85
78867697\C,-1.5746289234,-0.2334572552,1.3035814495\N,-1.9326758814,-1
.2833248434,2.1219858682\C,-2.9930694425,-1.3948448426,2.9877186338\O,
-3.82729366,-0.5295014396,3.2066931687\C,-2.4557720649,0.9346819454,1.
0614990051\S,-2.1717949182,2.3631086976,2.2411457874\H,0.03978583,1.57
28463075,0.2738559675\H,1.2585537679,0.5019828303,-0.2505281741\H,-2.6
985153558,1.7306904795,3.3106703055\H,-2.2589689063,1.3525642035,0.071
145776\H,-3.5079375009,0.6648343024,1.128751391\H,-1.2452344999,-2.037
9303518,2.0873320884\H,-3.0070649306,-2.3810259481,3.483230941\Versio
n=EM64L-G09RevA.02\State=2-A\HF=-814.7656571\S2=0.75616\S2-1=0.\S2A=0.
75003\RMSD=4.483e-09\RMSF=2.689e-05\Dipole=0.4066088,-0.0457659,-0.318
0033\Quadrupole=-2.3593142,0.5031832,1.856131,5.6433506,1.0685514,-4.7
11079\PG=C01 [X(C4H7N2O2S1)]\@

CYS_2

1\1\GINC-V1361\FOpt\RB3LYP\Gen\C3H7N1O1S1\GXG501\06-Jul-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\cys2.freq\0,1\C,0.0380294074,-0.1168215662,-0.0302714715\O,0.09
49434607,-0.1497621523,1.1792729415\C,1.2657559412,0.0414451717,-0.927

5652038\N,2.5295071211,-0.0628964763,-0.2091785429\C,1.1587031573,1.40
56170841,-1.6465490016\S,2.4493441846,1.6296202766,-2.9323500521\H,3.4
538362673,1.2149583296,-2.1285063087\H,0.1969609058,1.4982130701,-2.16
17135647\H,-0.9400145025,-0.1703439125,-0.5589414705\H,1.2214598981,-0
.7396092901,-1.6983041438\H,2.4067506865,0.3492908617,0.7166439569\H,2
.7513213642,-1.0421693478,-0.0422058552\H,1.2237371995,2.215565433,-0.
911872826\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-646.6720086\\RMSD=8.3
68e-09\\RMSF=7.358e-06\\Dipole=-0.2844967,-0.4764489,0.0722766\\Quadrupol
e=2.4283563,2.5904949,-5.0188512,-1.755103,4.4604623,2.1073483\\PG=C01
[X(C3H7N1O1S1)]\\@

CYS_200

1\1\GINC-V1308\FOpt\UB3LYP\Gen\C3H6N1O3S1(2)\GXG501\08-Jul-2010\0\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\cys200.freq\0,2\C,-0.0097250166,0.1089425453,0.029308323\O,-
0.1200145206,-0.1601319279,1.2036387961\C,1.3252660243,0.0734765721,-0
.704001703\N,2.4160935323,-0.0038471002,0.2434852531\C,1.4430606925,1.
2928392357,-1.6450962989\S,1.8184859811,2.8368397252,-0.7973492718\H,2
.5537020658,2.1952766349,0.1487492385\H,-0.8917975483,0.3670544051,-0.
5913764704\H,1.2640015177,-0.7920106295,-1.3896151002\H,2.0675712003,-
0.3675463839,1.1287669668\H,3.1728379072,-0.5905017882,-0.0923422655\H
,0.5365941133,1.416480022,-2.2425089151\O,2.5292320798,1.0286044423,-2
.6253328737\O,2.1993867028,0.0298863289,-3.4250879621\\Version=EM64L-G
09RevA.02\\State=2-A\\HF=-796.3783314\S2=0.753249\S2-1=0.\S2A=0.750007\R
MSD=5.492e-09\RMSF=4.167e-06\\Dipole=-0.200536,-0.6141293,0.1802353\\Qua
drupole=2.324598,1.918683,-4.243281,-1.8949747,6.293952,-0.4313202\\PG=
C01 [X(C3H6N1O3S1)]\\@

CYS_200H

1\1\GINC-V1292\FOpt\RB3LYP\Gen\C3H7N1O3S1\GXG501\08-Jul-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\cys200h.freq\0,1\C,0.0172664848,0.1054847014,-0.0348382559\O,0.
0178173681,0.1111758226,1.1747063803\C,1.2940944855,-0.0181205264,-0.8
590593296\N,2.4481918389,0.2790383905,-0.0348459647\C,1.2153455382,0.8
868765734,-2.1055938751\S,1.2802391032,2.6775530315,-1.6634806268\H,2.
1856068485,2.4554508168,-0.6784151505\H,-0.9266475517,0.1469871389,-0.
6154385369\H,1.2839041772,-1.052780147,-1.2545605877\H,2.2327446213,0.
058316321,0.9356207502\H,3.2645812484,-0.245611177,-0.3314842913\H,0.2
717519769,0.7378231719,-2.6424869255\O,2.2953393905,0.475077163,-2.922
2201687\O,2.1572068503,1.1185626488,-4.2077766379\H,2.5339010547,2.000
0491536,-4.006100902\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-797.01450
14\\RMSD=7.173e-09\\RMSF=8.562e-06\\Dipole=0.2214322,-0.4989603,-0.001532
3\\Quadrupole=2.8804055,2.5256091,-5.4060146,1.2516682,4.0700492,-2.406
8488\\PG=C01 [X(C3H7N1O3S1)]\\@

CYS_2R

1\1\GINC-V1319\FOpt\UB3LYP\Gen\C3H6N1O1S1(2)\GXG501\06-Jul-2010\0\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26
8435456\cys2r.freq\0,2\C,-0.1959703263,-0.1956509349,-0.0398265167\O
,-0.3223686166,-0.3454775907,1.1565728936\C,1.1517552694,0.0760180684,
-0.7206101196\N,2.2041182783,0.1168683699,0.2833943191\C,1.0134454124,
1.3852649646,-1.4730502935\S,1.4472708087,2.896405665,-0.7380294606\H,
2.1827908137,2.2781373839,0.2282514793\H,-1.0696741076,-0.1981004765,-
0.722373755\H,1.2903148783,-0.7246817566,-1.4692461045\H,1.8633742317,
-0.302204445,1.1471086197\H,3.0410072134,-0.3666517874,-0.0244097599\H
,0.4062528963,1.4342732935,-2.3703254983\\Version=EM64L-G09RevA.02\\Sta
te=2-A\\HF=-646.0155169\S2=0.755279\S2-1=0.\S2A=0.750021\\RMSD=4.133e-09
\\RMSF=5.389e-06\\Dipole=0.3823789,-0.8467523,-0.6286185\\Quadrupole=1.03
19398,-0.0827137,-0.9492261,-2.3786668,4.0566449,2.7094886\\PG=C01 [X(C
3H6N1O1S1)]\\@

DEF_1

1\1\GINC-V1285\FOpt\RB3LYP\6-31G(d)\C6H12Cl2\GXG501\02-Jun-2010\0\#B3
LYP/6-31G* OPT Freq=noraman maxdisk=268435456\defl.freq\0,1\C,0.0146
448618,-0.0161580741,-0.0114588755\C,0.0166699176,0.0025996434,1.53126
35146\C,1.3988666472,-0.0018330909,2.17420805\C,-1.4111686543,-0.04380
58956,-0.6016770169\C,-1.4832355884,0.2008502292,-2.1039744807\C,0.912
6606503,-1.1451614601,-0.550839626\Cl,-0.871719763,1.5071930507,2.1344
860718\Cl,-2.2514756516,-1.6419845716,-0.2173023862\H,0.6179527234,-2.
118543887,-0.1462008561\H,0.4373284953,0.9441674682,-0.3427059043\H,1.
9614749697,-0.9681236653,-0.2988962724\H,0.8472566889,-1.2059641963,-1.
6408968059\H,-1.0100869289,1.1626855683,-2.338686556\H,-0.9796469099,
-0.582881574,-2.6763012625\H,-2.5249195192,0.2437127948,-2.4331165359\H,
-2.02126075,0.6961665522,-0.083333712\H,-0.5824066254,-0.8284902407,
1.9101962419\H,2.016917919,0.8181867046,1.7928991808\H,1.3135542618,0.
1081378128,3.2582654594\H,1.9091403755,-0.9489626776,1.9702910544\Ver
sion=EM64L-G09RevA.02\State=1-A\HF=-1156.2784377\RMSD=3.177e-09\RMSF=6
.788e-06\Dipole=0.9273631,0.0182164,-0.5348969\Quadrupole=0.7912182,-2
.2179474,1.4267292,-2.0122771,1.0461433,-3.4339613\PG=C01 [X(C6H12Cl2)]\@

DEF_100

1\1\GINC-V1285\FOpt\UB3LYP\6-31G(d)\C6H11Cl2O2(2)\GXG501\02-Jun-2010\0
\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\defl.oo.freq\0,2\C
, -0.0149726354,-0.0168495761,-0.0203188677\C,0.0015484781,-0.036601994
1,1.5298653474\C,1.3913307915,0.0498317326,2.1549837451\C,-1.453372099
3,-0.0040039387,-0.6129593841\C,-1.5508220913,0.1463842149,-2.12561860
87\C,0.8678261129,-1.1273703253,-0.5860956825\Cl,-1.0206334161,1.32268
16773,2.2228299237\Cl,-2.3257666803,-1.5436270777,-0.1121140258\H,0.54
35917338,-2.092504414,-0.1887763581\H,1.9129734062,-0.9629732974,-0.31
85939997\H,0.8058165252,-1.1600800436,-1.6734193756\H,-1.0515129545,1.
0659475084,-2.4441047341\H,-1.1014540016,-0.697480196,-2.6552438995\H,
-2.6037876218,0.2068909289,-2.4135355621\H,-2.0114967839,0.7926995006,
-0.122599784\H,-0.5084182594,-0.9458912715,1.8500588023\H,1.9208760633
,0.9447431081,1.8180419265\H,1.3034218943,0.0860486076,3.2434161618\H,
1.9843229833,-0.8328971209,1.8948934846\O,0.550670644,1.3205271136,-0.
3609469863\O,1.2017973583,1.3557507483,-1.5083714178\Version=EM64L-G0
9RevA.02\State=2-A\HF=-1305.979818\S2=0.753317\S2-1=0.\S2A=0.750007\RM
SD=7.250e-09\RMSF=8.807e-06\Dipole=0.4453082,-0.6809835,-0.1039781\Qua
drupole=0.3749559,-1.7577607,1.3828048,-4.3300104,4.0157706,-0.8808735
\PG=C01 [X(C6H11Cl2O2)]\@

DEF_100H

1\1\GINC-V1284\FOpt\RB3LYP\6-31G(d)\C6H12Cl2O2\GXG501\02-Jun-2010\0\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\defl.oo.h.freq\0,1\C,0
.0033466008,0.0168921216,0.0881128574\C,-0.0043823047,-0.1157691903,1.
6392867597\C,1.3789020904,-0.1504317861,2.2792905496\C,-1.4238610247,0
.0950722183,-0.5237961695\C,-1.4751051408,0.3310664564,-2.0274859372\C
,0.8314597057,-1.1419046421,-0.4965644852\Cl,-0.9528151492,1.258314589
8,2.4461410425\Cl,-2.3486212702,-1.446414475,-0.1245551798\H,0.4996446
661,-2.1028589951,-0.0958913815\H,1.8887901879,-1.0025247343,-0.260625
7608\H,0.733189107,-1.1638555225,-1.5831475281\H,-0.9387837667,1.25238
11057,-2.2687272362\H,-1.0364820443,-0.4958983469,-2.592072414\H,-2.51
61892329,0.4397039057,-2.343499076\H,-1.9805046344,0.8757133463,-0.010
9486894\H,-0.5795085865,-1.0025555075,1.9068010484\H,1.9772755943,0.71
03403686,1.9685428353\H,1.290505204,-0.1464169698,3.3682191158\H,1.907
2930659,-1.0641696955,1.9890391525\O,0.7744812858,1.1658895414,-0.3300
040304\O,-0.0022818661,2.3934781289,-0.2801271088\H,0.0803277689,2.638
9049344,0.6614580156\Version=EM64L-G09RevA.02\State=1-A\HF=-1306.6147
816\RMSD=6.931e-09\RMSF=4.595e-06\Dipole=0.6752396,-0.2989261,0.139621

4\Quadrupole=-0.6392908,0.0792152,0.5600756,-3.6819621,2.7781274,0.475
2164\PG=C01 [X(C6H12Cl2O2)]\@

DEF_1R

1\1\GINC-V1309\FOpt\UB3LYP\6-31G(d)\C6H11Cl2(2)\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def1r.freq\0,2\C,-0.0796554719,-0.1082556201,0.0527941372\C,0.0559945509,0.2854755342,1.4787389282\C,1.0342073533,-0.523423585,2.3202856369\C,-1.4432918058,-0.2451193578,-0.4888205141\C,-1.6381846331,-0.1080822533,-1.9889570615\C,1.1326202919,-0.4760127935,-0.743267275\C,0.6017132042,2.0984598413,1.5290811034\C,1.20827366302,-1.9971606471,0.007186155\H,1.3392390031,-1.5567262758,-0.6810227487\H,2.0193262968,0.0492593249,-0.3749086078\H,1.0180900187,-0.2352384997,-1.8043903376\H,-1.3085562431,0.889249482,-2.3066540923\H,-1.0690283968,-0.8581183504,-2.5437334048\H,-2.6941258127,-0.2221371096,-2.246042748\H,-2.1435588877,0.3910803453,0.0554555343\H,-0.9212100833,0.3177334708,1.9629256718\H,2.0469577541,-0.4923519494,1.9102150395\H,1.0655458928,-0.1403761988,3.3437696985\H,0.6988772482,-1.5674643191,2.3465823424\Version=EM64L-G09RevA.02\State=2-A\HF=-1155.6258708\S2=0.755774\S2-1=0.\S2A=0.750026\RMSD=9.225e-09\RMSF=5.838e-06\Dipole=0.3088038,-0.1016187,-0.4091806\Quadrupole=0.9551691,-5.310106,4.3549369,-5.1367084,-0.0959132,-2.6210301\PG=C01 [X(C6H11Cl2)]\@

DEF_2

1\1\GINC-V1343\FOpt\RB3LYP\6-31G(d)\C6H12Cl2\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def3.freq\0,1\C,0.0197232957,0.014610685,0.0102144509\C,-0.0133152887,0.0311632417,1.5439237444\C,1.456779369,0.0244734093,-0.5505692506\C,2.3114972533,-1.1782690404,-0.1334450474\C,-0.8561549496,1.1335370678,-0.5972691193\C,-2.2503938604,1.2774333448,0.0023272635\C,0.6412666263,1.572304287,2.2732771942\C,1.0535216668,0.8271471804,-2.4058437778\H,-0.4512500541,-0.9442081023,-0.2596153776\H,-1.0252219734,-0.0754702174,1.9341700537\H,0.6003200341,-0.7728595254,1.9502822304\H,1.3931894513,0.0515399802,-1.6423362804\H,1.820294187,-2.125760654,-0.3883938489\H,3.2751141835,-1.1571286134,-0.6536669416\H,2.5279293973,-1.1884293523,0.9408026458\H,-2.7928734453,0.3259122189,-0.0181863504\H,-2.8307618775,2.0128407393,-0.5604708984\H,-2.1829445437,1.6275876291,1.0380264634\H,-0.3251767195,2.0865908593,-0.5446193523\H,1.9516765525,0.9542042394,-0.2422559485\Version=EM64L-G09RevA.02\State=1-A\HF=-1156.274535\RMSD=5.595e-09\RMSF=6.441e-06\Dipole=-0.1371665,-0.5549972,0.417212\Quadrupole=2.3220788,2.3485127,-4.6705915,-0.8734911,-3.1357863,-1.9885128\PG=C01 [X(C6H12Cl2)]\@

DEF_200

1\1\GINC-V1380\FOpt\UB3LYP\6-31G(d)\C6H11Cl2O2(2)\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def3oo.freq\0,2\C,0.0685167996,0.0160684511,0.0665210966\C,0.0593515012,-0.0602757712,1.6019929725\C,1.4741776952,0.0320515489,-0.5620296646\C,2.3818962213,-1.1325875561,-0.1472729333\C,-0.8341843693,1.09299905,-0.5766525077\C,-0.3368225832,2.5340477564,-0.516558978\C,1.066949933,1.2102020863,2.4063423564\C,-2.5316773059,1.0280018968,0.1205033706\H,-0.9531696339,0.045520257,1.9874469596\H,0.4640068492,-1.0227608483,1.9145830483\H,1.3423494923,0.025991446,-1.6495974564\H,1.9270489614,-2.1003066138,-0.3773906069\H,3.3284274446,-1.0691183499,-0.6937608317\H,2.6199956516,-1.1044928417,0.9209857154\H,-0.231020417,2.8872404906,0.5109666324\H,-1.0478492527,3.1811404774,-1.0368977349\H,0.6316110109,2.6243484377,-1.0192722129\H,-0.9672693563,0.7827313685,-1.6146296032\H,1.9538779679,0.9785885459,-0.2983609005\O,-0.5559242523,-1.3151272759,-0.2453695693\O,-0.677835043,-1.5339089163,-1.5384559635\Version=EM64L-G09RevA.02\State=2-A\HF=-1305.9771434\S2=0.75333\S2-1=0.\S2A=0.750008\RMSD=9.030e

-09\RMSF=9.002e-06\Dipole=0.8764957,0.3431472,-0.1783443\Quadrupole=-0.8326071,0.4273385,0.4052686,-1.3941761,-2.6268749,-4.42542\PG=C01 [X(C6H11Cl2O2)]\@

DEF_200H

1\1\GINC-V1297\FOpt\RB3LYP\6-31G(d)\C6H12Cl2O2\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def3ooh.freq\0,1\C,0.0374370905,-0.0106162647,-0.0750284546\C,0.0072721139,0.0729089111,1.4675603001\C,1.4542446132,-0.0176626755,-0.6899078973\C,2.3584496622,-1.1422809505,-0.1728324659\C,-0.8327572515,1.0563154151,-0.7894728032\C,-0.462810255,2.5187238297,-0.5729186298\Cl,1.1177348418,1.310653425,2.1903749417\Cl,-2.6128360826,0.8329951042,-0.3490206192\H,-0.9979548526,0.3050390139,1.8169601941\H,0.3142853499,-0.8892070935,1.8772058232\H,1.334717267,-0.1196294794,-1.774569238\H,1.8947508841,-2.1207053728,-0.3250017336\H,3.3111659927,-1.1284575361,-0.7128637291\H,2.5846817042,-1.0258471619,0.8922961525\H,-0.5769497043,2.8206002192,0.4700931184\H,-1.1038366533,3.1528740194,-1.1914323352\H,0.5767740711,2.6929735984,-0.8686771229\H,-0.8096482033,0.8192964027,-1.8530607921\H,1.9306529694,0.9502235526,-0.508308553\O,-0.5631300211,-1.3208996482,-0.2211567629\O,-0.8218144206,-1.5945176553,-1.6221598217\H,-1.790923157,-1.4706264824,-1.6338238194\Version=EM64L-G09RevA.02\State=1-A\HF=-1306.6114186\RMSD=7.042e-09\RMSF=5.115e-06\Dipole=0.1233994,0.2301322,-0.509081\Quadrupole=-0.2871576,-0.5451716,0.8323292,1.1035194,-0.4859489,-2.6171836\PG=C01 [X(C6H12Cl2O2)]\@

DEF_2R

1\1\GINC-V1468\FOpt\UB3LYP\6-31G(d)\C6H11Cl2(2)\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def3r.freq\0,2\C,0.6979082178,-0.7236689494,0.5935354514\C,0.7742184494,-0.7758731965,2.0621325772\C,1.772214859,-0.039946392,-0.203194233\C,1.3519903851,1.3402824792,-0.7586167713\C,-0.4244424944,-1.3684283378,-0.1274772926\C,-1.8123535161,-1.2714958329,0.4894700369\Cl,0.0363119824,0.7713527467,2.8524925791\Cl,0.0041296568,-3.2172822093,-0.3047908859\H,0.2113343937,-1.5975388244,2.5033576921\H,1.7994393593,-0.782502187,2.4323657847\H,2.6698077959,0.0838922639,0.4143225018\H,1.1058103706,2.0298068536,0.0542225905\H,2.1669181149,1.7746553018,-1.3480942418\H,0.4750088171,1.2587317783,-1.4108582934\H,-1.844431426,-1.6985942478,1.4951623667\H,-2.5401889719,-1.8012391327,-0.1306840078\H,-2.1040002196,-0.2171660189,0.5581977312\H,-0.4447629452,-1.0450924044,-1.1694723657\H,2.0558094953,-0.6880075418,-1.0456732898\Version=EM64L-G09RevA.02\State=2-A\HF=-1155.622164\S2=0.755562\S2-1=0.\S2A=0.750025\RMSD=4.545e-09\RMSF=6.672e-06\Dipole=0.1859012,0.3388304,-0.4302624\Quadrupole=4.399402,-4.3838957,-0.0155063,0.6626272,0.9486481,-5.1577066\PG=C01 [X(C6H11Cl2)]\@

DEF_3

1\1\GINC-V1341\FOpt\RB3LYP\6-31G(d)\C5H9Cl3\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def2.freq\0,1\C,0.03608671,-0.519819229,-0.0241085669\C,0.109694764,0.4093050031,1.2045144071\C,1.3312332396,0.1827154713,2.0878895444\C,-1.2549706514,-0.398446724,-0.8511245647\C,-1.5047089291,0.9484390222,-1.5149076921\Cl,1.5022706269,-0.1653474391,-1.0583542805\Cl,-1.3921666805,0.1463502266,2.2382473035\Cl,-1.2941880697,-1.7270978473,-2.1063974311\H,0.1548751594,-1.5559451125,0.2991818281\H,0.0499154654,1.4513917267,0.8855588712\H,2.2445776869,0.410321201,1.5322064511\H,1.2837847316,0.8338585267,2.9643771247\H,1.3768196672,-0.8561359005,2.4298860122\H,-2.0785329678,-0.6450956953,-0.1804645099\H,-1.5663366429,1.7357542427,-0.7542759423\H,-2.4557959123,0.9266081067,-2.0526699901\H,-0.7086532263,1.1982922553,-2.2201998749\Version=EM64L-G09RevA.02\State=1-A\HF=-1576.5559937\RMSD=3.664e-09\RMSF=9.060e-06\Dipole=0.1353932,0.6280976,0.534574\Quadrupole=0.8258167,1.5452129,-2.3710296,-0.5670559,3.1402066,-2.2415763\PG=C01 [

X(C5H9Cl3)]\@

DEF_300

1\1\GINC-V1291\FOpt\UB3LYP\6-31G(d)\C5H8Cl3O2(2)\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def2oo.freq\0,2\C,-0.0142247297,0.0732160696,-0.091184661\C,-0.0137925441,0.0462729122,1.4640900588\C,1.3718013077,-0.0867412875,2.089554577\C,-1.4000603021,-0.0783750202,-0.7466838465\C,-2.4264607075,0.9532034171,-0.2920196605\Cl,0.7824654752,1.6219418696,-0.5733661404\Cl,-1.071310854,-1.3012101704,2.1100078522\Cl,-1.2557390205,-0.0418781492,-2.5594747745\H,-0.5008851502,0.962874863,1.7981871784\H,2.020251163,0.7264320342,1.7524419413\H,1.2803703449,-0.0330870902,3.1770713426\H,1.8321405492,-1.0401531954,1.8227963498\H,-1.7342315111,-1.0886160504,-0.5163281951\H,-2.6068366007,0.8661919905,0.7843152613\H,-3.372443859,0.767277739,-0.8061950732\H,-2.0999588737,1.9701176906,-0.5245249417\O,0.9267465828,-0.9350578349,-0.5951537202\O,0.4000194871,-2.1501084872,-0.6032573458\Version=EM64L-G09RevA.02\State=2-A\HF=-1726.2496192\S2=0.753211\S2-1=0.\S2A=0.750007\RMSD=6.422e-09\RMSF=8.502e-06\Dipole=-0.292142,0.8088845,1.0059483\Quadrupole=2.7851891,-1.1727072,-1.6124819,0.034173,2.1279284,1.3950904\PG=C01 [X(C5H8Cl3O2)]\@

DEF_300H

1\1\GINC-V1293\FOpt\RB3LYP\6-31G(d)\C5H9Cl3O2\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def2ooh.freq\0,1\C,0.0564836494,-0.0380912555,0.0496486114\C,0.0165779217,0.0058107091,1.6091309005\C,1.399557912,-0.009593164,2.247758451\C,-1.3055354641,-0.3619173134,-0.6034178661\C,-2.430599383,0.6152193632,-0.2906030902\Cl,0.6332782399,1.6183619712,-0.4607588075\Cl,-0.9625311381,-1.3823279748,2.3122803326\Cl,-1.1094939987,-0.5205669581,-2.4147423961\H,-0.5407659329,0.8952374876,1.9032083434\H,1.9926415215,0.8314669571,1.8774380642\H,1.3008596733,0.0808427505,3.3323756822\H,1.9235756378,-0.9376284876,2.0120351479\H,-1.5722897595,-1.364220468,-0.2747772057\H,-2.6149411858,0.6423912163,0.7884997158\H,-3.3490961346,0.2795800291,-0.7785331118\H,-2.1955694171,1.6226849531,-0.6414513202\O,1.1158912527,-0.8470323367,-0.4406386401\O,0.7183515537,-2.2462160918,-0.3671065308\H,0.5466594827,-2.4092022921,-1.3159959001\Version=EM64L-G09RevA.02\State=1-A\HF=-1726.887761\RMSD=8.009e-09\RMSF=3.272e-06\Dipole=-0.4256052,0.2350281,0.2846788\Quadrupole=0.8257643,0.754449,-1.5802134,-0.5443051,1.1314894,4.7321672\PG=C01 [X(C5H9Cl3O2)]\@

DEF_3R

1\1\GINC-V1398\FOpt\UB3LYP\6-31G(d)\C5H8Cl3(2)\GXG501\02-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def2r.freq\0,2\C,0.6855665754,0.796037622,-0.0718384939\C,0.1691238649,-0.0149443282,1.0503508698\C,0.9638149011,0.0158673138,2.3479296576\C,-0.1783387603,1.5755749487,-0.9867600164\C,-1.4291217281,0.8629830356,-1.4904387919\Cl,2.3979361605,0.9155025421,-0.3071676734\Cl,0.0207004614,-1.8112334146,0.4917324359\Cl,-0.720318266,3.148223009,-0.0887743279\H,-0.8681249906,0.270863641,1.2320146106\H,1.0205920763,1.0491497618,2.7097724842\H,0.4663923603,-0.5961524942,3.1043882804\H,1.9784407334,-0.3609695592,2.2026912346\H,0.4089347823,1.9613730429,-1.8189747193\H,-1.1342378102,-0.0250870446,-2.0600132219\H,-1.9983831017,1.5317543718,-2.1411413523\H,-2.0795650037,0.5452898287,-0.6717081548\Version=EM64L-G09RevA.02\State=2-A\HF=-1575.9030426\S2=0.755547\S2-1=0.\S2A=0.750024\RMSD=4.809e-09\RMSF=6.613e-06\Dipole=-0.1236584,0.0314154,-0.0563465\Quadrupole=1.3986779,-7.090442,5.6917641,1.002233,1.2160291,-0.4940686\PG=C01 [X(C5H8Cl3)]\@

DEF_4

1\1\GINC-V1299\FOpt\RB3LYP\6-31G(d)\C4H7Cl1\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def4.freq\0,1\C,-0.0056710868,0.0211253449,0.0033053886\C,-0.0091169866,-0.0075682979,1.3332558725\C,1.2519728323,-0.0042103252,-0.8239703413\C,1.3164268416,-1.2194583668,-1.7644742574\Cl,-1.4759858239,0.0121363339,2.2960224032\H,0.8869107707,-0.0423853696,1.9435584821\H,-0.9535049408,0.0522913941,-0.5325929787\H,1.3021637436,0.9153858388,-1.4251031991\H,2.1301193613,0.0060571194,-0.166456069\H,2.2250090501,-1.1902965283,-2.3760769103\H,1.3161386299,-2.1557391206,-1.1961046218\H,0.4559824981,-1.2407223658,-2.4436199875\Version=EM64L-G09RevA.02\State=1-A\HF=-616.8189309\RMSE=9.543e-09\RMSEF=1.057e-05\Dipole=0.6089496,-0.0255245,-0.5741353\Quadrupole=0.5208028,-0.8282605,0.3074578,0.1361589,1.3213393,-0.3642989\PG=C01 [X(C4H7Cl1)]\@

DEF_400

1\1\GINC-V1448\FOpt\UB3LYP\6-31G(d)\C4H6Cl1O2(2)\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def4oo.freq\0,2\C,0.1011199906,-0.3715047318,0.2412622154\C,-0.2271775472,0.4438120578,1.2409083537\C,1.3164332258,-0.1365103747,-0.6013289474\C,2.140614252,-1.3901290304,-0.8592098739\Cl,-1.633975186,0.2109159381,2.2462426055\H,0.3480704657,1.3206161707,1.5172141935\H,-0.5193007299,-1.2308563173,-0.0026015796\H,1.926544052,0.6738001502,-0.1934358168\H,2.9796163075,-1.1688208883,-1.5256529633\H,2.5346503539,-1.7760655446,0.0860516304\H,1.5263251609,-2.1706756715,-1.3203567667\O,0.8968031223,0.3320726967,-1.9514751606\O,0.4722440218,1.5802936493,-1.9186324526\Version=EM64L-G09RevA.02\State=2-A\HF=-766.5252653\S2=0.753087\S2-1=0.\S2A=0.750007\RMSE=1.926e-09\RMSEF=4.279e-06\Dipole=0.8214179,-0.6489362,0.4321338\Quadrupole=2.5310701,1.4048896,-3.9359598,-0.0425939,0.9027481,3.3486287\PG=C01 [X(C4H6Cl1O2)]\@

DEF_400H

1\1\GINC-V1350\FOpt\RB3LYP\6-31G(d)\C4H7Cl1O2\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def4ooh.freq\0,1\C,0.0309899509,0.0501475663,-0.0163793609\C,0.0250660662,0.0617243555,1.3143241864\C,1.308272671,0.0419065556,-0.8178381415\C,1.2773287949,-0.9701108053,-1.9614772998\Cl,-1.4379933555,0.0963822454,2.2743159313\H,0.9236771396,0.044968232,1.9215618802\H,-0.9037825056,0.0761370224,-0.5737444992\H,2.1675662619,-0.1451094272,-0.1627282138\H,2.208246893,-0.921152435,-2.5336217316\H,1.1577086679,-1.981996885,-1.561860147\H,0.4416422057,-0.7643446014,-2.6389470401\O,1.5065630931,1.3151407017,-1.4617013053\O,1.862699273,2.276448257,-0.4376976825\H,0.992355851,2.6722092506,-0.244239125\Version=EM64L-G09RevA.02\State=1-A\HF=-767.1587694\RMSE=8.317e-09\RMSEF=1.025e-05\Dipole=-0.1399651,-0.3914922,-0.0623986\Quadrupole=-1.5635597,1.948574,-0.3850143,-3.7053854,3.3172484,2.5802465\PG=C01 [X(C4H7Cl1O2)]\@

DEF_4R

1\1\GINC-V1281\FOpt\UB3LYP\6-31G(d)\C4H6Cl1(2)\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def4r.freq\0,2\C,0.0575522643,-0.2952512151,0.1309486695\C,-0.0401383219,0.2207379932,1.4145569487\C,1.2525885075,-0.6366731827,-0.477747497\C,1.3635767543,-1.1931339691,-1.8616466412\Cl,-1.5690252979,0.6331281578,2.1313937702\H,0.8106498734,0.4041233128,2.0597803752\H,-0.8682798532,-0.4373070918,-0.425455732\H,2.1796596105,-0.4951785743,0.0773743635\H,1.982263006,-0.5507503046,-2.5051675517\H,1.8452559066,-2.1818340827,-1.8602397423\H,0.38185238,-1.2980571508,-2.3355997303\Version=EM64L-G09RevA.02\State=2-A\HF=-616.1796123\S2=0.778605\S2-1=0.\S2A=0.750181\RMSE=5.073e-09\RMSEF=8.046e-06\Dipole=0.5954715,-0.2319931,-0.4597494\Quadrupole=0.8184721,-1.3576639,0.5391918,0.1296748,0.8560158,0.7982076\PG=C01 [X(C4H6Cl1)]\@

11)\@

DEF_5

1\1\GINC-V1361\FOpt\RB3LYP\6-31G(d)\C4H7Cl1\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def5.freq\0,1\C,0.01719 50347,0.0204007226,0.0157086703\C,0.0163740641,-0.0164177667,1.3518930 868\C,1.2425008145,-0.0036135062,-0.8489927468\C,-1.2258087019,-0.0178 56067,2.1734586915\Cl,-1.3623115206,1.5028446099,3.2036216013\H,-1.250 8846668,-0.8390663924,2.8931500716\H,-2.1263995629,-0.0476750362,1.558 0127022\H,0.9576902145,-0.0537293343,1.8991922291\H,-0.9396747888,0.07 0673019,-0.5073335257\H,2.1585478233,-0.0495847423,-0.2514018269\H,1.2 915819751,0.8921027881,-1.4824111801\H,1.2320088482,-0.8673008771,-1.5 272076869\Version=EM64L-G09RevA.02\State=1-A\HF=-616.8218893\RMSD=8.7 19e-09\RMSF=1.172e-05\Dipole=0.2341906,-0.7211925,-0.7519694\Quadrupol e=0.9231144,-1.0070543,0.0839399,0.974918,0.5565461,-1.4832408\PG=C01 [X(C4H7Cl1)]\@

DEF_500

1\1\GINC-V1473\FOpt\UB3LYP\6-31G(d)\C4H6Cl1O2(2)\GXG501\03-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def5oo.freq\0,2\C, 0.011078257,0.1241829718,0.0606874722\C,-0.0350358676,-0.4270301981,1. 2771879397\C,1.2224333608,0.1629902497,-0.8202086017\C,-1.2715120877,- 0.4349423575,2.0994373388\Cl,-1.8319676882,-2.1334544463,2.4521443775\ H,-2.1162027203,0.0876317998,1.653496106\H,0.8378831192,-0.9014042364, 1.7206398708\H,-0.8933503158,0.581494183,-0.3436036501\H,2.0866667443, -0.3097901711,-0.3439127269\H,1.4887253326,1.1981220141,-1.0704768953\ H,1.0284786264,-0.350658663,-1.7709386058\O,-0.975693586,0.2065244059, 3.3648642914\O,-2.0674157468,0.7030183848,3.9254347439\Version=EM64L- G09RevA.02\State=2-A\HF=-766.5245261\S2=0.752905\S2-1=0.\S2A=0.750006\ RMSD=7.941e-09\RMSF=6.554e-06\Dipole=0.6411218,0.3053091,-1.3634631\Qu adrupole=1.3963473,-1.3686766,-0.0276706,-0.3733595,0.0520442,-2.76211 04\PG=C01 [X(C4H6Cl1O2)]\@

DEF_500H

1\1\GINC-V1296\FOpt\RB3LYP\6-31G(d)\C4H7Cl1O2\GXG501\04-Jun-2010\0\#B 3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def5ooh.freq\0,1\C,0. 0014751459,0.0320293467,0.0563534865\C,0.0935299725,0.0602175403,1.388 8801705\C,1.1655059834,-0.0536177943,-0.8835078991\C,-1.1016329119,0.1 447551962,2.268208674\Cl,-1.2901052422,-1.4685479631,3.2412689618\H,-2 .0515155533,0.2310797873,1.7403976967\H,1.0553911358,0.0209833969,1.89 5104064\H,-0.9874372449,0.0675025026,-0.4031142248\H,2.1189302984,-0.0 841933525,-0.3472475236\H,1.18040855,0.8066670633,-1.5654028353\H,1.09 41528152,-0.9515694256,-1.511271444\O,-0.9139789623,1.186860984,3.1599 782099\O,-2.1581181208,1.42370011,3.8609681956\H,-2.0838947947,0.76328 23337,4.5795978111\Version=EM64L-G09RevA.02\State=1-A\HF=-767.165727\ RMSD=6.644e-09\RMSF=1.029e-05\Dipole=0.2837713,0.0002273,-0.7722057\Qu adrupole=0.853251,-6.0098836,5.1566326,0.2447383,-1.7579965,-0.2443589 \PG=C01 [X(C4H7Cl1O2)]\@

DEF_5R

1\1\GINC-V1279\FOpt\UB3LYP\6-31G(d)\C4H6Cl1(2)\GXG501\03-Jun-2010\0\# B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def5r.freq\0,2\C,0.0 103081638,0.1727996045,-0.0263131044\C,0.0072241409,0.1214043362,1.355 6120122\C,1.2254103712,-0.0500945813,-0.8689526537\C,-1.0654759139,0.3 137774801,2.2134484478\Cl,-2.678566145,0.6722518059,1.6649964764\H,-0. 9824769615,0.2560244775,3.290679561\H,0.9494374521,-0.0948141381,1.861 4888497\H,-0.9233456724,0.38784213,-0.541421352\H,2.1120307389,-0.2581 167604,-0.2603906423\H,1.4438767962,0.8261919316,-1.4965238868\H,1.084

0469187,-0.8937477052,-1.5601388825\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-616.1801484\\S2=0.778059\\S2-1=0.\\S2A=0.750174\\RMSD=8.430e-09\\RMSF=1.028e-05\\Dipole=0.665361,-0.1365504,-0.0731592\\Quadrupole=-0.3518018,-1.9123444,2.2641461,-0.3585232,0.3727372,-0.2379842\\PG=C01 [X(C4H6Cl1)]\\@

DEF_6

1\\1\\GINC-V1282\\FOpt\\RB3LYP\\6-31G(d)\\C5H9Cl1\\GXG501\\03-Jun-2010\\0\\#B3LYP\\6-31G* OPT Freq=noraman maxdisk=268435456\\def6.freq\\0,1\\C,0.1621728893,-0.1411325447,0.0324776126\\C,0.1147963881,-0.2078759424,1.5285265857\\C,1.125965871,0.064750014,2.3586282535\\C,1.0481008015,-0.0312106644,3.854590863\\Cl,-1.1380300287,1.0656768383,-0.5367563372\\H,-0.1956556916,-1.0845940869,-0.3897651186\\H,2.0866936835,0.3791845539,1.9525688094\\H,1.7848105593,-0.7457788319,4.2456185234\\H,0.0546383257,-0.3478699506,4.1883292849\\H,1.272226639,0.9372015351,4.3216143694\\H,-0.8448096741,-0.5177583344,1.9412226238\\C,1.4921301114,0.2423491449,-0.5984085132\\H,1.4042312607,0.2677707516,-1.6873407024\\H,2.2541544624,-0.4990422945,-0.3299660221\\H,1.8241429109,1.2267248089,-0.2563217615\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-656.1374987\\RMSD=2.111e-09\\RMSF=4.718e-06\\Dipole=0.7801725,-0.554268,0.4700325\\Quadrupole=-0.3666229,-0.6583028,1.0249258,1.2999461,-1.2889498,1.1455968\\PG=C01 [X(C5H9Cl1)]\\@

DEF_600

1\\1\\GINC-V1308\\FOpt\\UB3LYP\\6-31G(d)\\C5H8Cl1O2(2)\\GXG501\\03-Jun-2010\\0\\#B3LYP\\6-31G* OPT Freq=noraman maxdisk=268435456\\def600.freq\\0,2\\C,0.0186513828,0.2726028249,-0.0452496968\\C,0.340555428,0.525968958,1.3930254886\\C,0.6858994308,-0.4076607447,2.28326688\\C,1.0157622398,-0.1279485669,3.71915873\\Cl,1.2584201689,1.1536790386,-1.085641961\\H,0.7481794165,-1.450223833,1.974205565\\H,0.3493762235,-0.6868287401,4.3891192604\\H,0.9279027631,0.9368032732,3.9557036062\\H,2.0391342021,-0.4492603981,3.9537911474\\H,0.281738246,1.5725995501,1.6852260427\\C,-0.0915416185,-1.1638440527,-0.5137949646\\H,-0.3951382832,-1.1795558382,-1.5610531632\\H,-0.8445775455,-1.6865423807,0.0848647497\\H,0.8701837275,-1.6704366067,-0.4112328051\\O,-1.2637131325,0.9738410227,-0.241258028\\O,-1.7660202655,0.8278343738,-1.4522353649\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-805.8425901\\S2=0.753013\\S2-1=0.\\S2A=0.750007\\RMSD=9.831e-09\\RMSF=1.011e-05\\Dipole=0.3945712,-0.9107792,1.1706965\\Quadrupole=-3.3929059,1.9047744,1.4881315,0.5186453,0.0208121,0.9981583\\PG=C01 [X(C5H8Cl1O2)]\\@

DEF_600H

1\\1\\GINC-V1307\\FOpt\\RB3LYP\\6-31G(d)\\C5H9Cl1O2\\GXG501\\03-Jun-2010\\0\\#B3LYP\\6-31G* OPT Freq=noraman maxdisk=268435456\\def600h.freq\\0,1\\C,0.2402125336,-0.3529409565,0.051976414\\C,0.127428153,-0.1860119245,1.5355820888\\C,1.1474347163,0.0435180675,2.3667897292\\C,1.0071309529,0.2114464886,3.850469253\\Cl,-0.6757309273,1.1475814419,-0.7313252323\\H,2.1584622966,0.1267327554,1.9709387781\\H,1.607661822,-0.5349241652,4.3869235068\\H,-0.0337540848,0.1121317455,4.1732662455\\H,1.3731844508,1.1967765206,4.1681124983\\H,-0.8885123283,-0.2680087301,1.9153120739\\C,1.6276432396,-0.3798191879,-0.5604600283\\H,1.5547375483,-0.5122693176,-1.6391672478\\H,2.1806621569,-1.226250473,-0.13876872\\H,2.1612136361,0.5481697962,-0.3472534565\\O,-0.5306773048,-1.4850856803,-0.2247085793\\O,-0.5454730877,-1.7650482219,-1.6444930803\\H,-1.2348458395,-1.1332490509,-1.9354769148\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-806.4827569\\RMSD=4.771e-09\\RMSF=5.942e-06\\Dipole=0.5825663,0.0813452,0.6342813\\Quadrupole=2.1196343,-5.951213,3.8315786,0.6398269,1.773241,0.3744049\\PG=C01 [X(C5H9Cl1O2)]\\@

DEF_6R

1\1\GINC-V1281\FOpt\UB3LYP\6-31G(d)\C5H8Cl1(2)\GXG501\03-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\def6r.freq\0,2\C,0.3
 357682363,0.1594046773,0.0614008451\C,0.3426002244,0.3788794896,1.4376
 317176\C,0.9821420832,-0.3905147089,2.3932153435\C,0.9444126971,-0.091
 2526809,3.8594001179\Cl,-0.5619119288,1.2960871617,-0.9413480435\H,1.5
 508880754,-1.2670531424,2.0894006867\H,0.5122845374,-0.9262314468,4.43
 02823698\H,0.3521008203,0.8044416356,4.074801396\H,1.9546087081,0.0674
 299486,4.2645712865\H,-0.2146926238,1.2465260603,1.7877807871\C,1.0038
 263603,-0.9376428302,-0.7004142884\H,0.2722621121,-1.531697959,-1.2635
 908393\H,1.5425887822,-1.6094317144,-0.0268834431\H,1.7205403774,-0.53
 53761368,-1.4282800451\Version=EM64L-G09RevA.02\State=2-A\HF=-.655.499
 5978\S2=0.777927\S2-1=0.\S2A=0.750179\RMSD=8.622e-09\RMSF=5.391e-06\Di
 pole=0.4005483,-0.5061676,0.4527263\Quadrupole=-0.9866476,-0.0075133,0
 .9941609,-0.9071065,-0.6056099,1.3024277\PG=C01 [X(C5H8Cl1)]\@

DEF_7

1\1\GINC-V1421\FOpt\RB3LYP\6-31G(d)\C7H12Cl2\GXG501\07-Jun-2010\0\#B3
 LYP/6-31G* OPT Freq=norman maxdisk=268435456\def7.freq\0,1\C,0.2636
 24914,0.439759634,0.1158074694\C,-0.1069507312,-0.3069683305,1.1603340
 932\C,1.5286947767,0.2281121283,-0.6516027718\C,2.4048877392,1.4726043
 615,-0.743895012\C,-1.3529787008,-0.0929912365,1.9774098683\C,-2.30369
 82814,-1.2997307018,1.902325404\C,-2.9198517951,-1.5218941394,0.528409
 9639\Cl,-3.6453260303,-1.0658483315,3.1384448604\Cl,1.0991195623,-0.31
 77815609,-2.373371167\H,1.8573924698,2.3029805867,-1.2008449964\H,3.30
 11683126,1.2785074861,-1.3395349875\H,2.7112415351,1.77326149,0.265307
 3356\H,-0.3586352672,1.2724714404,-0.212582295\H,2.0910599571,-0.61291
 19328,-0.2397895669\H,0.5287470997,-1.1414636143,1.4640659398\H,-1.884
 1150519,0.8052618925,1.6417647386\H,-1.0801684432,0.0650857769,3.02864
 28564\H,-1.7859223474,-2.2021311918,2.2395468886\H,-3.5843185205,-2.39
 00663241,0.5320941166\H,-3.4965663406,-0.6451781985,0.215569002\H,-2.1
 256613921,-1.6912125395,-0.2075622763\Version=EM64L-G09RevA.02\State=
 1-A\HF=-1194.3647815\RMSD=4.556e-09\RMSF=4.312e-06\Dipole=0.8198325,0.
 2364225,0.2447516\Quadrupole=0.9931107,5.1415641,-6.1346748,0.524936,6
 .9608238,-0.5010541\PG=C01 [X(C7H12Cl2)]\@

DEF_700

1\1\GINC-V1282\FOpt\UB3LYP\6-31G(d)\C7H11Cl2O2(2)\GXG501\08-Jun-2010\0
 \#B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\def7oo.freq\0,2\C
 , -0.111141954,0.0582905864,-0.0483550284\C,-0.1130164695,-0.5015878359
 ,1.1628739083\C,1.03151438,-0.0452619513,-1.0082434673\C,1.6109203166,
 1.3097368102,-1.4019854574\C,-1.2387229852,-0.3557946238,2.1382398812\
 C,-0.8713916235,0.2894195019,3.4878821609\C,-2.0299505754,0.3446336311
 ,4.4750247538\Cl,-0.268104712,1.983033354,3.158962846\Cl,0.4399644684,
 -0.9097227325,-2.5310639906\H,0.8415997848,1.9510194838,-1.8433623803\
 H,2.4214458704,1.1903554677,-2.1262362119\H,2.0056546182,1.8064132698,
 -0.5078343519\H,-0.955903355,0.6613466596,-0.3804023176\H,1.8096705872
 , -0.6989088069,-0.6083640645\H,0.7233984214,-1.1118665922,1.4991410517
 \H,-2.0897369553,0.1673770982,1.6928441823\H,-0.0208177534,-0.24457083
 33,3.9149107376\H,-1.7151790007,0.8326114782,5.4010118246\H,-2.8750696
 233,0.9029475649,4.059597265\H,-2.3624789979,-0.6705316531,4.712142084
 5\O,-1.8095176533,-1.6976119548,2.426741105\O,-0.9254422576,-2.4913023
 623,3.0086841735\Version=EM64L-G09RevA.02\State=2-A\HF=-1344.0671136\
 S2=0.753366\S2-1=0.\S2A=0.750007\RMSD=9.834e-09\RMSF=3.289e-06\Dipole=
 0.1363333,0.732305,0.4996795\Quadrupole=5.8793775,-4.4740966,-1.405280
 9,-1.7531652,-1.733458,-3.057813\PG=C01 [X(C7H11Cl2O2)]\@

DEF_700H

1\1\GINC-V1477\FOpt\RB3LYP\6-31G(d)\C7H12Cl2O2\GXG501\08-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\def7ooh.freq\0,1\C,0
 .0421862958,0.0059938881,0.1275517947\C,-0.0196018881,0.2557363538,1.4

374574935\C,1.3110246734,0.025994445,-0.6633422408\C,1.2635819274,0.96
6065303,-1.862424278\C,-1.3029526994,0.2339482514,2.2279314042\C,-1.39
86104314,1.3348649907,3.3001983767\C,-2.6942103611,1.2972248646,4.0952
800296\Cl,-1.2277907409,2.9618687341,2.4683354533\Cl,1.6594442978,-1.6
92862698,-1.2650434648\H,0.441100098,0.7018374731,-2.5344771474\H,2.19
94893537,0.9278494666,-2.4266264108\H,1.1068593347,1.9918376051,-1.508
173733\H,-0.8658380638,-0.207464602,-0.4366955128\H,2.1608320924,0.260
9329192,-0.0188345332\H,0.891966883,0.4668902054,1.9945499216\H,-2.166
0802345,0.3120564821,1.5551024257\H,-0.5347109921,1.2657886116,3.96424
1066\H,-2.711346319,2.0962687433,4.8412758009\H,-3.5621447174,1.417214
9999,3.4383829172\H,-2.7739401003,0.3330502615,4.6061648849\O,-1.53331
12844,-1.0503537314,2.8396040455\O,-0.3995130622,-1.3484423312,3.70566
39188\H,0.0561524759,-2.0149894991,3.159109491\Version=EM64L-G09RevA.
02\State=1-A\HF=-1344.7008137\RMSD=6.772e-09\RMSF=2.319e-06\Dipole=0.1
187006,0.1886619,0.0077653\Quadrupole=3.0197761,-4.1003041,1.080528,1.
7446044,1.9935109,-3.758799\PG=C01 [X(C7H12Cl2O2)]\@

DEF_7R

1\1\GINC-V1465\FOpt\UB3LYP\6-31G(d)\C7H11Cl2(2)\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def7r.freq\0,2\C,-0.0095105318,0.1775976865,-0.3805829474\C,-0.4660296147,0.8097671596,0.7667243627\C,1.4193851677,0.1063273754,-0.7647637617\C,1.6876909267,0.3780803111,-2.2398394723\C,-1.7963468943,0.8774380349,1.1542102573\C,-2.2602741546,1.5721399077,2.3775711049\C,-3.3002628734,0.8015890717,3.1815955982\Cl,-3.0172172403,3.2190173437,1.8801802941\Cl,2.0610314312,-1.6150549005,-0.367465367\H,1.1187995829,-0.3098255098,-2.8730956194\H,2.7502022221,0.2653936256,-2.4717397038\H,1.3821397329,1.4037267306,-2.480006935\H,-0.720042484,-0.3238370085,-1.0359172357\H,2.0290670604,0.7513889338,-0.1285932929\H,0.274229812,1.2880069141,1.410532752\H,-2.5620201142,0.4251874613,0.5257466894\H,-1.4164972305,1.8662561533,3.0053217469\H,-3.6376229352,1.3827695225,4.0440476996\H,-4.1704896338,0.5595919576,2.5635337558\H,-2.8580976709,-0.1358297614,3.5403636385\Version=EM64L-G09RevA.02\State=2-A\HF=-1193.726268\S2=0.777451\S2-1=0.\S2A=0.750195\RMSD=7.799e-09\RMSF=7.121e-06\Dipole=-0.021747,-0.0139136,-0.0188697\Quadrupole=-0.5429661,-6.6562098,7.1991759,9.2375173,-0.7230956,-2.1119981\PG=C01 [X(C7H11Cl2)]\@

DEF_8

1\1\GINC-V1409\FOpt\RB3LYP\6-31G(d)\C8H12Cl2\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def8.freq\0,1\C,-0.1752703629,0.3550863871,0.1150152371\C,0.1752703629,-0.3550863871,1.4344947629\C,1.5799952474,-0.1676508339,1.9002961019\C,2.3759874248,-1.1746370281,2.2692074515\C,3.7907618371,-1.0254322402,2.7424334727\C,-1.5799952474,0.1676508339,-0.3507861019\C,-2.3759874248,1.1746370281,-0.7196974515\C,-3.7907618371,1.0254322402,-1.1929234727\Cl,-0.9708291657,0.3324894972,2.7246092052\Cl,0.9708291657,-0.3324894972,-1.1750992052\H,4.4820523409,-1.5774755815,2.0920163828\H,4.1031485796,0.0235455785,2.7606929438\H,3.9123575463,-1.4374106197,3.7531315574\H,1.9875692091,-2.1933432514,2.2249897749\H,1.9380732866,0.8609321925,1.9384367078\H,-0.0830298207,-1.4137758179,1.3660628652\H,-1.9380732866,-0.8609321925,-0.3889267078\H,0.0830298207,1.4137758179,0.1834471348\H,-1.9875692091,2.1933432514,-0.6754797749\H,-3.9123575463,1.4374106197,-2.2036215574\H,-4.1031485796,-0.0235455785,-1.2111829438\H,-4.4820523409,1.5774755815,-0.5425063828\Version=EM64L-G09RevA.02\State=1-AG\HF=-1232.4425382\RMSD=8.602e-09\RMSF=4.141e-06\Dipole=0.,0.,0.\Quadrupole=4.0740721,2.1012259,-6.175298,-1.6947369,6.5271043,-2.5904055\PG=CI [X(C8H12Cl2)]\@

DEF_800

1\1\GINC-V1285\FOpt\UB3LYP\6-31G(d)\C8H11Cl2O2(2)\GXG501\08-Jun-2010\0

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\\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\def8oo.freq\\0,2\\C
,0.1000364177,-0.1567190566,-0.0793552561\\C,0.0441927319,-0.1092113962
,1.4711799247\\C,1.3653944779,-0.0180645869,2.1623295509\\C,1.7397734959
,-0.870955789,3.1201515988\\C,3.0452915649,-0.8173667082,3.8547924416\\C
,-1.2328959246,-0.0956969124,-0.7696270103\\C,-1.9211962446,-1.12549771
73,-1.2637515225\\C,-3.2798553829,-1.0071764485,-1.887727957\\Cl,-0.9949
910661,1.3372659016,1.9711035727\\Cl,1.0373773637,-1.6610316055,-0.5161
9697\\H,3.6125010015,-1.7468461978,3.7137127671\\H,3.6662972323,0.017715
3857,3.5160893095\\H,2.8821034566,-0.7088231626,4.9352627825\\H,1.060289
3927,-1.6766280989,3.4035263437\\H,2.0138552647,0.8004058147,1.85981869
73\\H,-0.5184276362,-0.9844613425,1.7972941272\\H,-1.648179821,0.9079971
871,-0.8000808408\\H,-1.4877933977,-2.1232367554,-1.2336920937\\H,-4.010
3231372,-1.627796097,-1.3521702047\\H,-3.6414430527,0.0255918894,-1.887
6323324\\H,-3.2621842872,-1.3669105115,-2.9247613386\\O,0.9226818681,0.9
883314707,-0.4578272358\\O,0.908836984,1.2200845459,-1.7584806633\\Vers
ion=EM64L-G09RevA.02\\State=2-A\\HF=-1382.1393455\\S2=0.752983\\S2-1=0.\\S2
A=0.750006\\RMSD=4.537e-09\\RMSF=3.416e-06\\Dipole=-0.3917737,-0.9245162,
0.5472348\\Quadrupole=3.0623429,-2.4173221,-0.6450208,1.02787,7.7477013
,-0.8765573\\PG=C01 [X(C8H11Cl2O2)]\\@

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DEF_8OOH

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1\\GINC-V1287\\FOpt\\RB3LYP\\6-31G(d)\\C8H12Cl2O2\\GXG501\\08-Jun-2010\\0\\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\def8ooh.freq\\0,1\\C,0
.1193073005,-0.0218767524,-0.0173383448\\C,0.0579335692,-0.0235755059,1
.5354633946\\C,1.3760028856,-0.0456664748,2.2370914587\\C,1.67891331,-0.
9447076353,3.177534922\\C,2.978367196,-1.0025586211,3.9230039311\\C,-1.2
126876828,0.1242476314,-0.703333999\\C,-2.056261417,-0.8538289791,-1.03
45946422\\C,-3.4087354718,-0.6293694794,-1.6439339155\\Cl,-0.8837169333,
1.4764423141,2.0727258095\\Cl,0.9017559136,-1.6891796126,-0.4654663701\\
H,3.4783494222,-1.9675471061,3.7661998448\\H,3.6614624623,-0.2077769747
,3.6072080405\\H,2.8145004921,-0.9048405675,5.0044770616\\H,0.9404303842
,-1.7051630177,3.4370184924\\H,2.0847745363,0.7296271381,1.957369526\\H,
-0.5688567403,-0.8655480921,1.8288057193\\H,-1.4792484519,1.1644523371,
-0.8715102773\\H,-1.7644828497,-1.8901284508,-0.8731510148\\H,-4.1980001
95,-1.0523849082,-1.0083355093\\H,-3.6196405436,0.4348371689,-1.7877473
744\\H,-3.4869097226,-1.1314683523,-2.6172491541\\O,1.0222112849,0.97672
51573,-0.3598543102\\O,1.0607008544,1.1304572268,-1.795399508\\H,1.66891
26946,0.4008481439,-2.0331088815\\Version=EM64L-G09RevA.02\\State=1-A\\H
F=-1382.7799022\\RMSD=6.331e-09\\RMSF=1.048e-05\\Dipole=0.0093396,-0.8434
118,0.0080771\\Quadrupole=3.6882769,-5.3205351,1.6322581,1.1274737,3.92
767,-1.8932981\\PG=C01 [X(C8H12Cl2O2)]\\@

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DEF_8R

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1\\GINC-V1349\\FOpt\\UB3LYP\\6-31G(d)\\C8H11Cl2(2)\\GXG501\\08-Jun-2010\\0\\
#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\def8r.freq\\0,2\\C,0.
1463301103,-0.4436705413,0.0743856341\\C,0.0890712462,-0.4098114084,1.5
560808339\\C,1.3724378644,-0.1565235658,2.2722357115\\C,1.8409087416,-0.
9644325533,3.2288910219\\C,3.1287811947,-0.7615276852,3.9699221005\\C,-0
.5258831675,-1.4087649199,-0.6841169656\\C,-0.56321412,-1.5319525005,-2
.0545034217\\C,-1.306131788,-2.6108673803,-2.7749587871\\Cl,-1.166665972
3,0.9195045744,2.0977286767\\Cl,1.0410285507,0.8314356277,-0.7213496308
\\H,3.7996717802,-1.6211190613,3.8393035528\\H,3.6535078496,0.1368399139
,3.6298791091\\H,2.9481840763,-0.6649597799,5.0488818161\\H,1.2573444722
,-1.8427696928,3.5108647598\\H,1.9263342906,0.7309478334,1.9763043236\\H
,-0.3739682419,-1.3331121734,1.9071637112\\H,-1.0760109306,-2.143224920
1,-0.094764104\\H,-0.0254939609,-0.8073932836,-2.6613531976\\H,-0.629924
5239,-3.2072898444,-3.4041644419\\H,-1.8147732926,-3.2910545455,-2.0837
68736\\H,-2.061339124,-2.1872900442,-3.4523570762\\Version=EM64L-G09Rev
A.02\\State=2-A\\HF=-1231.8056949\\S2=0.775814\\S2-1=0.\\S2A=0.750181\\RMSD=
8.471e-09\\RMSF=4.014e-06\\Dipole=0.4718452,-1.2703622,-0.2510946\\Quadru
pole=-1.7546315,-1.4675979,3.2222294,3.5077723,5.4095194,-0.4875185\\PG
=C01 [X(C8H11Cl2)]\\@

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DEF_9

1\1\GINC-V1286\FOpt\RB3LYP\6-31G(d)\C5H10\GXG501\03-Jun-2010\0\#B3LYP
/6-31G* OPT Freq=noraman maxdisk=268435456\def9.freq\0,1\C,-0.1378139
553,-0.2019140253,0.2053691094\C,-0.0954926993,0.3073103121,1.41790318
47\C,1.4051202109,-0.0237014837,-0.5868240095\C,2.1108068135,-1.355855
5862,-0.8930372166\C,-1.3574670282,0.1202067814,2.2114140336\H,-1.8346
581143,1.0838594113,2.436848225\H,-2.0835255213,-0.4979147021,1.672221
4389\H,-1.1541990671,-0.3612630532,3.1778675262\H,0.6806567393,0.91490
55403,1.8883169342\H,-0.6360703838,-0.813376526,-0.2658997622\H,1.1745
262533,0.4781662511,-1.5388436004\H,2.0884234247,0.6416126864,-0.04338
4182\H,1.4514598217,-2.0341026136,-1.4482805501\H,3.0109254571,-1.1962
037018,-1.497842991\H,2.4060920275,-1.863797556,0.0318190815\Version=
EM64L-G09RevA.02\State=1-A\HF=-196.5404425\RMSD=3.751e-09\RMSF=3.972e-
06\Dipole=-0.0036305,0.007438,0.0145107\Quadrupole=0.1739205,-0.748147
2,0.5742267,0.5450247,-0.2823576,0.6092877\PG=C01 [X(C5H10)]\@

DEF_900

1\1\GINC-V1281\FOpt\UB3LYP\6-31G(d)\C5H9O2(2)\GXG501\03-Jun-2010\0\#B
3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def9oo.freq\0,2\C,-0.
0267703311,-0.0115246507,-0.0674092626\C,0.0390218094,0.3239761708,1.2
239288106\C,1.1273141607,0.0042116064,-1.0304484324\C,1.3958101514,-1.
3776000683,-1.6516038975\C,-1.1342550053,0.3089921575,2.1483260174\H,-
1.3226259449,1.2821472871,2.6119390699\H,-2.0418892502,-0.0600594126,1.
6627026644\H,0.9817257816,0.6415319162,1.6681361421\H,-0.9859515056,-
0.3334690934,-0.4803062272\H,0.9129719371,0.7197690096,-1.8382063322\H
,2.0284296484,0.3680339158,-0.5216656486\H,0.5128646462,-1.7519130268,
-2.1833461435\H,2.2221786434,-1.3281906447,-2.3691026928\H,1.656398162
4,-2.1100105805,-0.8800499512\O,-0.9180448177,-0.631530403,3.261272912
2\O,-0.0858244346,-0.1225072205,4.1529788333\Version=EM64L-G09RevA.02
\State=2-A\HF=-346.2439468\S2=0.753045\S2-1=0.\S2A=0.750006\RMSD=7.974
e-09\RMSF=9.157e-06\Dipole=-0.1895536,0.3371323,-1.2032468\Quadrupole=
3.3951185,0.5677715,-3.96289,-0.6136367,-0.3825166,1.5016596\PG=C01 [X
(C5H9O2)]\@

DEF_900H

1\1\GINC-V1292\FOpt\RB3LYP\6-31G(d)\C5H10O2\GXG501\03-Jun-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\def9ooh.freq\0,1\C,-0.0
471106565,0.0266979262,0.0299519091\C,-0.0781594855,0.0224517369,1.366
4785846\C,1.191076778,-0.0597224494,-0.8190958981\C,1.1806721325,-1.27
41843106,-1.7633990348\C,-1.3399204761,0.0915589937,2.1786489787\H,-1.
2650133289,0.846158083,2.9726543032\H,-2.2114067388,0.3194991977,1.553
2810086\H,0.8522609898,-0.0570843218,1.9313375311\H,-0.9930801676,0.09
76335908,-0.5123782441\H,1.2762800108,0.8553449587,-1.424027602\H,2.07
97637177,-0.0922579781,-0.1764088808\H,0.3060615341,-1.2549239404,-2.4
244136869\H,2.0766022103,-1.2875195462,-2.3937469138\H,1.1495980801,-2
.2120343261,-1.1974889091\O,-1.582947321,-1.113291555,2.9183625925\O,-
1.9790440407,-2.1314777567,1.9650506536\H,-1.1091888361,-2.4790670188,
1.6913072517\Version=EM64L-G09RevA.02\State=1-A\HF=-346.8759732\RMSD=
7.963e-09\RMSF=1.176e-06\Dipole=0.8232135,0.3710077,-0.7254031\Quadrup
ole=-1.1026243,1.7435069,-0.6408826,-2.6960589,2.3643582,1.8984526\PG=
C01 [X(C5H10O2)]\@

DEF_9R

1\1\GINC-V1280\FOpt\UB3LYP\6-31G(d)\C5H9(2)\GXG501\03-Jun-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\def9r.freq\0,2\C,-0.084
1423406,-0.0500099671,-0.1231504495\C,-0.1325785936,0.083354231,1.2583
437993\C,1.16673782,0.0049734486,-0.9463293649\C,1.4230126252,-1.28833
41034,-1.7442510999\C,-1.2818170025,0.0286387809,2.0304163372\H,-1.247
2435346,0.1414849712,3.1088058987\H,-2.2575930854,-0.1292632337,1.5785

421251\H,0.8153398473,0.2462080893,1.7750708973\H,-1.0195656019,-0.218
3191734,-0.6593578688\H,1.1039791301,0.8431181895,-1.6590685251\H,2.02
79041501,0.2159020096,-0.2990529262\H,0.5835582364,-1.5112106774,-2.41
34784339\H,2.3263737884,-1.1973104257,-2.3583934482\H,1.5500271588,-2.
144580683,-1.072863335\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-195.894
1106\\S2=0.779724\\S2-1=0.\\S2A=0.75018\\RMSD=9.954e-09\\RMSF=4.147e-06\\Dip
ole=0.1082432,-0.0065201,-0.1335189\\Quadrupole=0.8052098,-1.6888634,0.
8836536,0.3653892,0.2870256,0.0777492\\PG=C01 [X(C5H9)]\\@

DEF_10

1\1\GINC-V1308\FOpt\RB3LYP\6-31G(d)\C5H10\GXG501\03-Jun-2010\0\#B3LYP
/6-31G* OPT Freq=noraman maxdisk=268435456\\def10.freq\\0,1\C,-0.05615
50782,-0.2476183898,0.1083636456\C,0.1390129795,0.4735668201,1.2129795
152\C,1.3199083994,0.349411263,2.1366968594\C,0.9249192975,-0.05235239
69,3.5707938856\C,2.1255737122,-0.1349555459,4.5183262747\H,-0.9363022
016,-0.1159666466,-0.5156092337\H,0.6618614058,-0.9979960881,-0.217653
7468\H,-0.6110653833,1.2133746597,1.5003915866\H,1.853009038,1.3123511
028,2.179337422\H,2.0311632906,-0.3828856791,1.7315454662\H,0.19677762
43,0.6722111906,3.9616151986\H,0.4067490323,-1.0197776842,3.5396708771
\H,2.6414605449,0.8305804113,4.5903394052\H,2.8562378145,-0.8746819123
,4.1687350917\H,1.8167257844,-0.4241441348,5.5292568388\\Version=EM64L
-G09RevA.02\\State=1-A\\HF=-196.5349803\\RMSD=4.405e-09\\RMSF=2.702e-06\\Di
pole=0.0402223,0.0340081,0.1305909\\Quadrupole=0.1081732,0.1984319,-0.3
06605,-0.6781895,0.1117966,0.6802471\\PG=C01 [X(C5H10)]\\@

DEF_1000

1\1\GINC-V1344\FOpt\UB3LYP\6-31G(d)\C5H9O2(2)\GXG501\04-Jun-2010\0\#B
3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\def10oo.freq\\0,2\C,0.
0564215095,-0.114949382,-0.0865959263\C,-0.0158001233,0.0032910088,1.2
385584012\C,1.1816349361,0.0258752055,2.141522964\C,1.2607822762,-1.16
23989606,3.102872858\C,2.5125563851,-1.1569674432,3.9861998471\H,-0.83
63989554,-0.1554095607,-0.7043498958\H,1.0096815718,-0.1817374814,-0.6
072706589\H,-0.978143042,0.0737511492,1.7422576378\H,2.1052328375,0.11
96971613,1.560121672\H,0.3559189588,-1.1608007877,3.7207865875\H,1.229
1802601,-2.07343388,2.4924169971\H,2.5462514186,-0.2651986292,4.619422
7073\H,3.4277719953,-1.1767433931,3.382022798\H,2.5253478102,-2.035458
7188,4.6398963375\O,1.1901318386,1.2986798251,2.9134362264\O,0.1605759
237,1.381902473,3.7374651812\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-3
46.2429422\\S2=0.753295\\S2-1=0.\\S2A=0.750007\\RMSD=3.997e-09\\RMSF=7.697e
-06\\Dipole=0.2370645,-0.8416219,-0.6249694\\Quadrupole=1.3344871,-2.561
3898,1.2269027,0.2491474,0.8328409,-1.6187257\\PG=C01 [X(C5H9O2)]\\@

DEF_1000H

1\1\GINC-V1485\FOpt\RB3LYP\6-31G(d)\C5H10O2\GXG501\04-Jun-2010\0\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\\def10ooh.freq\\0,1\C,-0.
0191873837,-0.0056023135,-0.0004091256\C,-0.0227200495,-0.0896848295,1
.3297723369\C,1.214108902,-0.0270530499,2.1876856985\C,1.4506381997,-1
.3138397775,2.9912879675\C,2.7267184039,-1.272528952,3.8367129332\H,-0
.9346419587,-0.0763616273,-0.5821997088\H,0.9018317551,0.1320966418,-0
.5639763087\H,-0.9602917795,-0.2343068608,1.8650187488\H,2.0895782166,
0.1775253134,1.5556041763\H,0.5792520084,-1.4899816053,3.6325908573\H,
1.4910831299,-2.1473979834,2.2779894414\H,2.6910554704,-0.4487294769,4
.5551839398\H,3.6160233463,-1.1326982642,3.209370008\H,2.8548248373,-2
.2077645983,4.3927013281\O,1.2215641061,1.1433513922,3.0335937775\O,0.
1067413253,1.0345535979,3.9695089902\H,-0.4514383691,1.7608554992,3.63
90022481\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-346.8732408\\RMSD=4.47
7e-09\\RMSF=9.639e-06\\Dipole=-0.3876315,-0.0827703,-0.5163545\\Quadrupol
e=1.7024846,-0.4857712,-1.2167134,-2.3821484,-0.7635482,-0.3438498\\PG=
C01 [X(C5H10O2)]\\@

DEF_10R

1\1\GINC-V1396\FOpt\UB3LYP\6-31G(d)\C5H9(2)\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def10r.freq\0,2\C,0.1109986632,0.0155263505,-0.0613851028\C,-0.0612992721,0.06399487,1.3126113737\C,0.9526892494,-0.0466066314,2.2550891506\C,0.7539500409,0.0136876546,3.7390841025\C,-1.5288929256,1.1664171493,4.40672779\H,-0.7282110464,0.1084639889,-0.7425139415\H,1.0956649335,-0.117923065,-0.5017191676\H,-1.0771100867,0.198692432,1.6895165073\H,1.9763433306,-0.1769398018,1.9001239053\H,-0.3158195454,0.1078129576,3.9666589373\H,1.08419476,-0.933502652,4.195360068\H,1.1934637251,2.1369922237,4.0252638535\H,2.6043211174,1.0843401776,4.2094147345\H,1.3857159236,1.1571102192,5.4934339242\Version=EM64L-G09RevA.02\State=2-A\HF=-195.8941106\S2=0.779726\S2-1=0\S2A=0.75018\RMSD=9.953e-09\RMSF=5.934e-06\Dipole=0.0313177,0.0048393,0.1690543\Quadrupole=1.0796142,-1.6486179,0.5690037,-0.4910775,-0.0460639,-0.1260803\PG=C01 [X(C5H9)]\@

DEF_11

1\1\GINC-V1400\FOpt\RB3LYP\6-31G(d)\C6H12\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def11.freq\0,1\C,0.0397716302,0.4172846559,-0.0273176065\C,0.1360141464,0.5042146356,1.4716843748\C,1.0162103185,-0.1547583259,2.2301487363\C,-1.3155325962,-0.1279415041,-0.517253242\C,-1.4255536897,-0.1712000044,-2.044389979\C,1.1044298683,-0.0749585165,3.7278285708\H,0.9695005217,-1.0628968959,4.1892745974\H,2.0892168537,0.2890299854,4.0517308801\H,0.3439366515,0.5970636049,4.1402665537\H,1.7422651008,-0.8081468164,1.7415369057\H,-0.5927128686,1.1565236673,1.9595386096\H,0.8504666809,-0.2148872786,-0.4147870476\H,0.1899446086,1.4169058765,-0.4652883106\H,-1.4652179989,-1.1337881346,-0.1031851807\H,-2.1239846075,0.4940276684,-0.1077436045\H,-1.3092635829,0.829428046,-2.4790210803\H,-2.3981916766,-0.5623336143,-2.3639897619\H,-0.6493019504,-0.8123794648,-2.4801558312\Version=EM64L-G09RevA.02\State=1-A\HF=-235.8543394\RMSD=4.967e-09\RMSF=1.523e-05\Dipole=-0.0083544,-0.0170506,0.0154147\Quadrupole=-0.0444341,-0.2287752,0.2732093,-0.9508033,0.2637253,-0.043382\PG=C01 [X(C6H12)]\@

DEF_1100

1\1\GINC-V1467\FOpt\UB3LYP\6-31G(d)\C6H11O2(2)\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def1100.freq\0,2\C,-0.0219576529,0.1123763622,0.1262488709\C,-0.0206998895,0.098051862,1.6225951445\C,1.0882891386,0.0701629383,2.3671380787\C,-0.7942766932,1.2751861559,-0.5023377766\C,-0.1233673406,2.6312973401,-0.2627557969\C,1.1258264818,0.0800716379,3.8667042273\H,0.1195148782,0.1050411594,4.2969860933\H,1.6410026734,-0.8104200474,4.2504217802\H,1.6813303629,0.9496535659,4.2424108428\H,2.056027862,0.0399884615,1.8631731527\H,-1.0000345551,0.1258761711,2.1022736074\H,0.9964555035,0.0640370583,-0.2729490513\H,-0.8712735252,1.0734583897,-1.5763396071\H,-1.8156110882,1.2788987323,-0.0993824444\H,-0.0446512351,2.8585818586,0.8057869972\H,-0.698605364,3.4331439613,-0.7374458954\H,0.8889275373,2.6536837563,-0.6842211398\O,-0.6726465354,-1.160516801,-0.2889701891\O,-0.4915152187,-1.3976208606,-1.575483415\Version=EM64L-G09RevA.02\State=2-A\HF=-385.5635146\S2=0.753147\S2-1=0\S2A=0.750007\RMSD=8.176e-09\RMSF=3.615e-06\Dipole=0.4106556,0.8931337,0.8969923\Quadrupole=2.2945747,-2.5973663,0.3027916,-1.7231936,-0.0755456,-3.4429793\PG=C01 [X(C6H11O2)]\@

DEF_1100H

1\1\GINC-V1298\FOpt\RB3LYP\6-31G(d)\C6H12O2\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def1100h.freq\0,1\C,0.0743034944,0.0376403759,-0.1245190997\C,0.0576938455,0.0141093684,1.3809475273\C,1.1465032379,-0.1016958183,2.148260571\C,-0.7847149013,1.1551910154,-0.7288426961\C,-0.251526716,2.5558193571,-0.4097175809\C,1.15

44886379,-0.1481911506,3.6489319088\H,0.1413707146,-0.0958309091,4.061
1859454\H,1.6265277761,-1.069843133,4.014741623\H,1.7357345568,0.68534
15442,4.0654766613\H,2.1215037128,-0.1578509631,1.6605639515\H,-0.9301
676764,0.0670644514,1.8444052278\H,1.1066797135,0.1132135912,-0.491284
4133\H,-0.820743547,1.0003341681,-1.8133751193\H,-1.8135287298,1.04892
56379,-0.3605988763\H,-0.2214933173,2.7387516125,0.6699013994\H,-0.886
9358344,3.3231982355,-0.864511719\H,0.7650726626,2.6912094522,-0.79793
36647\O,-0.4974327065,-1.1797654183,-0.6490891721\O,0.4289588679,-2.26
07722808,-0.3809570962\H,0.2020815126,-2.4769177932,0.5438486774\Vers
ion=EM64L-G09RevA.02\State=1-A\HF=-386.195101\RMSD=4.065e-09\RMSF=7.46
0e-06\Dipole=0.1545813,0.5319576,0.9817742\Quadrupole=0.8528027,-0.935
4076,0.0826049,-0.5151681,0.2734815,-4.6835052\PG=C01 [X(C6H12O2)]\@

DEF_11R

1\1\GINC-V1280\FOpt\UB3LYP\6-31G(d)\C6H11(2)\GXG501\13-Jun-2010\0\#UB
3LYP\6-31G* OPT=tight SCF=tight Freq=noraman INT(grid=ultrafine) maxdi
sk=268435456\def11r.freq\0,2\C,-0.2442273366,0.6328870105,0.17073862
6\C,-0.0896039991,0.1796522711,1.4735167972\C,1.0652513577,0.286811597
.2.2364596802\C,-1.4993983272,0.5007553548,-0.6379930483\C,-1.30366194
19,-0.311330901,-1.9329534784\C,1.2041774277,-0.2108920739,3.640483030
9\H,2.0077998065,-0.9572462461,3.7298596837\H,1.4632218825,0.601323478
2,4.3362081955\H,0.2775553248,-0.6736964545,3.997930865\H,1.9376000733
.0.7652942246,1.7907039586\H,-0.952530498,-0.302234597,1.9401175477\H,
0.6061684924,1.1131007282,-0.3161497516\H,-2.2857992626,0.0369789906,-
0.0282402015\H,-1.8725240631,1.5009554843,-0.9122304267\H,-0.533237505
1,0.1411528044,-2.5686556562\H,-2.2328188734,-0.3561155121,-2.51308946
56\H,-0.9898004091,-1.336772454,-1.7089240608\Version=EM64L-G09RevA.0
2\State=2-A\HF=-235.2139722\S2=0.778427\S2-1=0.\S2A=0.750174\RMSD=6.10
9e-09\RMSF=3.011e-07\Dipole=-0.0021591,-0.0104749,0.0241917\Quadrupole
=0.6072064,-1.2508733,0.6436669,0.6229834,0.6075144,-0.9390965\PG=C01
[X(C6H11)]\@

DEF_12

1\1\GINC-V1486\FOpt\RB3LYP\6-31G(d)\C7H14\GXG501\04-Jun-2010\0\#B3LYP
/6-31G* OPT Freq=noraman maxdisk=268435456\def12.freq\0,1\C,-0.02186
26585,0.0053345072,0.0056589455\C,-0.0095187167,-0.007408837,1.5204124
077\C,1.3439506916,0.0172936339,2.1904848419\C,-1.1411783762,-0.059661
6974,2.231650143\C,0.526074339,1.2957718985,-0.6532618106\C,-0.3023039
781,2.5285877484,-0.2680071705\C,0.5870900606,1.1276786847,-2.17823715
58\H,-2.1167994279,-0.0860458531,1.7521626479\H,-1.1350159414,-0.08170
46849,3.3190194084\H,1.9676944328,-0.8198809138,1.8474918841\H,1.89759
6162,0.935209781,1.9531689375\H,1.2551023268,-0.0480173707,3.279244194
1\H,-0.3460747288,2.6621937068,0.817914251\H,0.1204249122,3.4395866229
,-0.7080311042\H,1.5545852658,1.45149108,-0.2959322802\H,0.5776102223,
-0.8431233509,-0.359862156\H,1.2109407763,0.2718213744,-2.4631983537\H
1.0028860673,2.0213025924,-2.6586573238\H,-1.334423052,2.4318838664,-
0.6304647528\H,-1.047453098,-0.1607096445,-0.3511025858\H,-0.415220292
1,0.9631946985,-2.595045715\Version=EM64L-G09RevA.02\State=1-A\HF=-27
5.1675751\RMSD=2.775e-09\RMSF=4.550e-06\Dipole=0.183917,0.0124937,-0.0
749498\Quadrupole=0.69376,-0.9007786,0.2070186,-0.0855711,0.5027286,0.
0966622\PG=C01 [X(C7H14)]\@

DEF_120O

1\1\GINC-V1467\FOpt\UB3LYP\6-31G(d)\C7H13O2(2)\GXG501\07-Jun-2010\0\#
B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\def12oo.freq\0,2\C,0
.0481600877,0.0078751122,0.0018118709\C,0.0212485219,0.0109005797,1.51
43420667\C,1.3385719862,0.0928261028,2.2433111766\C,-1.1125461729,-0.0
557931123,2.2217255761\C,0.5980605472,1.294945511,-0.6611126575\C,-0.2
388408708,2.5297507467,-0.3011276837\C,0.6751951121,1.1056139481,-2.18
26415951\H,-2.0843384469,-0.0905399745,1.735907468\H,-1.1141754348,-0.

073565222,3.3090062697\H,1.202054992,0.0487821162,3.3267951691\H,1.9283680207,0.9728398082,1.9739610314\H,-0.2856294115,2.691382144,0.7815794495\H,0.1781863495,3.434187313,-0.7592230306\H,1.6232708595,1.4482029682,-0.2977754889\H,0.6618321034,-0.8374724752,-0.3374019409\H,1.310047175,0.25180101,-2.4461802106\H,1.090744578,1.9956556522,-2.6694300587\H,-1.270253927,2.4199348714,-0.6623408492\H,-0.9701971133,-0.1749214809,-0.3660569612\H,-0.3209124058,0.9283833671,-2.6092531744\O,2.1852617963,-1.0702589619,1.9405630085\O,2.9522343624,-0.8556095044,0.884398794\Version=EM64L-G09RevA.02\State=2-A\HF=-424.8706376\S2=0.753238\S2-1=0.\S2A=0.750007\RMSD=6.490e-09\RMSF=6.306e-06\Dipole=-0.707318,0.5891658,0.3021999\Quadrupole=-1.5618408,-2.0847788,3.6466196,3.1220324,-0.1885093,0.7528812\PG=C01 [X(C7H13O2)]\@

DEF_12OOH

1\1\GINC-V1403\FOpt\RB3LYP\6-31G(d)\C7H14O2\GXG501\08-Jun-2010\0\#B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\def12ooh.freq\0,1\C,0.0327564064,0.0531823566,-0.076671433\C,0.0561116163,0.0080803762,1.4361574614\C,1.407857846,-0.191718913,2.0868209721\C,-1.0496980496,0.0745813085,2.1869974574\C,0.5688985273,1.3671604727,-0.7011928507\C,-0.3015923605,2.5752133161,-0.3307351944\C,0.683940098,1.2173496317,-2.2249819618\H,-2.0375919852,0.1843074513,1.7449581486\H,-1.005087144,0.0293305688,3.2726010934\H,1.3723995434,-0.0117087882,3.1666697409\H,2.1733576154,0.455740757,1.641172517\H,-0.3812951611,2.6992331564,0.7542121233\H,0.113469924,3.499706654,-0.7488315741\H,1.5812426818,1.5446857777,-0.3081705532\H,0.6396652091,-0.780744262,-0.4567171841\H,1.3415125226,0.3834712149,-2.4976621864\H,1.0881679384,2.1282791188,-2.681595598\H,-1.3186350538,2.4586929919,-0.7284782205\H,-0.9926837589,-0.110644023,-0.4343674737\H,-0.2994422203,1.0289123077,-2.6752524239\O,1.9265309563,-1.5068085401,1.8404207395\O,1.1720207639,-2.4310562386,2.6636421142\H,0.3953352943,-2.6015819611,2.0971650228\Version=EM64L-G09RevA.02\State=1-A\HF=-425.5026795\RMSD=5.106e-09\RMSF=2.818e-06\Dipole=-0.6775926,0.5463494,-0.405345\Quadrupole=0.7175911,-0.8768093,0.1592182,4.6590797,-2.0230296,2.6697521\PG=C01 [X(C7H14O2)]\@

DEF_12R

1\1\GINC-V1456\FOpt\UB3LYP\6-31G(d)\C7H13(2)\GXG501\07-Jun-2010\0\#B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\def12r.freq\0,2\C,0.0640208864,0.0198859862,0.026964831\C,0.0542359317,0.0508196606,1.5495594164\C,1.2685114372,-0.0035961379,2.2310503166\C,-1.151719902,0.1379243021,2.2312649938\C,0.547244237,1.3312548147,-0.6380976295\C,-0.3858017127,2.5104437555,-0.3317618327\C,0.7053998708,1.135107638,-2.1525629198\H,-2.1014907711,0.1716929857,1.706812216\H,-1.1836806996,0.1703147129,3.3168957208\H,1.3078931912,0.0356617307,3.3157742285\H,2.2141639388,-0.0921785917,1.704707014\H,-0.4852881503,2.6765902936,0.7457698877\H,-0.0092423449,3.4355733908,-0.7840623963\H,1.5377637674,1.5665103559,-0.2210729192\H,0.7155731237,-0.7985177588,-0.3075856275\H,1.4067796484,0.3237213787,-2.3818257959\H,1.0785840249,2.0473345105,-2.6329072934\H,-1.3904301207,2.3281513157,-0.7366446713\H,-0.9429648565,-0.2139773295,-0.3435184719\H,-0.2566277746,0.885270734,-2.6192233817\Version=EM64L-G09RevA.02\State=2-A\HF=-274.5185747\S2=0.781991\S2-1=0.\S2A=0.750195\RMSD=9.673e-09\RMSF=5.937e-06\Dipole=0.04092,0.0110287,-0.0740489\Quadrupole=1.0317435,-1.5390458,0.5073023,-0.0386565,0.0317268,0.1819025\PG=C01 [X(C7H13)]\@

DEF_13OO

1\1\GINC-V1468\FOpt\UB3LYP\6-31G(d)\C7H13O2(2)\GXG501\07-Jun-2010\0\#B3LYP\6-31G* OPT Freq=noraman maxdisk=268435456\def13oo.freq\0,2\C,0.1102172705,0.1315765421,0.0642850443\C,0.0986910002,-0.0516058162,1.5648849082\C,1.0093186743,0.8322508022,2.3811368795\C,-0.7130274111,-0.9590475955,2.1157777902\C,1.4671766824,-0.0730515661,-0.6335134673\C,1

.3461201458,0.1471448392,-2.1494882886\C,2.0281034227,-1.4694865486,-0.3237186372\H,-1.3788037342,-1.5731829034,1.5151798538\H,-0.7427299907,-1.1186094422,3.1908228477\H,2.0675560462,0.6458160315,2.1562545901\H,0.8199346036,1.8907171932,2.1662722122\H,0.8589380524,0.6673442264,3.4518916493\H,0.9659426115,1.1453383615,-2.3832247857\H,2.3237647041,0.0320597685,-2.6307325002\H,2.1622509587,0.6776924105,-0.2327811246\H,-0.6564767817,-0.4963613076,-0.3994253052\H,2.1650901692,-1.6308127787,0.7499546855\H,2.9973644363,-1.6045169441,-0.8160434722\H,0.6657336624,-0.5885024828,-2.5976216663\H,1.3554571027,-2.2532088635,-0.6944922267\O,-0.2843653914,1.53063548,-0.2435690122\O,-1.5904831822,1.7049487337,-0.1502328864\Version=EM64L-G09RevA.02\State=2-A\HF=-424.8747596\S2=0.75314\S2-1=0.\S2A=0.750007\RMSD=8.050e-09\RMSF=3.185e-06\Dipole=0.7883616,-0.7576438,0.19242\Quadrupole=-1.2572398,-1.4893422,2.7465821,3.2267174,-0.6437105,1.0550073\PG=C01 [X(C7H13O2)]\@

DEF_13OOH

1\1\GINC-V1455\FOpt\RB3LYP\6-31G(d)\C7H14O2\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def13ooh.freq\0,1\C,0.0084652085,0.0272924831,-0.0435426074\C,0.0140637515,0.0439249766,1.477151426\C,1.3554875478,-0.0539398145,2.1641450414\C,-1.1280576432,0.2134808007,2.1531685414\C,0.7413819513,-1.164178075,-0.6941557442\C,0.690761708,-1.0711674995,-2.2266445441\C,0.1458625545,-2.4936584604,-0.2049181875\H,-2.0848569152,0.2954194052,1.6429892892\H,-1.1510847539,0.2626637534,3.2396465428\H,1.8003513492,-1.0496712787,2.0397923331\H,2.0644489341,0.663941118,1.7347897882\H,1.2684926646,0.1416210358,3.2372267387\H,1.121743107,-0.1329437858,-2.5836222989\H,1.243853943,-1.902743785,-2.6784264791\H,1.7945823935,-1.1189349411,-0.3843587572\H,-1.0260208576,0.0556869202,-0.4089522365\H,0.2002657166,-2.5994900647,0.8835277079\H,0.6808369872,-3.3376258342,-0.65451381\H,-0.3450465021,-1.1257410166,-2.5858558384\H,-0.9094576779,-2.5779566649,-0.4936308852\O,0.6783597203,1.2118742654,-0.5253535473\O,-0.2074414563,2.34116917,-0.3316445553\H,-0.0869480073,2.5207005112,0.6212701371\Version=EM64L-G09RevA.02\State=1-A\HF=-425.507033\RMSD=6.288e-09\RMSF=8.652e-06\Dipole=-0.0101972,-0.5151898,0.7680403\Quadrupole=0.6279111,-1.3162194,0.6883083,-0.5601473,0.0942514,4.1292598\PG=C01 [X(C7H14O2)]\@

DEF_13R

1\1\GINC-V1438\FOpt\UB3LYP\6-31G(d)\C7H13(2)\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def13r.freq\0,2\C,0.7246904337,-0.7333185805,0.6555939931\C,0.0560417559,-0.0872734881,1.701300033\C,0.4396237859,1.3254650896,2.1091753759\C,-0.9688469739,-0.7256129335,2.384241795\C,1.8487647752,-0.1926004566,-0.1834069944\C,1.4364294081,-0.1193219818,-1.6692893678\C,3.1182651267,-1.0554260315,-0.0192198608\H,-1.2741230941,-1.7354738535,2.1246674622\H,-1.4998494541,-0.242231825,3.1981563455\H,1.4865260096,1.3835574535,2.4303640727\H,0.3167910811,2.0331534812,1.2805557956\H,-0.1816852369,1.6750946154,2.9388138767\H,0.5651873079,0.5299522331,-1.8084654742\H,2.2566266221,0.2708847272,-2.2845166335\H,2.0907788278,0.8251469115,0.147217894\H,0.4025159353,-1.7471389024,0.4108058021\H,3.4516124315,-1.0775484588,1.0240310644\H,3.9392143943,-0.6649862267,-0.6332788646\H,1.17591745,-1.114618852,-2.050889444\H,2.9292141626,-2.0901820458,-0.3317319634\Version=EM64L-G09RevA.02\State=2-A\HF=-274.5231781\S2=0.780205\S2-1=0.\S2A=0.750185\RMSD=7.743e-09\RMSF=4.105e-06\Dipole=0.1471836,0.1261907,-0.0784244\Quadrupole=-0.5464774,0.8002621,-0.2537847,0.3912225,-0.6713269,0.8582511\PG=C01 [X(C7H13)]\@

DEF_14

1\1\GINC-V1322\FOpt\RB3LYP\6-31G(d)\C7H14\GXG501\04-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def15.freq\0,1\C,0.1500377062,-0.4244254562,0.1060346519\C,0.006646306,0.0085812727,1.367977980

3\C,1.0577315756,0.7540794349,2.155268184\C,-1.2792446648,-0.231434076
 2,2.1251787897\C,1.3341831697,-0.2934838471,-0.821481015\C,0.949888104
 3,0.5163257274,-2.0750968457\C,1.8668306769,-1.684955398,-1.215344345\
 H,-2.0146170323,-0.7730495796,1.5218435142\H,-1.0973458163,-0.81151269
 93,3.0411645852\H,-1.7338838923,0.7171112181,2.4448109062\H,0.67808894
 25,1.7345206094,2.4757340119\H,1.3130413472,0.2074908162,3.0740356146\
 H,1.9824822294,0.9203099565,1.5980206211\H,0.1328975427,0.0272312699,-
 2.6211666536\H,0.6151467543,1.5246304035,-1.8078831044\H,1.801118081,0
 .6078754307,-2.7609436237\H,2.1444204761,0.2426347698,-0.3127853917\H,
 1.0904571997,-2.2713037957,-1.7235865591\H,2.187471131,-2.2503268369,-
 0.3334893932\H,2.7212136008,-1.6005816837,-1.8981664354\H,-0.698482540
 4,-0.9514376347,-0.3386346955\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-
 275.1710521\\RMSD=8.608e-09\\RMSF=7.393e-06\\Dipole=0.0383867,0.0535755,0
 .0960843\\Quadrupole=0.1936152,-0.6797142,0.4860991,0.4554376,-0.189311
 3,0.53178\\PG=C01 [X(C7H14)]\\@

DEF_1400

1\1\GINC-V1419\FOpt\UB3LYP\6-31G(d)\C7H13O2(2)\GXG501\07-Jun-2010\0\#
 B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl6oo.freq\\0,2\C,0
 .0249633693,0.3627934982,0.0221631486\C,0.0060277007,-0.003176143,1.31
 41793612\C,1.1411110588,-0.6539539571,2.0664119745\C,-1.2293723408,0.2
 420970913,2.1486172572\C,1.1354264769,0.2165842533,-0.9954423483\C,0.8
 813037157,1.1061054591,-2.2141823234\C,1.4083602551,-1.233770903,-1.40
 38164396\H,-2.0373937318,0.6966951057,1.5675038474\H,-1.6025601014,-0.
 6975230896,2.5789201158\H,-1.0040085136,0.9039113242,2.9961322682\H,1.
 4126513331,-0.0439979671,2.9385470731\H,0.8257859796,-1.6310630979,2.4
 582194014\H,2.0408193619,-0.7890150654,1.4673382202\H,-0.0107943001,0.
 7620981159,-2.7483312085\H,0.721407409,2.1446099362,-1.9065428389\H,1.
 7363748346,1.0658609231,-2.8931988214\H,0.5341102978,-1.6346180087,-1.
 9268571547\H,1.5980809543,-1.8639883199,-0.5309635901\H,2.2727024062,-
 1.2797327449,-2.0720790571\H,-0.873214458,0.8334860856,-0.3758750551\O
 ,2.3715353119,0.7563378086,-0.3178384147\O,3.4452449377,0.6762133843,-
 1.0800045513\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-424.880649\\S2=0.7
 53311\\S2=1-O\\S2A=0.750007\\RMSD=5.411e-09\\RMSF=1.553e-06\\Dipole=-1.043
 2194,-0.3635771,0.098591\\Quadrupole=-3.477987,0.2881589,3.1898281,-1.8
 166282,0.7616945,-0.3905387\\PG=C01 [X(C7H13O2)]\\@

DEF_1400H

1\1\GINC-V1435\FOpt\RB3LYP\6-31G(d)\C7H14O2\GXG501\08-Jun-2010\0\#B3L
 YP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl6oo.h.freq\\0,1\C,0.0
 287292788,0.0368265223,0.001084377\C,0.0125567264,0.0133503244,1.34363
 5206\C,1.2249301336,-0.0095165184,2.242272301\C,-1.3071357153,0.012018
 3012,2.0802289451\C,1.2198191924,0.0242120628,-0.9472271489\C,0.758207
 8525,0.3884529979,-2.36576632\C,1.9528594176,-1.3263021732,-0.94154628
 52\H,-2.1626048702,0.0055500295,1.397671591\H,-1.3866638557,-0.8652133
 982,2.7374285149\H,-1.3950110883,0.8942947593,2.7293828388\H,1.1825701
 646,0.8285668371,2.9515303695\H,1.2325379113,-0.9264112832,2.848671015
 \H,2.162063753,0.0668284313,1.6930638133\H,0.0548407756,-0.360376963,-
 2.7460078998\H,0.2547961864,1.3618742324,-2.3644656165\H,1.6121310305,
 0.4298326965,-3.0474280844\H,1.2795835854,-2.1176814389,-1.2884621197\
 H,2.2895366405,-1.5840306676,0.0659890593\H,2.822788082,-1.2920528607,
 -1.603719278\H,-0.934517839,0.0605265345,-0.5076086545\O,2.0849791378,
 1.0776939896,-0.4363820648\O,3.2957481891,1.1407747768,-1.2536953955\H
 ,3.1498602628,1.9979506759,-1.6916304511\\Version=EM64L-G09RevA.02\\Sta
 te=1-A\\HF=-425.5099653\\RMSD=3.212e-09\\RMSF=1.255e-05\\Dipole=-0.4661226
 ,0.077819,-0.2644997\\Quadrupole=-2.5991212,0.3155687,2.2835525,1.08699
 51,-1.2679781,-2.1154006\\PG=C01 [X(C7H14O2)]\\@

DEF_14R

1\1\GINC-V1432\FOpt\UB3LYP\6-31G(d)\C7H13(2)\GXG501\07-Jun-2010\0\#B3

LYP/6-31G* OPT Freq=norman maxdisk=268435456\\defl6r.freq\\0,2\C,0.32
 26117057,0.5668661005,-0.2462031082\C,0.0287195331,0.4527170927,1.1138
 068705\C,0.0564112497,-0.8202426718,1.9207867814\C,-0.3604873096,1.684
 7746327,1.8878910697\C,0.5988336561,-0.3781422377,-1.2359901987\C,1.01
 65235148,0.0913610819,-2.6048364249\C,0.5248308425,-1.8751159016,-1.07
 47039143\H,-0.3672316628,2.5830259778,1.2621796005\H,-1.3643224184,1.5
 796261644,2.3290733159\H,0.3230941066,1.8633225898,2.7321915226\H,0.33
 30623432,-0.6035710072,2.9607780401\H,-0.9311611476,-1.3073656281,1.96
 10111197\H,0.7679958935,-1.5544230142,1.5364624336\H,0.3299436688,-0.2
 746899826,-3.3836945183\H,1.0563660646,1.1831190766,-2.6747806777\H,2.
 0122235032,-0.2953705893,-2.8739228945\H,0.2442424323,-2.3452701231,-2.
 0261689922\H,-0.2045009373,-2.188493979,-0.324399488\H,1.4968931221,-
 2.3103961607,-0.7921616545\H,0.3398142228,1.5974877382,-0.6064288304\\
 Version=EM64L-G09RevA.02\State=2-A\HF=-274.5306164\S2=0.777552\S2-1=0.
 \S2A=0.750172\RMSD=3.013e-09\RMSF=1.332e-06\Dipole=-0.0019858,-0.11949
 92,0.04177\Quadrupole=-1.1813551,0.384398,0.7969571,-0.1929036,-0.6236
 367,0.1773989\PG=C01 [X(C7H13)]\\@

DEF_1500

1\1\GINC-V1434\FOpt\UB3LYP\6-31G(d)\C7H13O2(2)\GXG501\07-Jun-2010\0\\#
 B3LYP/6-31G* OPT Freq=norman maxdisk=268435456\\defl5oo.freq\\0,2\C,0
 .039717721,0.0022952915,0.0016143514\C,0.0812408107,0.0062136443,1.344
 282806\C,1.325914311,0.0185345583,2.1958987297\C,-1.2166463597,0.00697
 83302,2.1070827977\C,1.1813625038,0.0237300462,-0.982691567\C,1.093651
 3962,1.274681482,-1.8784523805\C,1.1742955101,-1.2614571584,-1.8340475
 755\H,-1.2618601087,0.7847722929,2.8750722897\H,-2.0826808081,0.073112
 9305,1.4434848939\H,1.3636565265,0.924908397,2.8151165586\H,1.32600221
 82,-0.8291405996,2.8910438408\H,2.2425227532,-0.0257786933,1.604004523
 5\H,0.1542660656,1.2867296403,-2.4458340244\H,1.1379356834,2.193759035
 1,-1.2840398017\H,1.9188120045,1.2941269524,-2.6001225458\H,2.13364288
 82,0.063696,-0.4413571874\H,0.2363320108,-1.3551915342,-2.3959670684\H
 ,1.2796620872,-2.1534197122,-1.2074006809\H,1.9974913546,-1.251313479,
 -2.5582877045\H,-0.9462987593,-0.0152099763,-0.4696992042\O,-1.4101809
 995,-1.2689659143,2.8198540706\O,-0.9305240866,-1.2228906264,4.0514734
 781\\Version=EM64L-G09RevA.02\State=2-A\HF=-424.8751822\S2=0.753238\S2
 -1=0.\S2A=0.750007\RMSD=5.404e-09\RMSF=4.782e-06\Dipole=0.2537246,0.70
 23481,-0.9581621\Quadrupole=3.223128,-0.0931632,-3.1299647,-1.9640498,
 1.8501047,3.4302572\PG=C01 [X(C7H13O2)]\\@

DEF_1500H

1\1\GINC-V1435\FOpt\RB3LYP\6-31G(d)\C7H14O2\GXG501\08-Jun-2010\0\\#B3L
 YP/6-31G* OPT Freq=norman maxdisk=268435456\\defl5ooh.freq\\0,1\C,-0.
 0619239478,0.0397740602,-0.0163342308\C,-0.0811206844,0.0478857988,1.3
 264836103\C,1.1250333988,-0.0164610051,2.2326074748\C,-1.4089184557,0.
 0865423113,2.0506387461\C,1.1221164535,-0.0025821871,-0.9502288139\C,1
 .157193776,1.2662792556,-1.824676399\C,1.0710875403,-1.2679085742,-1.8
 287248211\H,-1.3901521969,0.8075053968,2.8793022611\H,-2.2368821281,0.
 3353548523,1.3776530369\H,1.2475252904,0.9265861683,2.7837991657\H,0.9
 884340212,-0.802230514,2.9856919391\H,2.057438413,-0.2141960635,1.6987
 080759\H,0.2465298875,1.3498530525,-2.4313080986\H,1.2339154487,2.1699
 828041,-1.210460191\H,2.0133788504,1.243950556,-2.5093644843\H,2.05027
 82616,-0.0335206758,-0.3669963935\H,0.1518962486,-1.293261626,-2.42762
 47524\H,1.0978968163,-2.177818905,-1.2187128775\H,1.9211604288,-1.2971
 587424,-2.520710748\H,-1.0275461855,0.0829377664,-0.5268054997\O,-1.69
 88479682,-1.1497322174,2.7206293081\O,-2.0564593689,-2.1181953465,1.70
 26174499\H,-1.1753315167,-2.4087920215,1.3984663358\\Version=EM64L-G09
 RevA.02\State=1-A\HF=-425.507085\RMSD=7.234e-09\RMSF=5.694e-06\Dipole=
 0.9028195,0.4368478,-0.5655198\Quadrupole=-1.7066635,1.6386908,0.06797
 27,-3.4312254,2.988257,2.733841\PG=C01 [X(C7H14O2)]\\@

DEF_15R

1\1\GINC-V1424\FOpt\UB3LYP\6-31G(d)\C7H13(2)\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def15r.freq\0,2\C,-0.0358884674,0.0601479198,0.0130481717\C,-0.020326958,0.0354301333,1.4120168427\C,1.295741995,-0.0087588656,2.1705445098\C,-1.2065251437,0.0508428802,2.1310324618\C,1.1466574,0.0483538564,-0.9150084987\C,1.1807428272,1.3303324934,-1.7743626877\C,1.1216459954,-1.2038966794,-1.8174468595\H,-1.2162503762,0.0321737065,3.2162210343\H,-2.1689091404,0.0822568489,1.6278195397\H,1.9218566415,0.8628985107,1.9453284937\H,1.1240155322,-0.0235449189,3.250755502\H,1.8803707182,-0.9005165131,1.9145990021\H,0.2720242692,1.4153334908,-2.3835579951\H,1.2478694087,2.2267835585,-1.1483778625\H,2.0407482981,1.3225029134,-2.4553951155\H,2.0706896603,0.0167542594,-0.3243645161\H,0.2104401783,-1.2257161159,-2.4284615229\H,1.1464245533,-2.1232453278,-1.2223239182\H,1.9816321715,-1.213022926,-2.4984902716\H,-1.0129227694,0.0915984187,-0.4727111716\Version=EM64L-G09RevA.02\State=2-A\HF=-274.523178\S2=0.780205\S2-1=0.\S2A=0.750185\RMSD=3.185e-09\RMSF=2.797e-06\Dipole=0.1959802,-0.0033733,-0.0729389\Quadrupole=0.6309495,-1.4204706,0.7895211,-0.0579631,0.5625879,-0.0517003\PG=C01 [X(C7H13)]\@

DEF_16

1\1\GINC-V1394\FOpt\RB3LYP\6-31G(d)\C6H12\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def18.freq\0,1\C,0.0053947655,-0.0206585384,-0.0307011664\C,0.0102774444,0.024840798,1.3039364044\C,1.236569094,-0.0252180138,2.1708424483\C,-1.2212036444,0.028964835,-0.9084091511\C,-1.1911363117,1.2661038557,-1.8259040025\C,-1.3555772398,-1.2615892848,-1.7389298823\H,0.9593560169,-0.1008894054,-0.5598497903\H,2.1497716905,-0.1049641586,1.5710837243\H,1.3203166862,0.8734276144,2.7973952231\H,1.2063029856,-0.8825810344,2.8572592811\H,-2.103118318,0.1087329194,-0.2568450133\H,-0.4886426131,-1.3943546799,-2.3990596297\H,-2.2522005238,-1.2310390063,-2.3699658489\H,-1.4212673259,-2.143392924,-1.0923910421\H,-0.944240304,0.1049312782,1.8286708342\H,-2.087024916,1.3087981529,-2.4572811189\H,-1.1391550568,2.1912003153,-1.2415952242\H,-0.3173226597,1.2400305708,-2.4897969345\Version=EM64L-G09RevA.02\State=1-A\HF=-235.8547738\RMSD=4.531e-09\RMSF=4.336e-06\Dipole=-0.0061736,0.0017344,0.0396238\Quadrupole=0.5421541,-1.255662,0.7135079,-0.117498,0.0040519,0.0675066\PG=C01 [X(C6H12)]\@

DEF_1600

1\1\GINC-V1472\FOpt\UB3LYP\6-31G(d)\C6H11O2(2)\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def18oo.freq\0,2\C,0.0338898243,-0.0221296147,0.0078427473\C,0.0651819897,-0.0577334255,1.3426796711\C,1.3246966772,-0.107614461,2.1446075438\C,-1.2116783095,0.0053802927,-0.8405607327\C,-1.2551054404,1.2870972682,-1.694208327\C,-1.2928924298,-1.2506795067,-1.7291464316\H,0.9780872952,-0.0181136991,-0.5437822815\H,1.3738013948,-0.9786487879,2.8051669294\H,2.2193089219,-0.0581101387,1.5176868506\H,-2.0818663939,0.0087143351,-0.169864309\H,-0.4317515873,-1.3087487463,-2.4070929627\H,-2.2001495576,-1.232651589,-2.3443024337\H,-1.3070744657,-2.1644769343,-1.1253780941\H,-0.8582626555,-0.058509654,1.9206884769\H,-2.1651256334,1.3150993131,-2.3049130106\H,-1.2366289027,2.1835589014,-1.0654555007\H,-0.3953255747,1.3351188822,-2.3745669378\O,1.4394886364,1.0696637922,3.0227761171\O,0.6411694057,0.9554904861,4.0699670919\Version=EM64L-G09RevA.02\State=2-A\HF=-385.5583026\S2=0.753046\S2-1=0.\S2A=0.750006\RMSD=4.918e-09\RMSF=4.310e-06\Dipole=-0.0500118,-0.629568,-1.0986825\Quadrupole=3.7615797,0.2747936,-4.0363733,-1.5920647,-0.8389064,-3.2589655\PG=C01 [X(C6H11O2)]\@

DEF_1600H

1\1\GINC-V1468\FOpt\RB3LYP\6-31G(d)\C6H12O2\GXG501\08-Jun-2010\0\#B3L

YP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl8ooh.freq\\0,1\\C,-0.0370559074,-0.011660089,0.0037177444\\C,-0.052459098,-0.0522846868,1.3398464012\\C,1.1806469925,0.0075844604,2.1961668349\\C,-1.2456174567,-0.0567457542,-0.8966506921\\C,-1.3371221695,1.2210852088,-1.7523637247\\C,-1.2096905174,-1.3119961839,-1.7895706625\\H,0.9285350645,0.0474903208,-0.5059489879\\H,1.1649082796,-0.7636977647,2.9772555964\\H,2.0930409207,-0.1093625346,1.599249768\\H,-2.1424620773,-0.1117379041,-0.2638547256\\H,-0.3203524706,-1.3107828331,-2.4324993474\\H,-2.091298356,-1.3518507636,-2.4401183832\\H,-1.1868376827,-2.2265540988,-1.1873601478\\H,-1.0042297851,-0.1045115726,1.8713408736\\H,-2.217653402,1.1901183559,-2.4047730244\\H,-1.4099252321,2.1160711324,-1.1245814384\\H,-0.451837711,1.3306997992,-2.3914117053\\O,1.2600373438,1.2202708196,2.9589187132\\O,1.5682939051,2.2918488418,2.0321635824\\H,0.6742752433,2.5378989497,1.7276900513\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-386.1903128\\RMSD=5.075e-09\\RMSF=1.915e-06\\Dipole=-0.7634437,-0.4679747,-0.7571898\\Quadrupole=-0.0575621,1.3403008,-1.2827387,-3.2528676,-2.8402148,-3.0112694\\PG=C01 [X(C6H12O2)]\\@

DEF_16R

1\\G\\INC-V1447\\FOpt\\UB3LYP\\6-31G(d)\\C6H11(2)\\GXG501\\08-Jun-2010\\0\\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl8r.freq\\0,2\\C,-0.165855161,-0.081141707,0.0146156777\\C,-0.046577553,-0.0926144541,1.4024009537\\C,1.063788835,-0.1546439609,2.2297835879\\C,-1.2254196719,-0.0138828681,-0.8759744299\\C,-1.2038580025,1.2614209737,-1.7443073251\\C,-1.3292383593,-1.2705757424,-1.7653144133\\H,0.9538986928,-0.1239695611,-0.4842472197\\H,2.0697750574,-0.200262524,1.8209638523\\H,0.9669758446,-0.159591845,3.3102981434\\H,-2.1199057936,0.0250767014,-0.2378348087\\H,-0.4510190726,-1.3608162287,-2.4171133818\\H,-2.2177271597,-1.222694996,-2.4067613891\\H,-1.3919800257,-2.1811278988,-1.1598924995\\H,-1.0280311242,-0.048921244,1.8787506868\\H,-2.0921977857,1.312192968,-2.3857361102\\H,-1.1768281304,2.1635972231,-1.1238783864\\H,-0.3204920266,1.2752188695,-2.3952564614\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-235.2082976\\S2=0.779603\\S2-1=0.\\S2A=0.750179\\RMSD=8.367e-09\\RMSF=1.244e-05\\Dipole=-0.1077231,0.0064132,-0.1215539\\Quadrupole=0.9992155,-1.646692,0.6474764,-0.1263058,-0.4050578,-0.0009833\\PG=C01 [X(C6H11)]\\@

DEF_17

1\\G\\INC-V1391\\FOpt\\RB3LYP\\6-31G(d)\\C6H12\\GXG501\\04-Jun-2010\\0\\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl4.freq\\0,1\\C,-0.1229587329,0.1878179192,0.1616468819\\C,0.1673492959,-0.4601391658,1.2908526163\\C,1.343200819,-0.1771665586,2.1857068007\\C,0.9557263688,0.1937262517,3.6376423306\\C,2.2033192077,0.2572465466,4.5298010474\\C,0.1670312942,1.5089801019,3.6974335676\\H,0.4987443842,1.0023782745,-0.2053387833\\H,-0.9878233983,-0.0721357259,-0.4432390667\\H,-0.4885743807,-1.2705120433,1.6167078487\\H,1.9856899682,-1.0706789501,2.2212156749\\H,-0.727567579,1.4695600083,3.0673241294\\H,0.7832834799,2.3476769284,3.346974777\\H,-0.1471480818,1.7337224465,4.7235706001\\H,1.9531826597,0.6289823484,1.7541930648\\H,2.7466018506,-0.6954481363,4.5295345975\\H,2.8948143921,1.0355471447,4.1811563504\\H,1.9369118732,0.4921027432,5.567097723\\H,0.3070960384,-0.609137383,4.0215178718\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-235.8491047\\RMSD=7.968e-09\\RMSF=6.913e-06\\Dipole=0.032422,-0.0579519,0.1053687\\Quadrupole=0.0561397,0.1593064,-0.2154461,0.7431397,0.1606127,-0.7367069\\PG=C01 [X(C6H12)]\\@

DEF_170O

1\\G\\INC-V1388\\FOpt\\UB3LYP\\6-31G(d)\\C6H11O2(2)\\GXG501\\08-Jun-2010\\0\\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl4oo.freq\\0,2\\C,-0.2264214175,0.3246826211,0.2133539456\\C,0.0715936286,-0.4120268073,1.2821046077\\C,1.2786764287,-0.2479100075,2.1678826357\\C,0.9381387403,-0.0731393814,3.6637852667\\C,2.2066174353,-0.1199828614,4.5279540609\\C,0

.113337752,1.1950970386,3.9336192768\H,0.4068215658,1.1415105838,-0.1178441969\H,-1.1196133444,0.1248264476,-0.3713446773\H,-0.5855762039,-1.2294463801,1.5811292614\H,1.9546557966,-1.1021728815,2.040451327\H,-0.803219671,1.2156657685,3.335305621\H,0.6899144132,2.0953623323,3.6957202831\H,-0.1681819418,1.2454698159,4.9911532275\H,2.7660105565,-1.0496154289,4.369073133\H,2.8726545776,0.717609055,4.2942441472\H,1.9498193933,-0.0595771148,5.5912199896\H,0.3187064914,-0.9459636833,3.9193104126\O,2.0553718794,0.92654021,1.7606044288\O,2.953121535,0.6299030967,0.8332577971\Version=EM64L-G09RevA.02\State=2-A\HF=-385.5547102\S2=0.753169\S2-1=0.\S2A=0.750007\RMSD=9.817e-09\RMSF=5.465e-06\Dipole=-0.7410209,-0.5140631,0.5892136\Quadrupole=-1.0270715,0.696966,0.3301055,-0.1758388,2.7580822,-0.1867801\PG=C01 [X(C6H11O2)]\@

DEF_17OOH

1\1\GINC-V1422\FOpt\RB3LYP/6-31G(d)\C6H12O2\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def14ooh.freq\0,1\C,0.0102516985,0.0812282048,0.1456413995\C,0.0406387131,-0.1970327851,1.4503969312\C,1.2628245891,-0.0855850622,2.335652411\C,1.2455942024,1.162770433,3.2560749367\C,2.3382872669,1.0597439338,4.3306460165\C,1.3504311862,2.479496009,2.471899762\H,0.8939882204,0.4417926118,-0.3761122886\H,-0.8990761564,-0.022328739,-0.4392576757\H,-0.8655351909,-0.5383231215,1.9524000126\H,1.3186101707,-0.9789563826,2.973024622\H,0.5650582561,2.5622135834,1.7139088535\H,2.3189485225,2.5582151332,1.9669085239\H,1.2556000385,3.3324591783,3.1533338918\H,2.2198968202,0.1522921778,4.9347246139\H,3.3318271925,1.0314664784,3.8722488359\H,2.2973528979,1.9214235634,5.0065496396\H,0.2665660092,1.1402949949,3.7578032604\O,2.4716728177,-0.0196961075,1.5724859408\O,2.7674346675,-1.353797684,1.0866678314\H,2.1890897028,-1.3988300141,0.3005994631\Version=EM64L-G09RevA.02\State=1-A\HF=-386.1869643\RMSD=6.467e-09\RMSF=2.324e-06\Dipole=-0.8853092,0.052172,-0.0535216\Quadrupole=-2.0191721,-1.013576,3.032748,2.205578,0.6209606,1.2616842\PG=C01 [X(C6H12O2)]\@

DEF_17R

1\1\GINC-V1419\FOpt\UB3LYP/6-31G(d)\C6H11(2)\GXG501\07-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def14r.freq\0,2\C,-0.0749959723,-0.7799384354,0.192108676\C,-0.0018312603,-0.0063408364,1.3398362612\C,1.1451107471,0.6064113884,1.8257435113\C,1.2164352425,1.4441034791,3.0715721008\C,2.1749778771,0.8182629991,4.1061889042\C,1.6454085015,2.8895864431,2.7437133248\H,0.8025208329,-0.9603886008,-0.4232259245\H,-1.0077816552,-1.2303475664,-0.1302829411\H,-0.9211097775,0.1347985624,1.9117518568\H,2.0767837416,0.4793724324,1.2704110574\H,0.9467744648,3.3620917566,2.0449795294\H,2.6419451436,2.9060706016,2.284477201\H,1.6868994517,3.5005464543,3.6537483751\H,1.8554941868,-0.1921615314,4.3828679936\H,3.1932941872,0.7496319196,3.7029803377\H,2.2170238278,1.4268836438,5.0177637877\H,0.2123645991,1.4810672313,3.5180383512\Version=EM64L-G09RevA.02\State=2-A\HF=-235.2082976\S2=0.779598\S2-1=0.\S2A=0.750179\RMSD=8.317e-09\RMSF=2.551e-06\Dipole=0.0407236,0.0936206,0.1264733\Quadrupole=1.0081653,-0.9727978,-0.0353675,0.3016895,-0.5754492,0.9166612\PG=C01 [X(C6H11)]\@

DEF_18

1\1\GINC-V1323\FOpt\RB3LYP/6-31G(d)\C6H12\GXG501\08-Jun-2010\0\#B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\def17.freq\0,1\C,-0.0000027788,0.0000009211,-0.0193948703\C,0.000007475,0.0000010219,1.3174135214\C,1.2709233803,0.0000008585,-0.848996635\C,2.5954786357,0.0000009162,-0.0831928318\C,-1.2709416645,0.0000008586,-0.848977138\C,-2.5954851718,0.0000009164,-0.0831530153\H,0.9200863691,0.0000010653,1.8931298078\H,-0.9200625872,0.0000010653,1.8931439224\H,-2.6898456147,-0.8856287137,0.555030596\H,-3.4396143008,0.0000008638,-0.7812950653\H,-2.6898456146,0.8856306427,0.5550304625\H,-1.2426190862,0.8717050894,-1.5213843

994\H,1.2425904869,0.8717050893,-1.5214034618\H,2.6898488688,-0.885628
7139,0.5549893318\H,2.6898488688,0.8856306426,0.5549891983\H,3.4395970
546,0.0000008636,-0.7813478313\H,-1.2426190863,-0.8717034735,-1.521384
268\H,1.2425904868,-0.8717034736,-1.5214033304\\Version=EM64L-G09RevA.
02\\State=1-A\\HF=-235.8520345\\RMSD=4.618e-09\\RMSF=2.153e-05\\Dipole=-0.
0000017,0,-0.2161947\\Quadrupole=0.4418213,-0.7487961,0.3069747,0,-0.
000001,0\\PG=C02V [C2(C1C1),SGV(C4H4),X(H8)]\\@

DEF_1800

1\1\GINC-V1290\FOpt\UB3LYP\6-31G(d)\C6H11O2(2)\GXG501\08-Jun-2010\0\\#
B3LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl7oo.freq\\0,2\C,0
.0433696503,0.0011563512,-0.0121988623\C,0.0028052115,-0.090158216,1.3
202643256\C,1.3269554852,0.0771085838,-0.8169544266\C,2.6303608257,0.0
398794962,-0.018039523\C,-1.2195092745,0.0632236113,-0.8470103694\C,-2
.5572064334,0.0487183092,-0.1252640418\H,0.9079124851,-0.1123706124,1.
918348335\H,-0.9311025995,-0.13961336,1.870030066\H,-2.6565745646,-0.8
376569074,0.5085392286\H,-3.3598832026,0.0395976159,-0.8673708509\H,-2
.6673429676,0.9429116004,0.4961930898\H,-1.1707404742,0.9171699445,-1.
5326597013\H,1.2968877433,0.9962722662,-1.4226639485\H,2.7221996761,-0
.8881711829,0.5572489735\H,2.6994812874,0.8798467341,0.6825259418\H,3.
489767776,0.0982675954,-0.6940264911\H,1.3216512074,-0.7428405737,-1.5
479095646\O,-1.166017283,-1.1273991897,-1.7411456364\O,-1.9300716211,-
0.967238801,-2.8059607372\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-385.
5600747\\S2=0.753136\\S2-1=0\\S2A=0.750007\\RMSD=6.914e-09\\RMSF=3.021e-06
\\Dipole=0.313767,0.6151752,0.8077649\\Quadrupole=2.0674436,-0.4978484,-
1.5695952,-1.1710826,-2.7408442,-1.9264109\\PG=C01 [X(C6H11O2)]\\@

DEF_180OH

1\1\GINC-V1348\FOpt\RB3LYP\6-31G(d)\C6H12O2\GXG501\08-Jun-2010\0\\#B3L
YP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl7ooh.freq\\0,1\C,0.0
223955507,-0.0336458785,-0.038324949\C,-0.0152416913,-0.0656393922,1.2
969393232\C,1.3062933915,0.018159718,-0.8443721597\C,2.6093842218,0.04
32211224,-0.0442528894\C,-1.2462018939,-0.020903468,-0.881576334\C,-2.
5738377888,0.0384392054,-0.1347327642\H,0.891057607,-0.0494165232,1.89
38029167\H,-0.9473120751,-0.1020760686,1.8507853051\H,-2.6822417763,-0
.8134854285,0.5446084134\H,-3.3933840639,0.0138955843,-0.8586736477\H,
-2.6605736709,0.9640366357,0.4436248617\H,-1.1850843339,0.8274643365,-
1.5791455657\H,1.2629618349,0.9042398633,-1.4966363502\H,2.716638377,-
0.8525877174,0.577957459\H,2.6649697904,0.9183397119,0.6134809084\H,3.
4688957349,0.0811809971,-0.722020615\H,1.3100484956,-0.8366650648,-1.5
322850162\O,-1.1590723092,-1.2232974858,-1.6778733238\O,-2.0616176256,
-1.0614601463,-2.8117900295\H,-2.6982848331,-1.7729621226,-2.620226484
9\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-386.1904351\\RMSD=3.660e-09\\R
MSF=3.169e-06\\Dipole=-0.3528575,0.0505678,0.3680272\\Quadrupole=3.24446
96,-0.5356264,-2.7088432,2.1675663,0.5317687,0.514017\\PG=C01 [X(C6H12O
2)]\\@

DEF_18R

1\1\GINC-V1447\FOpt\UB3LYP\6-31G(d)\C6H11(2)\GXG501\08-Jun-2010\0\\#B3
LYP/6-31G* OPT Freq=noraman maxdisk=268435456\\defl7r.freq\\0,2\C,0.25
09051929,0.3975179754,0.4552014337\C,0.1781920396,-0.0878342842,1.7534
562968\C,1.5945980929,0.3358799909,-0.2639245057\C,1.7958803718,-0.977
1844506,-1.0379240091\C,-0.8400315185,0.9118440551,-0.2521759829\C,-2.
2547644154,1.025420603,0.223147918\H,1.0631899642,-0.4648323595,2.2570
279994\H,-0.7478698575,-0.1143765521,2.3174636599\H,-2.3819470922,0.71
99240624,1.2649831914\H,-2.928901305,0.4072251836,-0.3884923473\H,-2.6
188730907,2.0586965002,0.1316938927\H,-0.6535334367,1.2656337603,-1.26
59044182\H,2.4051288608,0.4532667112,0.4658755769\H,1.0169510016,-1.10
82247365,-1.7979191391\H,1.7490651742,-1.8399402876,-0.3638128171\H,2.
7688160054,-0.9922312665,-1.5431367259\H,1.6785718804,1.1810237135,-0.

9587487913\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-235.2087351\\S2=0.78
055\\S2-1=0.\\S2A=0.750186\\RMSD=5.416e-09\\RMSF=5.199e-06\\Dipole=-0.07796
61,0.0409388,-0.1076145\\Quadrupole=1.178857,-1.3004956,0.1216386,-0.59
28719,-0.0036038,-0.8612887\\PG=C01 [X(C6H11)]\\@

DEF_19

1\\G\\INC-V1374\\FOpt\\RB3LYP\\Gen\\C8H14O2\\GXG501\\27-Jun-2010\\0\\#B3LYP\\ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\\def19.freq\\0,1\\C,0.2818786167,0.1248505307,-0.0986464841\\C,0.10069
68554,-0.3481102933,1.3505663978\\C,1.5592899409,0.962045103,-0.2465381
561\\C,-0.9784270574,0.899540519,-0.5619958677\\C,-1.0039966647,1.247020
9891,-2.032337298\\C,-1.2617985008,0.1000454943,-2.9583701269\\O,-1.5102
059685,-1.0306860071,-2.583036308\\O,-1.1998800705,0.4392995613,-4.2671
310166\\C,-1.4583047821,-0.6300729908,-5.1883109765\\C,-0.8337167611,2.4
881570667,-2.5078727737\\H,-1.8585839203,0.2865262486,-0.3340426962\\H,-
1.3648880996,-0.1889916747,-6.1813073647\\H,-0.7320033968,-1.4365948806
,-5.0559315823\\H,-2.4639439301,-1.0329369564,-5.0398432336\\H,-0.782596
2267,-0.9891569089,1.453465781\\H,0.9722784239,-0.9200800396,1.69004504
31\\H,0.3708044392,-0.7645050828,-0.7353156179\\H,2.4417689416,0.3838358
147,0.0517265938\\H,1.7101499593,1.2959172129,-1.2787395932\\H,-0.666347
1066,3.3254576112,-1.8352464875\\H,-0.8600424769,2.7028545645,-3.570281
7408\\H,-1.0636309691,1.8247272672,0.0229778916\\H,1.5185605292,1.855843
9893,0.390935074\\H,-0.0216465343,0.5046584622,2.031741743\\Version=EM6
4L-G09RevA.02\\State=1-A\\HF=-463.7277691\\RMSD=8.561e-09\\RMSF=4.152e-06\\
Dipole=0.0988831,0.4680056,-0.4186034\\Quadrupole=-2.1345497,-1.8017714
,3.9363211,-0.9986017,1.0660294,1.9185723\\PG=C01 [X(C8H14O2)]\\@

DEF_1900

1\\G\\INC-V1299\\FOpt\\UB3LYP\\Gen\\C8H13O4(2)\\GXG501\\28-Jun-2010\\0\\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\\def1900.freq\\0,2\\C,-0.0018325609,0.0318804174,-0.020685067\\C,-0
.0290361841,0.0274351347,1.5155795339\\C,1.4369612517,0.0160390994,-0.5
596247749\\C,-0.836510501,1.2086841687,-0.5738427678\\C,-1.0425704458,1.
1944634794,-2.076966519\\C,-2.036045587,0.1796814458,-2.5386754928\\O,-2
.6558546049,-0.5452319207,-1.7811366634\\O,-2.1847979553,0.1470031505,-
3.8786975143\\C,-3.1465102863,-0.8028942453,-4.3667027013\\C,-0.43161351
03,2.0246307201,-2.9297504614\\H,-1.8109774924,1.2326185714,-0.07912244
27\\H,-3.1365960838,-0.6945381262,-5.4514402088\\H,-2.8630471426,-1.8183
667118,-4.0778530057\\H,-4.1396878214,-0.5833896149,-3.9663987718\\H,-1.
0566006404,-0.0115060548,1.8952788826\\H,0.5053303222,-0.8465335116,1.9
040019352\\H,-0.5195836422,-0.868440133,-0.3724127619\\H,1.9644664726,-0
.870528335,-0.1910148774\\H,1.4624585176,-0.0096593195,-1.6539648996\\H,
0.2640118138,2.7799715508,-2.5805623567\\H,-0.6280470603,1.973337898,-3
.994377805\\H,1.9950281369,0.8985807979,-0.2283669293\\H,0.4500519399,0.
9240947594,1.9235317729\\O,-0.1431967524,2.4372402887,-0.1757273494\\O,-
0.9706806499,3.4689395222,-0.1015533728\\Version=EM64L-G09RevA.02\\Stat
e=2-A\\HF=-613.4328294\\S2=0.753062\\S2-1=0.\\S2A=0.750006\\RMSD=4.596e-09\\
RMSF=3.597e-06\\Dipole=0.1160212,-0.7469601,-0.9365366\\Quadrupole=0.281
9517,-4.6185586,4.3366069,-0.0577252,3.2673607,-0.8859018\\PG=C01 [X(C8
H13O4)]\\@

DEF_1900H

1\\G\\INC-V1294\\FOpt\\RB3LYP\\Gen\\C8H14O4\\GXG501\\28-Jun-2010\\0\\#B3LYP\\ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\\def1900h.freq\\0,1\\C,0.0024066677,0.0007135401,-0.0052792765\\C,-0.0
24053404,-0.0483787379,1.5297449796\\C,1.4414651551,0.0570652105,-0.540
082058\\C,-0.8841900728,1.1606316765,-0.5327345809\\C,-1.1201260049,1.11
59710814,-2.0352417255\\C,-2.1065661132,0.0909454518,-2.4791139892\\O,-2
.7066572284,-0.6442874775,-1.7143218016\\O,-2.2788953321,0.0519034709,-
3.8191032701\\C,-3.2301244774,-0.9163064014,-4.2862253105\\C,-0.51764047

2,1.9418465509,-2.8978242951\H,-1.8560720751,1.1020739521,-0.028041603
5\H,-3.241080439,-0.8134594618,-5.3717567963\H,-2.9250396021,-1.926063
0213,-3.9984885509\H,-4.2211746396,-0.7144100917,-3.8709571485\H,-1.04
95798554,-0.1409073524,1.9066464754\H,0.545110285,-0.9101466388,1.8963
324769\H,-0.476915023,-0.9111764727,-0.3815626874\H,2.0015638185,-0.82
36397786,-0.2058900641\H,1.4665842096,0.0757608066,-1.634470657\H,0.17
23189292,2.6993524556,-2.5415346642\H,-0.7142401892,1.8881042661,-3.96
24987875\H,1.9655389956,0.9470069952,-0.1754196219\H,0.4184601638,0.85
59746185,1.9609259045\O,-0.2294996939,2.3662163152,-0.133357315\O,-1.1
861778978,3.4592238272,-0.2563986618\H,-1.3223109734,3.6594833446,0.68
76030141\Version=EM64L-G09RevA.02\State=1-A\HF=-614.0655176\RMSD=5.22
4e-09\RMSF=2.734e-06\Dipole=-0.0951472,-0.0593536,-0.1755502\Quadrupol
e=-2.6001677,-2.3845301,4.9846978,-1.2200235,2.0382587,4.7663778\PG=C0
1 [X(C8H14O4)]\@

DEF_19R

1\1\GINC-V1298\FOpt\UB3LYP\Gen\C8H13O2(2)\GXG501\27-Jun-2010\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843
5456\def19r.freq\0,2\C,0.5699127177,0.2999443693,-0.0509201812\C,0.3
28870332,-0.586444609,1.1895331239\C,1.0826938301,1.6941515327,0.36873
18484\C,-0.6918273563,0.4289082625,-0.8515763421\C,-0.8996724703,0.022
7379762,-2.1705931164\C,-2.28652452,0.2910006011,-2.6990389286\O,-3.17
99175312,0.8151080231,-2.0637942881\O,-2.4454538076,-0.1171552314,-3.9
783286438\C,-3.747666316,0.1127135685,-4.5359694669\C,0.0394530313,-0.
5856773157,-2.9980552274\H,-1.5395522982,0.8899438393,-0.349463164\H,-
3.7000947724,-0.2700379089,-5.5560332279\H,-4.5115199711,-0.4177928843
,-3.9610371894\H,-3.9833721192,1.1802574936,-4.5358788301\H,0.00516989
26,-1.5925192819,0.902336672\H,1.2465007387,-0.6776148724,1.7830873414
\H,1.3503404811,-0.1760387459,-0.6569177672\H,2.0011173203,1.605361397
1,0.9614168106\H,1.2978167675,2.3182239011,-0.5051701184\H,1.045490925
5,-0.793579854,-2.6517160918\H,-0.2095301655,-0.8683442295,-4.01174637
59\H,0.3368787378,2.2168866524,0.9800345138\H,-0.4469434343,-0.1544511
522,1.8334883194\Version=EM64L-G09RevA.02\State=2-A\HF=-463.0838654\S
2=0.783854\S2=1=0.\S2A=0.750212\RMSD=3.572e-09\RMSF=1.106e-05\Dipole=0
.4037988,-0.2400532,-0.297296\Quadrupole=-0.2290746,-2.6238962,2.85297
08,0.9889595,4.7455722,0.3316067\PG=C01 [X(C8H13O2)]\@

DEF_20

1\1\GINC-V1286\FOpt\RB3LYP\Gen\C6H10O2\GXG501\26-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\def20.freq\0,1\C,0.0925228443,0.2857583715,0.0667615057\C,-0.09831
13266,-0.1583793287,1.4848846428\C,0.7741368199,-0.1944994725,2.512510
8005\C,0.3459728984,-0.6908444607,3.8764265046\C,2.1923171241,0.247737
6638,2.3611886358\O,2.7327834155,0.6769624245,1.3578280205\O,2.8660107
059,0.1159502373,3.5343614217\C,4.2425442571,0.5157648782,3.4969993811
\H,4.79878387,-0.0823729843,2.7699799627\H,0.4794562704,0.0793723457,4
.6444358838\H,4.6234964093,0.34654126,4.5048953055\H,4.3308449813,1.57
10665561,3.2244422865\H,0.9411298122,-1.5541686804,4.1950011597\H,-1.1
073365766,-0.5065079123,1.7137789067\H,-0.1527605134,-0.5398584799,-0.
6160309087\H,1.1062824166,0.6266771452,-0.1312135374\H,-0.6145428368,1
.094251811,-0.1664240477\H,-0.707983236,-0.9852246426,3.8636439512\Ve
rsion=EM64L-G09RevA.02\State=1-A\HF=-385.1034757\RMSD=4.614e-09\RMSF=2
.220e-05\Dipole=-0.199842,-0.1790103,0.4420664\Quadrupole=3.3491916,-1
.6746143,-1.6745773,0.397321,3.542376,1.0501586\PG=C01 [X(C6H10O2)]\@

DEF_2000

1\1\GINC-V1296\FOpt\UB3LYP\Gen\C6H9O4(2)\GXG501\27-Jun-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\def20oo.freq\0,2\C,-0.0104430534,-0.1172918022,-0.0664652135\C,-
0.0407755081,-0.2081208443,1.4255346403\C,0.9735028868,-0.1662744021,2

.3147614539\C,0.6619464885,-0.2453271989,3.783223096\C,2.4006742572,0.0099654625,1.9134748782\O,2.8285376742,0.1465567006,0.7832614749\O,3.2126988349,-0.0022320875,2.9988763625\C,4.6097366744,0.1851740952,2.7248655595\H,4.9860731965,-0.61677496,2.0841560257\H,1.3975693781,-0.8224646492,4.3436748247\H,5.102094893,0.165040239,3.6973631769\H,4.7763668708,1.1443088252,2.2280100009\H,-0.3443893662,-0.6292781497,3.9607159535\H,-1.0375001109,-0.3216240825,1.8529177283\H,-0.5180311901,-0.9899641078,-0.4995301942\H,1.000280775,-0.0444600626,-0.4616305275\H,-0.5878521657,0.7613302392,-0.3865319363\O,0.7206740959,1.0833990459,4.4251110679\O,-0.3137216939,1.8230379849,4.0703606964\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-534.8057255\\S2=0.753045\\S2-1=0.\\S2A=0.750007\\RMSD=5.945e-09\\RMSF=1.351e-06\\Dipole=0.1321459,-0.9667055,-0.0724196\\Quadrupole=5.2479007,-2.0250933,-3.2228075,3.0869834,5.0627909,-3.0553851\\PG=C01 [X(C6H9O4)]\\@

DEF_200OH

1\I\GINC-V1296\FOpt\RB3LYP\Gen\C6H10O4\GXG501\27-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\def200oh.freq\\0,1\C,0.0131868577,0.0062564658,0.05233627\C,-0.0089722006,0.0057172747,1.5492291011\C,1.0116530858,0.069726854,2.4279822288\C,0.7286779345,0.0627313126,3.9135602791\C,2.4346783095,0.1965132687,1.9912148661\O,2.8275266964,0.5187094888,0.8851419107\O,3.2854928008,-0.1008069502,3.0028561197\C,4.6810569941,0.0075618206,2.6855254633\H,4.9483628447,-0.6867533835,1.8843208221\H,1.4239768554,-0.5853859562,4.4538991717\H,5.2092845761,-0.244672694,3.6053826202\H,4.9245703355,1.0248609011,2.3680235163\H,-0.2985191641,-0.2632530801,4.111258761\H,-1.0040670413,-0.0721168927,1.9898499383\H,-0.5681618007,-0.8444226555,-0.327179656\H,1.0228993155,-0.0204639129,-0.3529573995\H,-0.4868848946,0.9102205739,-0.3235057697\O,0.9451320725,1.3396809025,4.5249451896\O,-0.1277387362,2.2125124201,4.0799145728\H,0.3304675239,2.7214152639,3.3861980516\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-535.438203\\RMSD=5.345e-09\\RMSF=4.963e-06\\Dipole=0.1032425,-0.4447779,-0.411226\\Quadrupole=4.652245,1.4263465,-6.0785914,0.6808026,5.3571222,-2.5034217\\PG=C01 [X(C6H10O4)]\\@

DEF_20R

1\I\GINC-V1307\FOpt\UB3LYP\Gen\C6H9O2(2)\GXG501\27-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\def20r.freq\\0,2\C,0.0390512899,-0.0897945771,-0.0008515543\C,-0.065780831,-0.0256442139,1.4915635735\C,0.9662607161,0.0499020973,2.4350912184\C,0.7049561398,0.1033592643,3.8017432261\C,2.3919608581,0.0740787483,1.9620692857\O,2.7462740322,0.0348099669,0.799711287\O,3.275282844,0.1461468764,2.9855687013\C,4.6568971721,0.1729274678,2.5994615728\H,4.9203418954,-0.7331008681,2.0470375501\H,-0.3190009856,0.0871471397,4.1627941638\H,5.2190309766,0.2308038091,3.5321418851\H,4.8645384301,1.0428325975,1.9704777614\H,1.4999198795,0.1616653416,4.5322043605\H,-1.0704758723,-0.0386057996,1.9110076149\H,-0.9580426723,-0.1437664477,-0.4483593993\H,0.6192897959,-0.9588042604,-0.3341916063\H,0.5602447098,0.7828289176,-0.4130906171\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-384.4533261\\S2=0.78576\\S2-1=0.\\S2A=0.750236\\RMSD=8.965e-09\\RMSF=8.451e-06\\Dipole=0.0221934,0.0199256,0.446934\\Quadrupole=4.6752402,-2.1497091,-2.525531,0.3025921,1.9868848,0.0530038\\PG=C01 [X(C6H9O2)]\\@

DEF_21

1\I\GINC-V1293\FOpt\RB3LYP\Gen\C10H16O4\GXG501\27-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\def21.freq\\0,1\C,-0.8268747737,-1.1942254001,0.5994193281\C,-0.4284737998,-0.6303037942,1.966790834\C,0.8953150109,0.1780414409,1.9403056454\C,2.0489620707,-0.741222075,1.5410852258\O,2.3209624683,-1.7837900652,2.097297099\O,2.7414610321,-0.2469751456,0.4939828668\C,3.863609

1022,-1.0408850334,0.0684424747\C,1.1981244027,0.738427525,3.308164695
6\C,1.1749112017,2.0289504398,3.6863683819\C,1.478091819,2.3963842994,
5.1034598355\O,1.4817823621,3.5432153023,5.5104841245\O,1.7505507972,1
.3360167503,5.900666869\C,2.0500864697,1.6592097517,7.2655750862\C,0.8
620982741,3.2172502629,2.8132139164\H,0.6470373115,2.9302880733,1.7821
487952\H,0.0005092908,3.767163005,3.2081081822\H,2.2415419024,0.704216
2401,7.7561677394\H,2.9304123389,2.3051039699,7.3250037229\H,1.2053628
188,2.1704710805,7.735418557\H,1.6998469283,3.9232124951,2.8107971407\H,
1.4432520268,-0.0116007841,4.05541788\H,4.3002471901,-0.5017806208,-
0.7725488513\H,3.5335714363,-2.0361165649,-0.240602735\H,-1.2169416174
,0.0319010757,2.3436237405\H,-0.319602258,-1.4455319315,2.6911335597\H
, -0.0825202972,-1.9079041789,0.228217662\H,-1.7846021177,-1.7219575143
,0.6644002007\H,0.8208387707,0.9728321758,1.1945871106\H,4.5889164963,
-1.1432537132,0.8797717072\H,-0.9336596767,-0.3981602439,-0.1472909649
\Version=EM64L-G09RevA.02\State=1-A\HF=-691.6033322\RMSD=4.137e-09\RM
SF=5.463e-06\Dipole=0.058854,-0.3468183,-0.5775533\Quadrupole=3.470113
5,-10.4899308,7.0198173,0.0228057,-1.0689749,-1.6861441\PG=C01 [X(C10H
16O4)]\@

DEF_2100

1\1\GINC-V1298\FOpt\UB3LYP\Gen\C10H15O6(2)\GXG501\28-Jun-2010\0\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\def2100.freq\0,2\C,-0.6476827731,-0.649098953,0.16381304\C,-0.
2876439706,-0.6426035917,1.6534950666\C,1.1568882406,-0.2179480144,1.9
737784226\C,2.2083929236,-1.1408942546,1.3250479591\O,1.987657741,-2.2
809682337,0.9782235759\O,3.3993766135,-0.5377972474,1.237498715\C,4.45
79784758,-1.3313808564,0.6662516531\C,1.4140605426,-0.0511070537,3.458
1783686\C,1.4457708801,-0.9966136576,4.4127222583\C,1.6842853311,-0.58
2919311,5.8344353764\O,1.7175079936,-1.3719348631,6.7589029224\O,1.858
3594635,0.7480790283,5.9972305547\C,2.082924493,1.1760595622,7.3488588
97\C,1.2554201665,-2.4831148016,4.2481502279\H,1.1785381964,-2.7862327
062,3.2043921597\H,2.0908915864,-3.0210626943,4.7084351268\H,2.1993322
245,2.2588622999,7.2957008308\H,1.2323216119,0.9106660524,7.9823406722
\H,2.9853377481,0.7108181164,7.7544577113\H,0.3554828159,-2.8098143234
,4.782332633\H,1.5577549093,0.9826675637,3.7524648269\H,5.3337302476,-
0.683237343,0.6631347876\H,4.1974925054,-1.6361974963,-0.3501738134\H,
-0.9387727605,0.0485547906,2.198031573\H,-0.4390078473,-1.6361778198,2
.0842258672\H,-0.0322853301,-1.3610985859,-0.3929339648\H,-1.695401787
6,-0.9437316485,0.0422342574\H,4.6350120926,-2.221332949,1.2752107184\H,
-0.526052438,0.3429821026,-0.2811701688\O,1.4108884742,1.1034577792,
1.3248412746\O,0.6472471493,2.0532076986,1.8273358967\Version=EM64L-G
09RevA.02\State=2-A\HF=-841.3013559\S2=0.753365\S2-1=0.\S2A=0.750008\R
MSD=8.957e-09\RMSF=7.288e-06\Dipole=0.5362641,0.021939,-0.1441434\Quad
rupole=6.5662355,-6.3803792,-0.1858563,0.1061026,-2.2221444,7.6983359\
PG=C01 [X(C10H15O6)]\@

DEF_2100H

1\1\GINC-V1439\FOpt\RB3LYP\Gen\C10H16O6\GXG501\28-Jun-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684354
56\def2100h.freq\0,1\C,0.1440012994,-0.0819178958,0.0335016204\C,0.1
129749287,-0.0492064236,1.5660704092\C,1.5059444675,-0.0272956055,2.24
53662627\C,2.2950441415,-1.3047278661,1.8645183359\O,1.8065190286,-2.4
044939352,1.7366856815\O,3.6164555427,-1.0681486744,1.6815979195\C,4.4
087699824,-2.2199232822,1.322816436\C,1.4009494396,0.1419819693,3.7540
168873\C,0.8310550479,-0.6544900469,4.6763913517\C,0.8123679014,-0.198
5034985,6.1056442754\O,0.3191165627,-0.8504140238,7.0063154064\O,1.391
7460691,1.0076186537,6.3092658192\C,1.3848091225,1.46780948,7.66781570
16\C,0.1665030303,-1.9932537828,4.4771341723\H,0.2923214615,-2.3770104
804,3.4663143473\H,0.5790292086,-2.7225414803,5.1821974524\H,1.8838112
523,2.4372625439,7.6495494859\H,0.3599020328,1.5693630162,8.0350226521
\H,1.9236105213,0.7696220445,8.3142603678\H,-0.9031116481,-1.922364028
5,4.7092331725\H,1.843146567,1.0717926549,4.0908231081\H,5.4305102168,
-1.852044426,1.2313683408\H,4.0608844101,-2.6368248049,0.3750807322\H,

-0.4143929306,0.8442939204,1.9160119558\H,-0.428057779,-0.9176012478,1.9489484544\H,0.6318605516,-0.9901280571,-0.3359867876\H,-0.8797467182,-0.0761476068,-0.3560041729\H,4.3385443665,-2.9830042828,2.1009794738\H,0.6678952378,0.785923462,-0.3755759597\O,2.1277910318,1.1356013339,1.6677106927\O,3.3330168824,1.5048307366,2.3815940543\H,3.958380331,0.8532292714,2.0067223722\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-841.9366386\\RMSD=5.648e-09\\RMSF=7.117e-06\\Dipole=0.9184809,-0.1433792,-0.5106766\\Quadrupole=5.6521864,-5.102822,-0.5493644,-6.0953732,0.2637812,7.6661648\\PG=C01 [X(C10H16O6)]\\@

DEF_21R

1\1\GINC-V1440\FOpt\UB3LYP\Gen\C10H15O4(2)\GXG501\29-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=268435456\\def21r.freq\\0,2\C,1.5878401647,0.8728580958,0.4034988487\C,0.4796095022,0.2230536871,1.2598158365\C,1.0199212668,-0.638306874,2.3730419539\C,1.4327041555,-2.0331639909,2.0512225726\O,1.8875278164,-2.8380481189,2.8460406383\O,1.2480573464,-2.3344756798,0.7396384676\C,1.6261170575,-3.665966369,0.3617524104\C,1.2049407421,-0.2812373286,3.7107437675\C,0.9849831774,0.926687752,4.3781274767\C,1.2344173412,0.9858633458,5.8446801941\O,1.0950586078,1.9942633202,6.5177270207\O,1.6318949829,-0.1936329828,6.378745678\C,1.8847797334,-0.1722717175,7.7899254085\C,0.5144635928,2.223213882,3.7766833607\H,1.0602082929,2.4713402475,2.8616563603\H,-0.5537476859,2.1831206065,3.5220949163\H,2.1928278906,-1.1865839103,8.0453999461\H,2.6768717069,0.5427369073,8.0289865573\H,0.9809294473,0.1057959863,8.3389894173\H,0.6477622301,3.0282792905,4.4999431308\H,1.5866662911,-1.0888791237,4.3265709286\H,1.4194051596,-3.7363568673,-0.7067331629\H,1.0407593308,-4.4041205509,0.9167331298\H,-0.1706022877,0.9994618135,1.6661420022\H,-0.1392021076,-0.3992183749,0.6059182803\H,2.2185927381,0.1069548843,-0.0575239539\H,1.1448278899,1.4769705375,-0.3961164617\H,2.6875812492,-3.8362870617,0.5612384747\H,2.230389764,1.5236693549,1.0068095623\\Version=EM64L-G09RevA.02\\State=2-A\\HF=-690.9725635\\S2=0.776628\\S2-1=0.\\S2A=0.750237\\RMSD=8.083e-09\\RMSF=6.779e-06\\Dipole=-0.119222,-0.2698056,-0.8515174\\Quadrupole=-1.2125913,-4.23688,5.4494713,0.575538,1.5398743,-1.4329724\\PG=C01 [X(C10H15O4)]\\@

DEF_22

1\1\GINC-V1360\FOpt\RB3LYP\Gen\C11H14GXG501\08-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=268435456\\def23.freq\\0,1\C,1.0374918539,0.0661585475,-0.9024369185\C,0.9457940022,0.7871783123,0.2255652577\C,1.7196463372,0.4084949676,1.4425531713\C,3.2264378251,-0.3283705005,3.7163771282\C,1.9144533394,-0.9430815852,1.779073236\C,2.2839336452,1.3814863369,2.2860710748\C,2.6610590696,-1.308000768,2.8978081256\C,3.0326149997,1.0181620674,3.4052480081\C,0.0379510884,2.0007541228,0.2964161198\C,-1.1413224347,1.8381188504,1.2746888162\C,-2.0386189319,3.0782423785,1.3280296246\H,2.7916010536,-2.3603279571,3.1370504129\H,2.1554314853,2.4352969028,2.0566622735\H,1.4541541852,-1.7113945051,1.1646199395\H,3.4666717264,1.790900456,4.0346067881\H,3.8050340668,-0.6113935541,4.5916098617\H,1.6994358272,-0.7908265163,-0.9884663402\H,0.4622073874,0.3257534497,-1.7873209159\H,-0.3507654287,2.2112458128,-0.7076125774\H,0.6162020866,2.8896230967,0.5881440961\H,-1.7325200614,0.9633301902,0.9731524106\H,-0.7550015023,1.6171563617,2.2775006097\H,-2.8726009669,2.9358308127,2.0245651667\H,-1.4769050264,3.9612586183,1.657623405\H,-2.4631232828,3.306071466,0.3423762595\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-427.5910004\\RMSD=8.027e-09\\RMSF=7.424e-06\\Dipole=-0.0572283,0.0641663,0.1101499\\Quadrupole=-1.8508811,1.6601142,0.1907669,-0.5441446,2.8080402,0.0730298\\PG=C01 [X(C11H14)]\\@

DEF_22OO

1\1\GINC-V1289\FOpt\UB3LYP\Gen\C11H13O2(2)\GXG501\08-Jul-2010\0\#B3LYP
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\def23oo.freq\0,2\C,0.2470754066,1.0321269777,-0.0336234018\C,0
.1791491015,0.4369734457,1.1667348031\C,1.3882564245,0.2747651147,2.02
38916989\C,3.7165195096,-0.00573854,3.5900612299\C,1.6384999974,-0.911
5484657,2.736729448\C,2.3240098869,1.3194694026,2.1234830507\C,2.79261
92636,-1.0486765143,3.5078544784\C,3.476746317,1.1806463751,2.89479916
22\C,-1.1751866887,-0.0320553137,1.6635736709\C,-1.5692898224,0.420059
179,3.0709048303\C,-1.7544883303,1.9378932311,3.1694465438\H,2.9707009
628,-1.9777181056,4.0428870073\H,2.1321710545,2.2547134502,1.604977563
6\H,0.9375646417,-1.7365712377,2.6682851269\H,4.1829339811,2.004248889
7,2.9598422038\H,4.6128579984,-0.1144058316,4.1946762137\H,1.188406050
2,1.3841356822,-0.4454308151\H,-0.6371155005,1.1760266986,-0.648574193
9\H,-1.9479927983,0.2597641391,0.9469329801\H,-2.5049747868,-0.0923822
298,3.3203617919\H,-0.8104914405,0.0843506214,3.786249231\H,-2.0825103
545,2.2167659124,4.1762350483\H,-0.8215254026,2.4724417463,2.961466560
3\H,-2.5116617182,2.2950699125,2.4609455764\O,-1.1658253691,-1.5196785
865,1.6217127563\O,-2.3911424426,-2.0084805161,1.6748207544\Version=E
M64L-G09RevA.02\State=2-A\HF=-577.2981715\S2=0.753147\S2-1=0.\S2A=0.75
0007/RMSD=3.273e-09/RMSF=3.048e-06/Dipole=0.5213199,1.0063583,0.152393
5\Quadrupole=0.371351,-2.0341236,1.6627727,-3.6938492,1.3369161,-3.366
5158\PG=C01 [X(C11H13O2)]\@

DEF_22OOH

1\1\GINC-V1395\FOpt\RB3LYP\Gen\C11H14O2\GXG501\09-Jul-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=6710886
40\def23ooh.freq\0,1\C,0.0759602142,-0.0496712234,-0.0138897716\C,0.
0589800063,0.0049704232,1.3274648322\C,1.3247799682,0.0438869645,2.114
4093476\C,3.7566002467,0.1070782941,3.5437287105\C,1.4883779169,-0.705
9858043,3.2939449607\C,2.4025575533,0.8338965836,1.6764180867\C,2.6927
341779,-0.6747285776,3.9968602571\C,3.6055070866,0.8634480819,2.380258
8543\C,-1.2872443168,0.0003994563,2.0463351413\C,-1.4471330584,1.05000
63243,3.1522657902\C,-1.367751623,2.4845147842,2.6182646668\H,2.799506
8752,-1.2680078824,4.9013077023\H,2.284331514,1.4441346321,0.785345675
3\H,0.670020527,-1.3231071194,3.649572119\H,4.4222031507,1.4857939306,
2.0237281283\H,4.6926964504,0.1314054815,4.0951026612\H,1.0039635117,-
0.09408368,-0.5777616584\H,-0.8456617366,-0.0555599197,-0.5898749669\H
,-2.0786879802,0.138881494,1.2996523236\H,-2.4195185152,0.8756594143,3
.6271905055\H,-0.6833339891,0.8953101607,3.9218420222\H,-1.53504249,3.
2029675546,3.4276061097\H,-0.3867440126,2.697169292,2.1803133075\H,-2.
1262792737,2.666386489,1.84745956\O,-1.523907149,-1.2701006859,2.69065
57002\O,-1.7800007075,-2.2573001405,1.6623064733\H,-0.8719428494,-2.49
30063896,1.389537832\Version=EM64L-G09RevA.02\State=1-A\HF=-577.93102
72/RMSD=5.136e-09/RMSF=2.525e-06/Dipole=0.7312192,0.5030126,-0.291265\
Quadrupole=-1.2851009,-1.291159,2.5762599,-3.6580626,1.3992002,-0.1953
598\PG=C01 [X(C11H14O2)]\@

DEF_22R

1\1\GINC-V1363\FOpt\UB3LYP\Gen\C11H13(2)\GXG501\08-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\def23r.freq\0,2\C,0.0170282222,-0.828692591,0.4631402463\C,0.195
5180862,-0.6683350322,1.8325069853\C,1.5249259304,-0.1910233051,2.3303
117622\C,4.0290108666,0.7099809781,3.262820584\C,2.7193519945,-0.69974
13244,1.7958212717\C,1.6117573288,0.7788148444,3.3417879427\C,3.958344
1269,-0.2546867856,2.2562578175\C,2.8497904704,1.2250987621,3.80379941
78\C,-0.8036749709,-0.9391739748,2.7781808888\C,-2.2087263019,-1.38203
94081,2.4947341853\C,-3.2212993791,-0.8124831475,3.5016409795\H,4.8700
567666,-0.6685224369,1.8329208062\H,0.6986474366,1.2006253553,3.753002
5742\H,2.6725572115,-1.4661129323,1.0269650208\H,2.8924644402,1.982656
6726,4.5822386593\H,4.9940917469,1.0571499576,3.6222152726\H,0.7979399
521,-0.5570250127,-0.2384328053\H,-0.908304401,-1.2086921872,0.0448283
039\H,-0.5313925589,-0.8659174168,3.8297324734\H,-2.5067842213,-1.0988
776321,1.4783736893\H,-2.2629733324,-2.4835213602,2.5276876149\H,-4.23

22008458,-1.1796178738,3.2927031255\H,-2.9646532666,-1.104235672,4.527
1006628\H,-3.2431954984,0.2823824186,3.4621349736\\Version=EM64L-G09Re
vA.02\State=2-A\HF=-426.9470396\S2=0.782844\S2-1=0.\S2A=0.750221\RMSD=
7.738e-09\RMSF=2.995e-06\Dipole=-0.154037,-0.0625127,0.0741593\Quadrup
ole=2.7613149,-2.2271784,-0.5341365,1.1142276,-0.138088,2.3675837\PG=C
01 [X(C11H13)]\\@

DEF_23

1\1\GINC-V1414\FOpt\RB3LYP\Gen\C10H12O1\GXG501\08-Jul-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684354
56\def24.freq\0,1\C,0.49199676,0.5022629941,0.0931712372\C,0.2600483
171,0.2503943209,1.5558433686\C,-0.0607323396,-0.2691665577,4.29282131
72\C,-0.9302337697,0.6004551529,2.2113733586\C,1.2872021756,-0.3634316
068,2.290286628\C,1.1289491896,-0.6216065112,3.6482809502\C,-1.0889539
763,0.3416582619,3.5727920975\C,-0.6109564452,1.1683132251,-0.72435883
85\C,-0.2440075118,1.3649943241,-2.1968033456\C,-1.3653670787,2.034580
0584,-2.9963649666\H,1.9304144665,-1.0971654829,4.2071885987\H,2.20126
40137,-0.6278950613,1.7686918992\H,-1.7385815607,1.0759771239,1.664852
2558\H,-2.0146321045,0.6166850916,4.0709772189\H,-0.1856029223,-0.4702
975155,5.3535804615\H,-0.8558993158,2.1343542863,-0.2578588433\H,-1.52
55612741,0.5632112553,-0.6345767025\H,0.6733414394,1.9615018811,-2.260
0881942\H,0.0046260766,0.3922186112,-2.6363303472\H,-1.0778182168,2.16
36612695,-4.0457633599\H,-2.2853329206,1.4367084232,-2.9759038844\H,-1
.6078848505,3.026508143,-2.5947263188\O,1.5481311543,0.1775662103,-0.4
297213881\\Version=EM64L-G09RevA.02\State=1-A\HF=-463.5239417\RMSD=5.3
31e-09\RMSF=1.310e-05\Dipole=-0.8399925,0.1996363,0.6603408\Quadrupole
=-1.4350322,-1.3968403,2.8318725,-0.9273047,2.289941,-2.2118515\PG=C01
[X(C10H12O1)]\\@

DEF_2300

1\1\GINC-V1360\FOpt\UB3LYP\Gen\C10H11O3(2)\GXG501\08-Jul-2010\0\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\def24oo.freq\0,2\C,-0.1422307157,0.7498908856,0.186870502\C,-0
.0519947756,0.2592271748,1.5954869725\C,0.2519784561,-0.5554627874,4.2
592693342\C,-1.1475015436,-0.2506997078,2.3107203827\C,1.1971734876,0.
3547896862,2.23249034\C,1.3489697577,-0.0519029022,3.5534185993\C,-0.9
936965785,-0.6526575435,3.6368363322\C,-1.4772528094,0.6232815079,-0.5
867494549\C,-1.3818425181,1.0927117659,-2.0327034702\C,-2.7267128021,1
.0675974804,-2.7647545038\H,2.3196469597,0.0230517027,4.0356421046\H,2
.033090292,0.7546079735,1.6681938431\H,-2.1180116953,-0.3509640019,1.8
376880789\H,-1.8467543645,-1.0460142417,4.1823899635\H,0.3688914977,-0
.8727875088,5.2920777644\H,-2.2639916711,1.1667702462,-0.047650167\H,-
0.964919381,2.1048732245,-2.0209665851\H,-0.645588212,0.4622671601,-2.
5416596516\H,-2.6056259653,1.4141408972,-3.7962953622\H,-3.1460051515,
0.0569112244,-2.79747865\H,-3.4616685307,1.7212389915,-2.2786517938\O,
0.8013653809,1.2964188023,-0.3581053499\O,-1.9654468568,-0.7621012703,
-0.5225585343\O,-1.0717342045,-1.6111156922,-1.0097300454\\Version=EM6
4L-G09RevA.02\State=2-A\HF=-613.2256221\S2=0.753265\S2-1=0.\S2A=0.7500
07\RMSD=2.885e-09\RMSF=6.608e-06\Dipole=-0.5499388,0.455335,0.8722603\
Quadrupole=0.2073408,-5.0739708,4.86663,-2.6130571,3.338494,-3.6627553
\PG=C01 [X(C10H11O3)]\\@

DEF_2300H

1\1\GINC-V1336\FOpt\RB3LYP\Gen\C10H12O3\GXG501\09-Jul-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=6710886
40\def24ooh.freq\0,1\C,0.0483358095,0.1647890523,-0.0251428051\C,0.0
161780021,0.0601186619,1.4731068543\C,0.1471554667,-0.1360074226,4.269
411185\C,-1.0416159601,0.5328375856,2.2697742292\C,1.1404923525,-0.505
9868498,2.0992975116\C,1.2037573833,-0.6087638349,3.4848053457\C,-0.97
03860484,0.4365321806,3.6602371223\C,-1.2228412509,0.5726363199,-0.804

5765684\C,-1.0805774248,0.3693149729,-2.3129412909\C,-2.2931876041,0.8
847839438,-3.0920402303\H,2.0759787207,-1.0533656429,3.956157777\H,1.9
550052161,-0.8542326519,1.4727251001\H,-1.9201354305,0.9694107532,1.80
97518593\H,-1.790420373,0.810160656,4.2672616306\H,0.1964918258,-0.212
7757311,5.352367518\H,-1.4263180296,1.6345522219,-0.5906801547\H,-0.16
54216322,0.8752290151,-2.6368550417\H,-0.9258656148,-0.6981660077,-2.5
020908125\H,-2.1684537084,0.7019118228,-4.1647105519\H,-3.2113460849,0
.3864565192,-2.7664667599\H,-2.4299234325,1.9650065561,-2.9532696137\O
,1.0829168188,-0.0476120156,-0.6359899007\O,-2.3954731791,-0.055073902
2,-0.2709922288\O,-2.1789740286,-1.4961485453,-0.3189139339\H,-2.05510
85121,-1.6765297137,0.6321478024\\Version=EM64L-G09RevA.02\\State=1-A\\H
F=-613.8593637\RMSD=4.287e-09\RMSF=3.696e-06\Dipole=-0.154613,0.24916,
1.1756996\\Quadrupole=-4.3982329,0.0305758,4.3676571,-2.2064852,1.13530
04,-2.9329499\\PG=C01 [X(C10H12O3)]\\@

DEF_23R

1\1\GINC-V1289\FOpt\UB3LYP\Gen\C10H11O1(2)\GXG501\08-Jul-2010\0\\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\\def24r.freq\\0,2\C,-0.5005590639,1.4940471569,1.1201664054\C,-0
.1689618883,0.5566998549,2.2477416445\C,0.5722924308,-1.1141046035,4.3
805506596\C,-1.0334867397,-0.4533341816,2.6972317992\C,1.0676768987,0.
7232962099,2.8906144562\C,1.4381930893,-0.1074862056,3.94405924\C,-0.6
656167147,-1.2812454072,3.7578454815\C,-1.6023523351,1.2038920679,0.23
39820499\C,-1.9829268735,2.1126017406,-0.8822643365\C,-1.8298547012,1.
451437047,-2.2687775522\H,2.4016272343,0.0292964242,4.4279727078\H,1.7
219549905,1.5161143061,2.5436234959\H,-2.0085784256,-0.5895666963,2.23
96188136\H,-1.3480564879,-2.0549046858,4.0994030572\H,0.8593918257,-1.
7621972406,5.2043840595\H,-2.1466573985,0.2683763429,0.3355793217\H,-3
.0362608509,2.4096462402,-0.7550069294\H,-1.3739355244,3.0186804801,-0
.8231191265\H,-2.156290638,2.1396871815,-3.0559616446\H,-0.7852206751,
1.1856594798,-2.4607206487\H,-2.4317636776,0.5385287752,-2.3475131153\
O,0.1966545658,2.510326247,0.9358374091\\Version=EM64L-G09RevA.02\\Stat
e=2-A\\HF=-462.8725356\\S2=0.764374\\S2-1=0.\\S2A=0.750069\\RMSD=7.408e-09\
RMSF=2.398e-06\\Dipole=-0.6555714,-0.8593424,0.0008843\\Quadrupole=1.567
8806,-3.832077,2.2641964,-0.9471189,3.9574435,-2.3523026\\PG=C01 [X(C10
H11O1)]\\@

DEF_24

1\1\GINC-V1391\FOpt\RB3LYP\Gen\C5H8O2\GXG501\08-Jul-2010\0\\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456
\\def22.freq\\0,1\C,0.3935073069,-0.7414590926,-0.2221212462\C,0.04176
31735,-0.204763837,0.9459412559\C,1.0229598834,0.1708849598,2.01633170
09\O,1.0119185674,1.5995584783,2.2842086322\C,0.0448863988,2.044296652
9,3.1208368642\C,0.1646059294,3.536373072,3.3281879565\O,-0.7936508997
,1.3293837309,3.6260262844\H,-0.629621428,3.8753120906,3.9940447803\H,
0.094062782,4.0560556187,2.3671268591\H,2.0486167966,-0.0432952025,1.7
076795666\H,0.8011767778,-0.3528872486,2.9512869029\H,1.1414663907,3.7
793243136,3.7591289323\H,-0.3450049539,-1.0274299196,-0.966126069\H,1.
4355081306,-0.9240401286,-0.4781501012\H,-1.0057793204,-0.0319588964,1
.1846105169\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-345.7818762\\RMSD=6
.918e-09\\RMSF=3.538e-05\\Dipole=0.5057414,0.1919715,-0.3962847\\Quadrupo
le=-1.3787833,2.4406093,-1.061826,-1.2303487,2.2820019,2.5580951\\PG=C0
1 [X(C5H8O2)]\\@

DEF_240O

1\1\GINC-V1292\FOpt\UB3LYP\Gen\C5H7O4(2)\GXG501\08-Jul-2010\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\\def22oo.freq\\0,2\C,-1.2423608885,0.0774342088,0.5305442896\C,-0.
1317793142,-0.5213977236,0.9570151234\C,1.1049934062,0.235701937,1.308
0288532\O,2.2228004531,-0.3079380822,0.646215881\C,3.1255880105,0.5780

161512,0.0963370366\C,4.3502442389,-0.1650076197,-0.3660892757\O,2.927
1599236,1.7624115084,0.0019100326\H,5.0002367616,0.5131901414,-0.91946
50463\H,4.067113344,-1.0172015512,-0.9912339373\H,1.0401784536,1.30921
12333,1.1277308134\H,4.8832932726,-0.5590565607,0.5060377665\H,-2.1326
188939,-0.4902282255,0.2762945756\H,-1.3035386684,1.1572370471,0.41655
94497\H,-0.0714124262,-1.6017639,1.0679891856\O,1.3156939058,0.0435906
136,2.7562740448\O,2.4544391469,0.5904433345,3.1467535744\\Version=EM6
4L-G09RevA.02\State=2-A\HF=-495.4903904\S2=0.752966\S2-1=0.\S2A=0.7500
06\RMSD=2.603e-09\RMSF=4.071e-05\Dipole=-0.4296703,-0.714772,-0.856286
7\Quadrupole=6.5986047,-2.1358253,-4.4627795,-2.0981031,-0.7973601,1.5
77245\PG=C01 [X(C5H7O4)]\\@

DEF_24OOH

1\1\GINC-V1475\FOpt\RB3LYP\Gen\C5H8O4\GXG501\09-Jul-2010\0\#B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640
\\def22ooh.freq\0,1\C,-0.4135642879,-0.2160304701,-0.0625538447\C,-0.
2692438661,-0.0152312629,1.2452330112\C,1.06533347,0.164077937,1.90071
33956\O,1.2003155861,-0.9849484612,2.8106417326\C,2.315358386,-1.13151
7695,3.5464029136\C,2.2934785381,-2.429939414,4.3138529377\O,3.2319504
073,-0.328405742,3.5922409849\H,3.1917028211,-2.5074856749,4.926922154
\H,2.2403545892,-3.2741272594,3.6185540862\H,1.8993892945,0.1480147159
,1.1960263937\H,1.4015246608,-2.4726742154,4.9470217074\H,-1.394748806
,-0.323716013,-0.5155196862\H,0.4412249329,-0.2777487576,-0.7320877786
\H,-1.1271517328,0.0487681521,1.9107916084\O,1.0655165935,1.3747055657
,2.5987727097\O,2.3727870766,1.9969981633,2.5012570032\H,2.8998936672,
1.3660376544,3.0481605709\\Version=EM64L-G09RevA.02\State=1-A\HF=-496.
1310189\RMSD=4.682e-09\RMSF=2.454e-05\Dipole=-0.3701368,-1.4173636,-0.
1771763\Quadrupole=-0.1334015,-3.5803034,3.7137049,-1.2184446,0.940509
7,-1.627584\PG=C01 [X(C5H8O4)]\\@

DEF_24R

1\1\GINC-V1363\FOpt\UB3LYP\Gen\C5H7O2(2)\GXG501\08-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\\def22r.freq\0,2\C,-0.2414469579,-0.5037832338,0.1682163969\C,0.0
543538909,0.4391899916,1.1341516986\C,1.2430947949,0.4822907274,1.8424
71439\O,1.4103429612,1.4762963438,2.7791557059\C,2.5904656707,1.517295
2227,3.4812287435\C,2.5763215987,2.6720650884,4.4489003756\O,3.4883605
751,0.7262767183,3.3196039006\H,3.5139227699,2.6880688378,5.0051174655
\H,1.7333428095,2.5754152816,5.1411698574\H,2.0715140951,-0.2055576886
,1.7281137033\H,2.4479915134,3.6159216361,3.9084237636\H,-1.1897549465
,-0.4904327951,-0.3566989172\H,0.4637165108,-1.2865769922,-0.096203626
6\H,-0.6817607646,1.2069269274,1.3683484326\\Version=EM64L-G09RevA.02\
State=2-A\HF=-345.1441335\S2=0.777968\S2-1=0.\S2A=0.750162\RMSD=6.266e
-09\RMSF=1.813e-05\Dipole=-0.4802437,0.5146203,0.1620243\Quadrupole=-2
.8450827,1.2896642,1.5554185,1.5676168,0.4992934,3.1516294\PG=C01 [X(C
5H7O2)]\\@

Solution-phase conformers

PAN_2OOH

1\1\GINC-V1296\FOpt\RB3LYP\Gen\C7H10N2O2\GXG501\27-Jun-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\\pan2ooh.freq\0,1\C,0.2235075112,0.3009561063,0.0276823008\C,0.07
42640008,-0.1731603537,1.4901103827\C,1.4524912189,-0.30406975,2.18681
01137\C,1.4893161974,-1.1263150283,3.5104264583\C,0.6793901394,-0.5365
702121,4.6820671159\C,-0.8553723628,0.7156310343,2.2063330976\C,1.0978

530818,-2.5125508435,3.2211667558\N,-1.6189141171,1.4216374024,2.72169
5389\N,0.766842345,-3.5949599508,2.9605888581\H,-0.7549477385,0.370159
2324,-0.4549940233\H,0.7005022387,1.2835374147,-0.0116156419\H,0.83533
35349,-0.4135810456,-0.532316514\H,2.1237500947,-0.7988590419,1.473030
9985\H,-0.3970900532,-0.5862996898,4.5055067197\H,0.9027524064,-1.0885
255376,5.5995372096\H,0.9598126566,0.5098501442,4.8236571855\H,2.54716
93846,-1.1445533867,3.8004264952\H,-0.3699002648,-1.1774161195,1.49097
98342\O,1.9066897323,1.025157833,2.4042650668\O,3.3200691034,0.9417183
087,2.7472429482\H,3.689855784,1.5000225879,2.0392195733\Version=EM64
L-G09RevA.02\State=1-A\HF=-532.5810811\RMSE=4.440e-09\RMSE=1.643e-05\Di
pole=1.431903,0.4910503,-0.9406296\Quadrupole=1.6852805,-10.1262396,8
.4409591,5.5300108,0.0347847,-2.3576804\PG=C01 [X(C7H10N2O2)]\@

PMMA_300H

1\1\GINC-V1362\FOpt\RB3LYP\Gen\C9H18O4\GXG501\19-Jun-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pmma300h.a2b3.freq\0,1\C,-0.1051074472,-0.1699640765,0.0852938905\
C,-0.2088365515,-0.1288291112,1.6175631144\C,1.1591383465,-0.272248906
6,2.295040828\C,-1.4440040803,-0.0592720521,-0.7026395593\C,-1.1373083
022,-0.3101364074,-2.2089145757\C,-2.3489711219,-0.3203214166,-3.14833
58246\C,-2.405202307,-1.1364518512,-0.1984094508\O,-1.8634911875,-2.39
04582433,-0.3439002398\O,-3.5035559828,-0.9463519688,0.2689549516\C,-2
.5921359482,-3.4824042041,0.2257166618\C,-2.0922369112,1.319917253,-0.
4953539945\H,-2.2994420783,1.5128964421,0.5601636729\H,-1.4211333022,2
.1032042272,-0.8664050226\H,-3.0762173145,-1.0898445513,-2.8634881109\
H,-2.8706515747,0.6419845735,-3.1624586234\H,-2.0287580737,-0.53570283
69,-4.1737331476\H,-3.0447025817,1.3996034218,-1.0246241792\H,-3.64953
46304,-3.2273271056,0.3145988994\H,-2.4078713681,-4.3373393381,-0.4262
66829\H,-0.8740972223,-0.9306141577,1.9681710155\H,-0.6726519707,0.810
6905185,1.9412815382\H,1.0673910345,-0.2472238468,3.3864266931\H,1.644
5790663,-1.2185041864,2.0225882802\H,1.8360369242,0.5380441838,1.99817
55601\H,0.3939014774,-1.1015195428,-0.2101283974\H,0.5441300591,0.6490
637401,-0.2547026107\H,-0.608004441,-1.2654075053,-2.2980049769\H,-0.4
327699887,0.4687324897,-2.530455159\O,-2.1770916015,-3.7468945608,1.53
1583478\O,-0.8614343639,-4.3627431637,1.4550980443\H,-0.2922972527,-3.
5776685626,1.5605493585\Version=EM64L-G09RevA.02\State=1-A\HF=-654.61
2715\RMSE=4.663e-09\RMSE=7.995e-06\Dipole=0.7814312,0.4959067,-0.64760
22\Quadrupole=0.1337448,-1.1938088,1.060064,2.163899,2.871779,2.845375
\PG=C01 [X(C9H18O4)]\@

PVA_400H

1\1\GINC-V1478\FOpt\RB3LYP\Gen\C9H16O6\GXG501\06-Jul-2010\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545
6\pva200h.freq\0,1\C,-0.0353645697,0.1074612566,0.0264169878\C,0.027
8323656,0.0669073988,1.5651987428\C,1.3457809221,0.0109467022,-0.64022
75947\C,-1.3079867708,0.307891918,2.253945544\C,1.290036658,-0.0965802
383,-2.1591913456\O,0.9520664899,1.1175553435,1.9638471816\C,1.9405485
726,0.7947111927,2.8376783235\O,2.0730199256,-0.3020847011,3.338021904
1\O,2.0246385688,-1.1569821438,-0.1108040061\C,3.2969771527,-0.9928356
164,0.3348124036\O,3.9085579045,0.0528569674,0.2640834227\H,0.75161048
21,0.7594968314,-2.5822516843\H,0.7841784744,-1.0152484716,-2.46630798
67\H,2.3048678166,-0.0949509165,-2.5679549761\H,-0.4993098881,1.041657
3521,-0.3115600688\H,0.4471050028,-0.8922426062,1.8712445276\H,1.91931
84901,0.8913720433,-0.3458809551\H,-1.1769817155,0.2522291573,3.339310
5658\H,-1.7092306276,1.2949114938,1.9996594154\H,-2.0348881279,-0.4495
026237,1.9501110973\O,-0.8330810846,-0.9871058411,-0.4454208982\O,-2.2
173624819,-0.5363595984,-0.5310412322\H,-2.3734805071,-0.6881309795,-1
.4807580404\C,3.8126584594,-2.2603831399,0.9658445686\C,2.8684009537,1
.9635102866,3.0545460524\H,3.3746542453,1.8536301148,4.0150618051\H,2.
3331298303,2.9145839373,3.0057879278\H,3.6198287919,1.9466747416,2.256
3562931\H,4.9037910253,-2.2589585331,0.9498185285\H,3.4178107087,-3.14
60928556,0.4628910391\H,3.4738194522,-2.2751589856,2.0083971791\Versi
on=EM64L-G09RevA.02\State=1-A\HF=-803.8695391\RMSE=8.999e-09\RMSE=7.39

0e-06\Dipole=-0.5206041,0.3514975,-0.8620573\Quadrupole=-2.0031088,0.2559251,1.7471837,-2.6842514,4.4802029,2.5287798\PG=C01 [X(C9H16O6)]\@

PMVC_300H

1\1\GINC-V1361\FOpt\RB3LYP\Gen\C8H16O5\GXG501\19-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545 6\pva4ooh.a3b2.freq\0,1\C,0.1180275741,0.0508111506,-0.0029387949\C,0.2274693724,0.0807456955,1.5268827172\C,1.6670061344,0.2793493475,2.0121024376\C,-1.2957982679,-0.1919435777,-0.5305901871\C,-1.3664626929,-0.273556402,-2.0565652005\C,-2.7728295228,-0.5239108622,-2.6097923259\O,-2.1212788421,0.9361668087,-0.094994669\C,-3.2408873912,0.6639408707,0.5783225665\O,-3.682995355,-0.4260471798,0.86254545\O,-3.8024630347,1.8547387361,0.9121994687\C,-5.1029936618,1.7912160054,1.5118972387\H,-3.4459856834,0.3073858825,-2.3755602825\H,-2.7457417976,-0.6302870408,-3.6995907333\H,-3.2112419696,-1.4365371844,-2.1908743842\H,-0.9547477321,0.6526963731,-2.4789764526\H,-0.6960124126,-1.0849779361,-2.3695689357\H,-1.7223601536,-1.0949122921,-0.0842622145\H,0.496259658,0.9934423906,-0.422289126\H,0.7597518531,-0.7477201422,-0.4009454945\H,-0.174318039,-0.8556110797,1.9385029769\H,-0.404480106,0.8877672852,1.9175397706\H,2.0843925811,1.2230384679,1.64005895\H,2.3201860142,-0.531024345,1.6654796211\H,1.7171572938,0.3021190247,3.1063502859\H,-5.1427157976,2.6302457126,2.2076801614\H,-5.2525330069,0.8225337454,1.9915890463\O,-6.1084654961,1.8820090041,0.5530911847\O,-6.1301944746,3.2544564194,0.0737488252\H,-5.4830924201,3.1991876723,-0.6547944306\Version=EM64L-G09RevA.02\State=1-A\HF=-690.5315321\RMSD=9.169e-09\RMSF=3.549e-06\Dipole=1.1134244,-0.0509809,-0.2934368\Quadrupole=-4.9450967,-0.6793295,5.6244262,-0.7144474,-0.8912482,0.5819245\PG=C01 [X(C8H16O5)]\@

PMVC_400H

1\1\GINC-V1351\FOpt\RB3LYP\Gen\C9H16O8\GXG501\19-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=26843545 6\pva2ooh.a2b2.freq\0,1\C,0.0867298368,0.1026552493,0.0687556265\C,0.1583581998,0.1832956828,1.6046660895\C,1.4523878979,-0.1428760956,-0.5868875503\C,-1.1856119341,0.3857090746,2.2889720916\C,1.3969231008,-0.2253227664,-2.1072593832\O,1.0174804052,1.3306300119,1.8652346017\C,1.7416678112,1.2927667032,2.995621981\O,1.7639595675,0.3958482371,3.8098752394\O,2.4442227421,2.4337419414,3.0652301334\C,3.2878381991,2.5454664795,4.2218359499\O,1.9594929498,-1.3927419856,-0.047872744\C,3.2956650073,-1.4978885793,0.0394077123\O,3.5776460972,-2.7097135199,0.5365299451\C,4.9785326931,-2.975369089,0.707469933\O,4.1061447546,-0.6521565453,-0.2738718097\H,0.9935580188,0.705472284,-2.5221395102\H,0.7642476378,-1.0577208102,-2.4261109022\H,2.4052478859,-0.364750357,-2.5063719145\H,-0.3069535657,1.0444031212,-0.3302168083\H,0.6509117405,-0.7108381178,1.9915255175\H,2.1259310246,0.6586023397,-0.2756598466\H,5.5025658631,-2.9125984647,-0.2498997515\H,5.4228308739,-2.262847318,1.40736295\H,5.0314740854,-3.9879325922,1.1079224351\H,3.7750010073,3.5164142754,4.1291273155\H,4.0309059959,1.7437995303,4.2355914839\H,-1.0377800908,0.4385661237,3.3715918356\H,-1.6659066367,1.3084003144,1.9473076712\H,-1.8505778661,-0.4528264043,2.0680745642\H,2.6938432029,2.4994719962,5.1384366998\O,-0.7844025331,-0.9613718629,-0.3285598131\O,-2.1316749084,-0.4168453272,-0.458075142\H,-2.2977317756,-0.6332502783,-1.393495609\Version=EM64L-G09RevA.02\State=1-A\HF=-954.3061375\RMSD=9.001e-09\RMSF=8.648e-06\Dipole=0.1455788,0.2501887,-0.5179114\Quadrupole=1.4976849,-2.8987275,1.4010427,-4.0106648,8.7056456,4.1934805\PG=C01 [X(C9H16O8)]\@

PU_100H

1\1\GINC-V1447\FOpt\RB3LYP\Gen\C7H15N1O4\GXG501\19-Jun-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\pu1ooh.a3b2.freq\0,1\C,-0.0669567754,0.0562889529,-0.2877260374\

O,-0.1370289247,-0.5373485472,0.7714368379\O,1.1081563583,0.4116230237
 ,-0.9128864571\C,2.3237377972,0.1408888265,-0.1969874881\C,3.370946734
 6,-0.3421077728,-1.1901701425\C,3.0044892853,-1.683525053,-1.832249552
 3\N,-1.1201774342,0.4417818939,-1.0555594405\C,-2.4981779302,0.2898836
 105,-0.608163351\C,-3.0429406923,1.5126820543,0.1422204419\C,-4.495847
 2514,1.3192392729,0.5866991999\H,2.0748256166,-1.6061729299,-2.4050901
 878\H,2.8701171426,-2.46754995,-1.0772189682\H,3.7953673076,-2.0113082
 599,-2.5150604513\H,4.3156083685,-0.4245466193,-0.6401190471\H,2.11280
 74481,-0.5916314224,0.5874326013\H,-2.5253622608,-0.5902725248,0.03994
 31261\H,-3.1189586025,0.0732637489,-1.4863447273\H,-2.4027442052,1.697
 4689129,1.0135204946\H,-4.5933010349,0.4568111017,1.2568619828\H,-5.15
 79256118,1.1500931939,-0.2716737897\H,-4.8653997825,2.1999163811,1.122
 5244177\H,-2.9640408115,2.3990423282,-0.5027271189\H,3.510837431,0.428
 3675683,-1.9537604799\H,-0.9163468898,0.9983550211,-1.8733665988\O,2.7
 024345455,1.2738256092,0.5488838206\O,3.0810473629,2.342206233,-0.3651
 847181\H,2.2157461384,2.7743540914,-0.4885005007\Version=EM64L-G09Rev
 A.02\State=1-A\HF=-631.3593993\RMSD=3.869e-09\RMSF=1.190e-05\Dipole=-0
 .9554951,0.3413521,-1.1427056\Quadrupole=0.84961,0.8843194,-1.7339294,
 -5.2065244,-0.4165299,-0.4203273\PG=C01 [X(C7H15N1O4)]\@

PES_100H

1\1\GINC-V1284\FOpt\RB3LYP\Gen\C7H14O4\GXG501\19-Jun-2010\0\#B3LYP/ge
 n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=26843545
 6\pes100h.a1b3.freq\0,1\C,-0.089874843,-0.266254445,-0.1386509816\O,
 -0.1450036935,-1.081720248,0.7526743478\C,1.1785444538,0.3047427361,-0
 .7358030159\C,2.4503573818,-0.3627408325,-0.2084101994\C,3.7206764547,
 0.2481768786,-0.8067573194\O,-1.183042603,0.265786827,-0.7642414641\C,
 -2.4739025085,-0.0028315804,-0.2093782892\C,-3.4476548291,-0.332439922
 2,-1.3345606275\C,-3.0632113869,-1.6069141394,-2.0916517445\H,-2.08178
 53718,-1.5023488496,-2.5641520293\H,-3.0265482774,-2.4748999322,-1.423
 0698478\H,-3.7960368452,-1.81935728,-2.8767471533\H,-3.4819260307,0.52
 57828803,-2.0152952064\H,-4.4449719819,-0.4353247787,-0.8917604858\H,-
 2.3720409454,-0.8095593905,0.5216410182\H,1.1799790302,1.382521282,-0.
 5203212719\H,1.1071112318,0.2267048729,-1.828671589\H,4.6168115361,-0.
 2452729424,-0.4148229225\H,3.7372335999,0.1487281775,-1.899245951\H,3.
 7994341789,1.3167533406,-0.5712867111\H,2.4106203212,-1.4366972989,-0.
 4274524345\H,2.4694920962,-0.2803664806,0.8842410318\O,-2.9736049807,1
 .1638202632,0.4030853666\O,-2.1236305656,1.4730129062,1.5402426679\H,-
 2.6636885442,1.11415445,2.2691790904\Version=EM64L-G09RevA.02\State=1
 -A\HF=-575.9955515\RMSD=3.297e-09\RMSF=4.872e-06\Dipole=-0.277376,-0.2
 556259,-0.2526213\Quadrupole=3.694372,-5.3388485,1.6444765,3.3749043,-
 2.5684973,1.7127427\PG=C01 [X(C7H14O4)]\@

PES_200H

1\1\GINC-V1280\FOpt\RB3LYP\Gen\C7H14O4\GXG501\19-Jun-2010\0\#B3LYP/ge
 n 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=26843545
 6\pes100h.a2b2.freq\0,1\C,0.003396802,0.2101271098,-0.0407857784\O,
 -0.0027039923,0.2867333941,1.1673335984\C,1.292140078,0.128786377,-0.8
 693076949\C,2.1024231762,-1.1170382647,-0.4775399983\C,3.4995896401,-1
 .1407652887,-1.1025892965\O,-1.1153489684,0.1828956513,-0.8007713359\C
 ,-2.3757311815,0.235719897,-0.0808132607\C,-3.5009282875,0.0767522678,
 -1.0914888016\C,-3.4985629458,-1.277425034,-1.8082733466\H,-2.56522185
 73,-1.4305197128,-2.3591580884\H,-3.604840153,-2.1016830955,-1.0925700
 637\H,-4.3277267665,-1.3440448213,-2.5204537238\H,-3.4432102886,0.8939
 248052,-1.8226995193\H,-4.4457089656,0.2146983216,-0.5491440297\H,-2.3
 79046487,-0.5648516828,0.6656284552\H,-2.4304532066,1.1912173256,0.450
 5656907\H,1.8691616244,1.0361154728,-0.6450226033\H,4.0396112418,-2.04
 41801096,-0.799458742\H,3.4436844298,-1.1242237988,-2.1945614115\H,4.0
 892186222,-0.2738487915,-0.7813149624\H,1.5345769998,-2.0069627592,-0.
 7779652868\H,2.1637434201,-1.1285840555,0.6156910397\O,1.0633372747,0.
 0433969458,-2.2659669478\O,0.5435686868,1.3211953548,-2.7163059814\H,-
 0.4102684013,1.1662703519,-2.5698592199\Version=EM64L-G09RevA.02\Stat
 e=1-A\HF=-575.9876154\RMSD=5.572e-09\RMSF=3.255e-06\Dipole=-0.8759339,

-0.2709988,0.1156587\Quadrupole=6.5687708,0.4225322,-6.9913031,-2.3050
868,1.9505114,0.0374431\PG=C01 [X(C7H14O4)]\@

PA_2OOH

1\1\GINC-V1287\FOpt\RB3LYP\Gen\C5H11N1O3\GXG501\06-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435
456\pa2ooh.freq\0,1\C,0.1158601962,-0.0117190114,0.0302567607\C,0.08
32983067,-0.055878535,1.560034193\C,1.4586796303,0.1669732463,2.194176
8518\N,1.3988329844,0.1034071354,3.6333987951\C,2.3556689637,-0.530234
7427,4.3926442696\O,3.2856293134,-1.1514840321,3.8999140899\C,2.166251
1042,-0.4219052048,5.8987846473\H,3.0373138958,0.0837921116,6.32759294
22\H,2.1353540394,-1.4301570225,6.3221630004\H,1.2608686378,0.11722633
5,6.1950845506\H,0.6744983428,0.6381777835,4.0909567105\H,2.1786146329
,-0.591476868,1.8717403079\H,0.7883012301,-0.7774802667,-0.3747642428\
H,0.4635377484,0.9623006949,-0.3247546125\H,-0.2847655498,-1.028935847
4,1.9079877422\H,-0.6105568041,0.7038470347,1.9410335549\H,-0.88276036
1,-0.1922766477,-0.3816911773\O,2.0850683793,1.3686171419,1.730141033\
O,1.2481622814,2.4880397762,2.1609904524\H,1.8922056942,2.9485445853,2
.7271594764\Version=EM64L-G09RevA.02\State=1-A\HF=-477.4992808\RMSD=2
.717e-09\RMSF=7.942e-06\Dipole=-0.9838176,0.5629916,0.8641451\Quadrupo
le=-3.3241731,-0.1004132,3.4245863,4.1157682,-0.7350535,3.8230179\PG=C
01 [X(C5H11N1O3)]\@

GLY

1\1\GINC-V1294\FOpt\RB3LYP\Gen\C4H8N2O2\GXG501\08-Jul-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684354
56\gly.freq\0,1\C,-0.2199790238,-0.0145854936,-0.133413699\C,0.03708
62014,0.219096247,1.3474414402\O,1.051858366,0.7654590735,1.7547958711
\N,-0.9529073714,-0.2309269857,2.1933073792\C,-0.9438441521,0.05683375
82,3.6169260232\C,-0.9406479465,-1.1669590877,4.5414422162\N,-0.521906
3938,-2.3353658103,3.9716023648\O,-1.2934729677,-1.0696370079,5.706034
358\H,-0.35108181,-3.1171640642,4.5887842565\H,-1.8092567798,-0.581689
1674,1.7871078398\H,-1.8001791679,0.6741285593,3.9077951525\H,-0.03400
99838,0.6339467479,3.8112621462\H,-0.4333212686,0.9476622515,-0.611600
4068\H,0.6903677563,-0.4110773076,-0.5903963783\H,-1.0518961052,-0.697
2043022,-0.3343886691\H,-0.0741488071,-2.3285613351,3.0669331086\Vers
ion=EM64L-G09RevA.02\State=1-A\HF=-417.2219845\RMSD=7.818e-09\RMSF=2.1
20e-06\Dipole=-0.5744113,-0.8494206,-1.5245884\Quadrupole=-0.9076263,4
.1229375,-3.2153112,-4.454444,5.186863,0.7232834\PG=C01 [X(C4H8N2O2)]\
\@

GLYOOH

1\1\GINC-V1394\FOpt\RB3LYP\Gen\C4H8N2O4\GXG501\09-Jul-2010\0\#B3LYP/g
en 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=4026531
84\glyooh.freq\0,1\C,-0.0983814805,0.0570181757,-0.0506308312\C,-0.0
517924065,0.1967324701,1.4611832198\O,0.9830037672,0.3441812668,2.0892
895963\N,-1.2896825333,0.1372663264,2.0841604556\C,-1.3778277857,-0.03
4085242,3.5018903862\C,-2.6073893635,-0.9188581594,3.815494561\N,-2.94
71236346,-0.9342739002,5.1280387744\O,-3.1618498469,-1.5714468231,2.94
11912807\H,-3.8142181071,-1.3905545356,5.3773270899\H,-2.068071324,-0.
276229809,1.5779841758\H,-0.454558131,-0.4817999392,3.8903900163\H,0.8
113435311,0.4852242504,-0.474325102\H,-0.1377649916,-1.0056835882,-0.3
200273939\H,-0.9759844691,0.5477053721,-0.4840726889\H,-2.6157513066,-
0.1865580408,5.7226970387\O,-1.4305513822,1.1913744302,4.2343118705\O,
-2.6498151394,1.8810193218,3.8436002999\H,-2.3309725662,2.3602658734,3
.0553106681\Version=EM64L-G09RevA.02\State=1-A\HF=-567.570415\RMSD=5.
375e-09\RMSF=4.660e-06\Dipole=-0.7565471,0.0970654,-0.1419185\Quadrupo
le=-6.8352668,-1.6778012,8.513068,-2.4197712,-3.49443,-3.8759577\PG=C0
1 [X(C4H8N2O4)]\@

ALA

1\1\GINC-V1336\FOpt\RB3LYP\Gen\C5H10N2O2\GXG501\09-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653
184\ala.freq\0,1\C,-0.0728078047,-0.0887311442,-0.0404979024\C,-0.42
96003446,0.3439050359,1.3738175813\O,-0.2707694565,1.49229502,1.762433
085\N,-0.9516100518,-0.6471976152,2.1768964339\C,-1.1351171452,-0.4644
476217,3.6149178515\C,-2.5692478309,-0.7905846817,4.0805884801\N,-3.52
45519249,-0.7681821896,3.1054856339\O,-2.8175230561,-1.0402630956,5.25
1068003\H,-4.4899491127,-0.8103997069,3.4010526161\H,-0.9155237063,-1.
5996234572,1.8361387526\H,-0.9932348806,0.6102198537,3.7789837301\H,-0.
433741415,0.6679691977,-0.7417058907\H,1.0180997958,-0.1282156947,-0.
1346485633\H,-0.4832769314,-1.0647840367,-0.3185576618\H,-3.3103703844
,-0.4041274854,2.1891427865\C,-0.1042507275,-1.2427926401,4.4383112255
\H,-0.3056180561,-1.1077380346,5.5027930602\H,0.9059292771,-0.88970434
88,4.2103622818\H,-0.1571819414,-2.3171451145,4.2228657414\Version=EM
64L-G09RevA.02\State=1-A\HF=-456.5389388\RMSD=5.907e-09\RMSF=4.796e-06
\Dipole=-0.1021043,-0.8874946,-1.4822039\Quadrupole=4.7789831,-3.18519
67,-1.5937864,-3.7914491,3.6763693,4.0298865\PG=C01 [X(C5H10N2O2)]\@

ALAOO

1\1\GINC-V1293\FOpt\UB3LYP\Gen\C5H9N2O4(2)\GXG501\11-Jul-2010\0\#B3LY
P/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2684
35456\alao0.freq\0,2\C,-0.0202621923,-0.0586092559,0.0005520824\C,-0.
.1574786297,-0.4481626213,1.4606231047\O,0.4102616423,-1.4051606725,1.
960160713\N,-0.9942620782,0.3672810933,2.2013012745\C,-1.3568692356,0.
0673255692,3.5429444756\C,-0.1104920721,-0.2462150945,4.4186152682\N,-
0.1209227379,-1.4347396401,5.0813461608\O,0.729176321,0.6242185764,4.5
648201939\H,0.7467890277,-1.6743269915,5.5445249688\H,-1.5694873663,1.
0402809731,1.7132478344\H,0.8647263623,-0.5468535371,-0.4094222944\H,-
0.8989070131,-0.4013813393,-0.5595989467\H,0.0648258694,1.0255501274,-
0.1286357993\H,-0.6576904663,-2.1997541123,4.6953759514\C,-2.147005929
1,1.2114650103,4.1662411606\H,-2.4635767693,0.9377411463,5.1759284719\H,
-3.0380364344,1.4178716274,3.5647210832\H,-1.5111465954,2.0975312712
,4.222038259\O,-2.2352820965,-1.1612739246,3.5830204918\O,-3.243632278
9,-1.0636976068,2.7406462164\Version=EM64L-G09RevA.02\State=2-A\HF=-6
06.2468747\S2=0.753126\S2=1=0\S2A=0.750007\RMSD=1.478e-09\RMSF=1.204e
-06\Dipole=-0.5711725,0.4531105,-0.4686861\Quadrupole=-6.2496303,0.696
1409,5.5534894,-5.0156908,-0.6967358,-6.0395022\PG=C01 [X(C5H9N2O4)]\@

ALAOOH

1\1\GINC-V1340\FOpt\RB3LYP\Gen\C5H10N2O4\GXG501\10-Jul-2010\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088
640\alaooh.freq\0,1\C,0.0324832381,0.1289495821,0.0259819503\C,0.022
6057671,-0.1410939897,1.5213502799\O,1.0407364451,-0.302233535,2.17488
85878\N,-1.2313695742,-0.1845085317,2.0980794422\C,-1.4243187006,-0.17
78719471,3.5349903425\C,-0.5049908618,0.8983572296,4.2010309336\N,0.18
41683129,0.4972157023,5.3000809664\O,-0.5401584949,2.042491367,3.78040
61446\H,0.870952435,1.1486681184,5.6573193439\H,-2.0255536266,0.082801
9853,1.5329527996\H,0.0777387018,1.2120236321,-0.1395980101\H,0.928070
7482,-0.3187959573,-0.4085267418\H,-0.8561502562,-0.2585313948,-0.4836
837844\H,0.3552433177,-0.4901932591,5.433202521\C,-2.8800972974,0.1681
166882,3.8534132834\H,-3.0342853448,0.1183413748,4.9342086895\H,-3.552
7966451,-0.5475256961,3.3736516937\H,-3.0988655519,1.1833957495,3.5122
255963\O,-1.0404440328,-1.4328384645,4.1079154834\O,-1.9058770616,-2.4
804975938,3.6059643137\H,-1.3955130842,-2.7594555989,2.8225414488\Ver
sion=EM64L-G09RevA.02\State=1-A\HF=-606.8805826\RMSD=7.231e-09\RMSF=1.
203e-05\Dipole=-0.6260257,-0.5018664,-0.7084102\Quadrupole=-1.40187,-5
.674256,7.076126,-0.9275689,5.0858699,1.7719615\PG=C01 [X(C5H10N2O4)]\@

PHE_100

1\1\GINC-V1385\FOpt\UB3LYP\Gen\C9H10N1O3(2)\GXG501\09-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1073741824\pheoo.freq\0,2\C,0.0533120072,0.0885648851,0.0074517404\O,0.0459957174,-0.2121444957,1.1742538348\C,1.317903115,0.0541602163,-0.8762752551\C,2.6028197074,0.1380510768,-0.0423377241\N,1.2629666863,-1.0821414245,-1.7156803452\C,3.8752167992,-0.0340440949,-0.8433522236\C,6.2288713338,-0.367766597,-2.3496700916\C,4.4507557469,1.0505828961,-1.5223329282\C,4.498077918,-1.2874771504,-0.9327152845\C,5.6178647789,0.8858605975,-2.2675530126\C,5.6660484581,-1.4547488668,-1.6803162077\H,6.0526187895,1.7383959104,-2.7825174257\H,4.0688347313,-2.1351397331,-0.403368368\H,7.1402162747,-0.4943124111,-2.9278040809\H,6.137709724,-2.432474426,-1.7323549558\H,3.9805032925,2.0283457438,-1.4623382033\H,2.1261212559,-1.2229075201,-2.234325871\H,-0.8731863094,0.3703741327,-0.5365793215\H,2.5846705033,1.1078188977,0.4642530684\H,0.4718540255,-1.0663065741,-2.3531905229\H,2.5204331373,-0.6291929319,0.7326154165\O,1.2183908752,1.2913313353,-1.7432912332\O,0.8680144946,2.3431709607,-1.0166560065\Version=EM64L-G09RevA.02\State=2-A\HF=-629.2527892\S2=0.753568\S2-1=0.\S2A=0.750009\RMSD=4.060e-09\RMSF=1.741e-05\Dipole=0.5519701,-0.6228747,-1.0095535\Quadrupole=3.1116808,-0.7175385,-2.3941424,1.2768268,3.0082799,2.0090628\PG=C01 [X(C9H10N1O3)]\@

PHE_200

1\1\GINC-V1282\FOpt\UB3LYP\Gen\C9H10N1O3(2)\GXG501\11-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\phe100.freq\0,2\C,-0.077317993,-0.0577388936,-0.1026113286\O,-0.2427422766,0.1513754993,1.078090182\C,1.2770927227,0.0761380037,-0.7950348129\C,1.1371489586,1.0644613139,-1.9821872299\N,2.3642202068,0.4203126422,0.1029045026\C,1.094937201,2.5269580618,-1.6269698991\C,0.9636203951,5.2436107239,-0.9502745004\C,-0.1126777141,3.2283226374,-1.734077199\C,2.2437735607,3.2009685106,-1.1872345938\C,2.1743569175,4.5539885297,-0.8557025528\C,-0.1818625723,4.5781178002,-1.3889502294\H,3.0697087582,5.0708846307,-0.5211544372\H,3.1787642995,2.6592089671,-1.1059390361\H,0.9144228487,6.2970689785,-0.6882088328\H,-1.1258419006,5.1094352362,-1.4726376089\H,-1.0043707201,2.7176495274,-2.0914490094\H,2.7541558064,-0.4265317444,0.5091668764\H,1.4831397223,-0.8896650102,-1.2796416059\H,-0.9259300075,-0.3619661907,-0.7551376635\H,1.986654145,0.9585131558,0.8823635175\H,0.2552078723,0.7872002455,-2.5698694494\O,2.2877483378,0.8745778296,-2.8937671339\O,2.3211685823,-0.3462408623,-3.3879915871\Version=EM64L-G09RevA.02\State=2-A\HF=-629.242085\S2=0.753185\S2-1=0.\S2A=0.750007\RMSD=7.115e-09\RMSF=1.955e-06\Dipole=-0.5029334,0.2485756,0.2352206\Quadrupole=0.6180061,6.2369845,-6.8549906,0.4633686,7.2839453,-0.7825589\PG=C01 [X(C9H10N1O3)]\@

CYS_100H

1\1\GINC-V1343\FOpt\RB3LYP\Gen\C4H8N2O4S1\GXG501\09-Jul-2010\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=939524096\cys100h.freq\0,1\N,0.0004720245,-0.0496798184,-0.0508411163\C,0.0116225321,0.1205914481,1.2965179712\O,1.0206527749,0.2622526395,1.9708323464\C,-1.4022976241,0.0682403957,1.9502958886\N,-1.2275162326,0.5601467821,3.2916200025\C,-2.1316686091,0.4672170404,4.3116519776\O,-3.26917904,0.0370766477,4.2283674649\C,-2.0629078512,-1.3297038016,1.8370413215\S,-1.2215909371,-2.6635633119,2.766757385\H,-0.8504594499,0.1591656017,-0.5561543141\H,0.8757561505,0.1081701476,-0.5326018328\H,-1.811566883,-2.4044720893,3.9520304738\H,-3.096495183,-1.2465147493,2.1703391869\H,-2.0520429436,-1.6341898728,0.7890762287\H,-0.2587594516,0.7827446773,3.5099291396\H,-1.7090421347,0.8513524463,5.2606651565\O,-2.3115570698,0.8737465968,1.1819996859\O,-1.7610946047,2.2137053076,1.0713545438\H,-2.154517529,2.631360844,1.8607330725\Version=EM64L-G09RevA.02\State=1-A\HF=-965.7422765\RMSD=7.070e-09\RMSF=3.553e-06\Dipole=0.2320086,0.7434609,-0.553184\Quadrupole=-7.7442716,-0.0703714,7.814643,0.5861202,0.0776979,2.2469676\PG=C01 [X(C4H8N2O4S1)]\@