Supporting Information for

Inherent and Transferable Stabilization Energies of Carbon- and Heteroatom-centered Radicals on the Same Relative Scale and Their Applications

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Table S1 Experimental data corresponding to the R–H, R–CH$_3$, R–Cl and R–R bond dissociation energies (BDE) in kcal mol^{-1} in Table 1.[1,2]

R	R-H BDE	R-CH$_3$ BDE	R-Cl BDE	R-R BDE
C(O)OH	96.6	92.0±2.0		80.0±1.5
C(O)OCH$_3$	92.7±1.0[3,4,5] **95.4±2.0** 95.1 94.0 96.9 100.0 98.5	92.6±3.0		88.4±2.5
C(O)OCH$_2$CH$_3$				
C(O)OC(CH$_3$)$_3$				
C≡N	126.1±0.4	125.2±2.2	100.8±1.2	137.7±1.6
C(O)H	88.0±0.2	84.8±0.4		72.0
C(O)Ph	88.7±2.6	85.0	81.5±2.0	
C(O)CH$_3$	89.4±0.3	84.1±0.5	84.6±2.0	73.4±1.0
C(O)N(CH$_3$)$_2$				
C(O)N(CH$_2$CH$_3$)$_2$				
C(O)NH$_2$		88.5±1.5		
Ph	112.9±0.5	102.0±1.0	95.5±1.5 95.1±2.5	114.4±1.5
C≡CH	134.9±1.2 132.9±0.7 133.1±0.2 **133.0±0.7** 133.3±0.1 131.3±0.7	121.3±3.2	104.1±2.0	160.2±2.0
CH=CH$_2$	111.1±2.2 110.1±2.0 110.2±2.0 **111.2±0.8** 110.2±0.3	101.9±1.5	91.7±1.0 **94.8±1.1** 95.6±2.0 93.5	116.9±1.5
C(O)NHCH$_3$				
(E)-CH=CHCH$_3$	109.0±2.4 **111.1**	102.6±2.0	95.2	
CH=C(CH$_3$)$_2$				
C(CH$_3$)$_3$	**95.7±0.7**	86.9±0.7	84.1±1.5	77.1±1.0
CH$_2$F	101.3±1.0	90.4±3.0 **93.2±2.0**	84.7±2.8	88.0±2.0
CH$_2$NO$_2$	99.3	87.1		
CH$_2$OC(O)H				
CH2OC(O)CH$_3$	96.7			
CH$_2$C≡N	96.0	83.2±3.0	63.9 66.4±0.7 70.5	70.7±4.0
CH(CH$_3$)$_2$	98.1±0.7	88.2±0.9	84.6±1.5	84.5±1.1
CH$_2$OH	96.1±0.1			85.6±1.5

[1] Luo, Y.-R., Comprehensive Handbook of Chemical Bond Energies. CRC Press: Boca Raton, FL, 2007

[2] Experimental data taken from Luo[1] unless otherwise noted. Where available, the bolded value is Luo's "recommended" value.

[3] NIST Chemistry WebBook, NIST Standard Reference Database Number 69, http://webbook.nist.gov/chemistry/ Accessed June 6 2013

[4] The experimental value may be wrong. The preferred value is 95.4±2.0. $\Delta_f H^0$(H) is 52.1, $\Delta_f H^0$(R-H) is -80.5, -83.4, -86.5 and -85.0 from NIST,[3] and $\Delta_f H°$(R) is -38.6 from Luo[1], which gives BDE(R-H) 94.0, 96.9, 100.0 and 98.5. (G3(MP2)-RAD gives 100.1)

R	R-H BDE	R-CH$_3$ BDE	R-Cl BDE	R-R BDE
CH$_2$SH	93.9±2.0	82.5±2.2		74.9±2.8
CH$_2$Cl	100.1±0.5	89.8±2.2	79.3 80.9 77.9 **80.8±0.8** 78.5	87.2±3.3 **86.2±2.0** 87.1±1.3
cyclo-C$_3$H$_5$	106.3±0.2	96.2		102.8
CH$_3$	105.0±0.1	90.2±0.2	83.7±0.4	90.2±0.2
CH$_2$SCH$_3$	93.7±1.4	82.0±2.0	72.0±0.6	
CH$_2$C≡CH	89.2±2.4 87.2±2.0 90.3±3.0 **88.9±1.0** 91.8±1.0	76.0±2.0 76.6±1.2		
CH$_2$CH=CH$_2$	88.1±0.7	76.5±2.2 **75.9±0.9**	71.3±1.2	61.5±1.0
CH$_2$Br	101.6±1.0			
CH$_2$CH$_3$	**100.5±0.3**	88.5±0.5	84.2±0.8	86.8±0.6
CH$_2$C(O)OH	95.3±2.9	84.5±3.0	66.6 74.3±0.5	81.9±1.0
CH$_2$SiH$_3$				
CH$_2$-cyclo-C$_3$H$_5$	97.4±1.6			
CH$_2$C(O)CH$_3$	95.9±0.7	86.5±3.0		
CH2C(O)NH$_2$			80.7	
CH$_2$Ph	88.5±1.5	76.4±1.7	72.9±2.0 71.6 **71.7±1.0**	62.6±2.2
CH$_2$S(O)CH$_3$	94.0			
CH$_2$S(O$_2$)CH$_3$	99.0			
CH$_2$NH$_2$	93.9±2.0	82.2		68.4±3.0
CH$_2$N(CH$_3$)$_2$	93.2			
N(CH$_3$)$_2$	94.6±2.0	75.6±2.5 79.3		59.6
NHCH$_3$	101.6±2.0	**82.2±2.5** 81.9		66.0±3.0
NH$_2$	108.2±0.3	85.7±0.5	60.5	67.4 **66.2±0.3**
NO$_2$		60.8 63.7 **62.3±0.5**	34.0	13.7±0.2
NHC(O)H	108.5			
NHC(O)CH$_3$	107.5			
OH	119.30±0.05	92.00±0.17	55.8	46.8±1.4
OCH$_2$CH$_3$	105.4±1.4	83.6±1.0		39.7
OCH$_3$	105.2±0.7	84.1±1.0	48.0	40.0±1.5
OC(O)H	112.0±3.0	91.7±3.0		
OC(O)CH$_3$	112.0±3.0	90.9±3.0		33.5±5.0
S(O$_2$)CH$_3$	≤94.9[5]	66.8	70.0	
SH	91.1±1.0 92.9±2.0 91.2±0.7 **91.2±0.7** 91.2±0.1	74.0±1.5 **74.7±1.0**		64.7±2.0
S(O)CH$_3$		53.0±2.0 55.1±2.4		

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[5] Not plotted in Figure 1.

R	R-H BDE	R-CH$_3$ BDE	R-Cl BDE	R-R BDE
SCH$_3$	88.3 86.4±2.2	77.2±2.0 73.6±0.8	70.0±3.0	64.0 62.9±2.6 65.2±0.9
SCH$_2$Ph	86.9 87.8			
F	136.157±0.003	109.8 112.8	62.3 61.2	37.923±0.023
Cl	103.098±0.003		57.978±0.001 57.939±0.461	57.978±0.001 57.939±0.461
Br	87.51±0.05	69.8	52.42±0.01	46.333±0.029
BH$_2$	82.6[5,67] 74.6[5,66] 107.1±3.6[8]			
SiH$_3$	91.7±0.5	90±1	109±2	77±1
PH$_2$	83.9±0.5			61.2

[6] Chase, M.W., Jr., *NIST-JANAF Themochemical Tables, Fourth Edition*, J. Phys. Chem. Ref. Data, Monograph

[7] Experimental value reported by Luo is wrong. Δ_fH^0(BH$_3$) is 25.50 from Chase[6], and should be 21.0±2.4 from NIST[6], and $\Delta_f H°$(•BH$_2$) is 48.00 from Chase[6], and should be 76.1±2.6 from NIST[3]. Using the corrected heats of formation gives BDE(R–H) 107.1±3.6 which is closer to the G3(MP2)-RAD value (104.7)

[8] From the NIST website.[3]

Table S2 Comparisons with known D[R–R′]. D[R–R′]$_{calc}$ by equation (8) with RSE$_{Et}$ and χ from Table 1. D[R–R′]$_{lit}$ literature values of bond dissociation energies, with reported uncertainties when significant, values reported in reference 9, and values obtained by D[R–R′] = D[CH$_3$–CH$_3$] – RSE$_H$[R·] – RSE$_H$[R′·]. Gas phase values in kcal mol^{-1} at 298 K.

R·[10]	·R′	D[R–R′]$_{calc}$	D[R–R′]$_{lit}$[11]	D[R–R′][12]	D[R–R′][13]
CH$_3$CH$_2$	CH$_2$CH=CH$_2$	73.2	74.3±1.5,[1] 74.3±2[14]		68.2
CH$_3$CH$_2$	CH(CH$_3$)$_2$	87.0	86.1,[15] 87.1[14]		79.9
CH$_3$CH$_2$	(CH$_3$)$_3$C	86.9	86.4,[16] 83.3,[15] 83.8[14]		78.6
(CH$_3$)$_2$CH	CH$_2$CH=CH$_2$	72.9	73.7,[15] 74.7[14]		65.9
(CH$_3$)$_3$C	CH$_2$CH=CH$_2$	72.9	72.9±1,[15] 72.4±1[14]		64.6
CH$_2$=CHCH$_2$	CH=CH$_2$	85.5	87.3±0.8,[16] 86.5[14]		77.8
HC≡CCH$_2$	CH$_3$	78.1	79.6,[15] 76.3±1[14]		76.0
HC≡CCH$_2$	CH$_2$CH$_3$	77.9	77±3,[16] 78.0,[15] 74.9±1[14]		72.8
N≡CCH$_2$	CH$_3$	83.0	84.3,[17] 83.2±3[15]	80.1	80.9
N≡CCH$_2$	CH$_2$CH$_3$	83.1	83.6,[17] 82.4±1.3[15]		77.7
N≡CCH$_2$	CH=CH$_2$	94.7	94.8,[17] 94.2±1[15]		87.3
PhCH$_2$	CH$_3$	76.9	77.6,[18] 77.2±1[14]	75.0	74.0
PhCH$_2$	CH$_2$CH$_3$	76.3	76.7,[16] 76.0[14]		70.8
PhCH$_2$	CH(CH$_3$)$_2$	76.1	76.4,[16] 75.8[15]		68.5
PhCH$_2$	Ph	91.3	97.0,[16] 91.7±2,[15] 91.1±2.2[14]		82.9
Ph	CH$_3$	103.0	102.9±1,[15] 103.8±2[14]	101.1	97.5
Ph	CH$_2$CH$_3$	102.4	100.2,[15] 102.3±2[14]		94.3
Ph	CH=CH$_2$	114.7	115.3±1,[15] 116.9±2.2[14]		103.9
Ph	cyclo-C$_3$H$_5$	112.6	112.4±1.5,[15] 111.9±3.2[14]		102.3
Ph	CH(CH$_3$)$_2$	102.2	100.7±1.5[1] 99.0±1,[15] 102.1±2[14]		92.0
Ph	CH$_2$OH	101.0	98.3±1,[15] 101.6±2.2[14]	95.1	89.8
Ph	CH$_2$NH$_2$	96.5	94.2±2.2,[15] 95.6±2.8[19]		86.8
Ph	CH$_2$NO$_2$	105.2	108.0±1[20]		94.6
Ph	CH$_2$Cl	103.1	102.7±2.1[15]		92.7
Ph	CH$_2$SH	97.7	92.9±2.2[25]		88.9
Ph[21]	CH$_2$S(O$_2$)CH$_3$	107.7	104.6±3.2[15]		98.1

[9] De Vleeschouwer, F.; Van Speybroeck, V.; Waroquier, M.; Greelings, P.; De Proft, F. *J. Org. Chem.* **2008**, *73*, 9109–9120.

[10] Standard enthalpies of formation, Δ$_f$H°[RR′], are from reference 14, unless indicated otherwise.

[11] Value either reported in the reference indicated or obtained by D[R–R′] = Δ$_f$H°[·R] + Δ$_f$H°[·R′] – Δ$_f$H°[RR′] with values of Δ$_f$H°[·R] and Δ$_f$H°[·R′] from the reference indicated.

[12] Reported in reference 9.

[13] Calculated using RSE$_H$[R·] values applicable to C–C bonds only (see text).

[14] Afeefy, H. Y.; Liebman, J. F.; Stein, S. E. Neutral Thermochemical Data. In *NIST Chemistry Webbbook*, NIST Standard Reference Database Number 69; Linstrom P. J., Mallard W. G. Eds.; National Institute of Standards and Technology, Gaithersburg, MD 20899 at http://webbook.nist.gov.

[15] *Handbook of Chemistry and Physics*, 90th ed.; Lide D. R., Ed., CRC Press; Boca Raton, FL, 2009–2010.

[16] Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255–263.

[17] Goos, E.; Burcat, A.; Ruscic, B. *Ideal Gas Thermochemical Database with updates from Active Thermochemical Tables*, available at http://garfield.chem.elte.hu/Burcat/BURCAT.THR or at ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics/

[18] Experimental value cited in reference 9.

[19] Lias, S. G.; Liebman, J. F.; Levin, R. D.; Kafafi, S. A. NIST Standard Reference Database 25; Stein, S. E., Ed.; 1994. Chemical Kinetics and Thermodynamics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899. Version 2.0.

[20] Using Δ$_f$H°[·CH$_2$NO$_2$] =36.4 kcal mol^{-1} and Δ$_f$H°[cyclo-C$_3$H$_5$NO$_2$] = 4.2 from the compilation of Burcat, A. *J. Phys. Chem. Ref. Data* **1999**, *28*, 63–130.

R· [10]	·R′	$D[R–R']_{calc}$	$D[R–R']_{lit}$ [11]	$D[R–R']$ [12]	$D[R–R']$ [13]
$CH_2=CH$	CH_3	100.3	101.6,[15] 101.0[14]	98.7	95.0
$CH_2=CH$	CH_2OH	98.4	97.0,[15] 98.6±1.4[14]	92.5	87.3
$CH_2=CH$	CH_2CH_3	99.8	100.1,[1] 99.6[14]		91.8
$CH_2=CH$	cyclo-C_3H_5	109.9	111.0,[22] 108.4±2.5[15]		99.8
$CH_2=CH$	$CH(CH_3)_2$	99.6	98.6,[15] 99.1±1.1[14]		89.5
$CH_2=CH$	$C(CH_3)_3$	99.6	98.1,[15] 97.1±1.2[14]		88.2
$HC\equiv C$	CH_3	124.6	126.4±1,[15] 123.5±2[14]		116.7
$HC\equiv C$	CH_2CH_3	125.1	125.1±0.5,[16] 124.5,[15] 121.9±2[14]		113.5
$HC\equiv C$	cyclo-C_3H_5	134.0	135.8,[22] 132.7±2.5[15]		121.5
$HC\equiv C$	$CH(CH_3)_2$	125.6	124.5,[16] 124.0,[15] 122.4±2.2[14]		111.2
$HC\equiv C$	$C(CH_3)_3$	125.9	124.1,[23] 121.7,[15] 118.6±2[14]		109.9
$HC\equiv C$	$CH=CH_2$	136.3	137.6,[15] 133.6±2.4[14]		123.1
$HC\equiv C$	$CH=CHCH_3$	137.3	137.9,[22] 137.2[17]		124.4
$HC\equiv C$	Ph	139.3	141.2,[15] 140.7±2.8[14]		125.6
$HC\equiv C$ [24a]	$C\equiv N$	151.6	151.5,[15] 148.1±2[14]		139.2
$HC\equiv C$ [24b]	CH_2Cl	122.9	120.7±2[15]		111.9
$HC\equiv C$ [24b]	CH_2Br	123.4	120.3±2[25]		113.1
$HC\equiv C$ [24b]	$CH_2C\equiv N$	116.2	114.0,[17] 112.8±1[15]		109.0
$N\equiv C$	CH_3	121.9	124.7±2.2,[15] 121.1[14]	123.1	111.1
$N\equiv C$	CH_2CH_3	122.9	121.6,[16] 121.1±1.8,[15] 120.1[14]		107.9
$N\equiv C$	cyclo-C_3H_5	131.3	130.9,[26] 131.2,[22] 128.2±2.8[15]		115.9
$N\equiv C$	$CH(CH_3)_2$	123.7	120.9,[16] 120.6±1,[15] 120.6[14]		105.6
$N\equiv C$	$CH_2CH=CH_2$	107.7	108.7,[16] 108.2,[15] 107.2[14]		93.9
$N\equiv C$	$C(CH_3)_3$	124.2	117.8,[16] 117.3,[15] 115.8[14]		104.3
$N\equiv C$	$CH=CH_2$	133.7	133±1,[16] 134.8,[15] 133.8±1[14]		117.5
$HOCH_2$ [19]	CH_2NH_2	79.8	80.2±2.5[15]		70.2
$HOCH_2$ [19]	CH_2F	90.2	88.3±2[25]		77.9
$HOCH_2$ [19]	CH_2Cl	87.1	86.2±2[15]		76.1
$HOCH_2$ [19]	CH_2SH	81.6	79.2±2.2[25]		72.3
FCH_2 [19]	CH_2NH_2	86.0	83.0±1.9[25]		74.9
$HC(O)$	CH_3	83.8	86.1,[15] 86.0[14]	84.1	73.2
$HC(O)$	CH_2CH_3	82.8	83.3,[16] 82.9[14]		70.0
$HC(O)$	$CH(CH_3)_2$	82.2	83.3,[16] 84.0[14]		67.7
$HC(O)$ [27]	$CH=CH_2$	95.5	97.7±1,[15] 97.4±1.4[14]		79.6
$HC(O)$	$CH=CHCH_3$	96.3	100.5,[22] 99.1[17]		80.9
$HC(O)$ [19]	$CH_2C\equiv CH$	74.0	74.3,[15] 71.4±1[14]		60.6
$HC(O)$	Ph	98.0	99.3,[16] 97.9±1,[15] 100.2±2[14]		82.1
$HOC(O)$	CH_3	95.2	92.0,[28] 94.8±1,[22] 95.2±1[17]		85.2

[21] Mackle, H.; O'Hare, P.A.G. *Trans. Faraday Soc.* **1961**, *57*, 1521–1526. $\Delta_fH°[PhCH_2S(O_2)CH_3] = -68.0 \pm 1.0$ kcal mol^{-1}.

[22] Goldsmith, C. F.; Magoon, G. R.; Green, W. H. *J. Phys. Chem. A* **2012**, *116*, 9033–9057.

[23] From CBS-QB3 calculations of Sabbe, M. K.; Saeys, M.; Reyniers, M.-F.; Marin, G. B.; Van Speybroeck, V.; Waroquier, M. *J. Phys. Chem. A* **2005**, *109*, 7466–7480. $\Delta_fH°[HC\equiv CC(CH_3)_3] = 23.0$ kcal mol^{-1}; $\Delta_fH°[(E)-CH_3CH=CH] = 65.3$; $\Delta_fH°[(CH_3)_2C=CH] = 57.9$.

[24] (a) Rayne, S.; Forest, K. *Comput. Theor. Chem.* **2011**, *974*, 163–179. G4 theoretical calculations. (b) Rayne, S.; Forest, K. *Comput. Theor. Chem.* **2011**, *970*, 15–22. G4 theoretical calculations.

[25] Sander, S. P.; Abbatt, J.; Barker, J. R.; Burkholder, J. B.; Friedl, R. R.; Golden, D. M.; Huie, R. E.; Kolb, C. E.; Kurylo, M. J.; Moortgat, G. K.; Orkin, V. L.; Wine, P. H. *Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 17*, JPL Publication 10-6, Jet Propulsion Laboratory, Pasadena, CA 2011. Standard enthalpies of formation available in Appendix A of the downloadable file at http://jpldataeval.jpl.nasa.gov.

[26] Using $\Delta_fH°[cyclo-C_3H_5\cdot] = 69.5$ of Sirjean, B.; Glaude, P. A.; Ruiz-Lopèz, M. F.; Fournet, R. *J. Phys. Chem. A* **2008**, *112*, 11598–11610.

[27] Using $\Delta_fH°[CH_2=CHC(O)H] = -16.0$ kcal mol^{-1} from the G3SX calculations of Asatryan, R.; da Silva, G.; Bozzelli, J. W. *J. Phys. Chem. A* **2010**, *114*, 8302–8311. No experimental value found.

[28] Berkowitz, J.; Ellison, G. B.; Gutman, D. *J. Phys. Chem.* **1994**, *98*, 2744–2765.

R· [10]	·R′	D[R–R′]$_{calc}$	D[R–R′]$_{lit}$ [11]	D[R–R′] [12]	D[R–R′] [13]
HOC(O)	CH$_2$CH$_3$	95.0	91.7,[25] 94.0,[17] 94.1,[22]		82.0
HOC(O) [29]	C(CH$_3$)$_3$	95.2	92.6,[17] 92.0[22]		78.4
HOC(O) [30]	CH$_2$OH	93.7	93.6±2.5,[22] 92.3±2.5[25]		77.5
HOC(O) [19]	CH$_2$CH=CH$_2$	80.5	78.7±1,[25] 80.9[22]		68.0
HOC(O)	CH=CH$_2$	106.9	106.7±1[17]		91.6
HOC(O) [19]	Ph	109.7	108.0±2[17]		94.1
CH$_3$C(O)	CH$_3$	83.9	84.8,[15] 85.0[14]	85.4	74.3
CH$_3$C(O)	CH$_2$CH$_3$	82.7	83.5,[16] 83.4[14]		71.1
CH$_3$C(O)	CH(CH$_3$)$_2$	82.0	81.3,[15] 82.8±1.1[14]		68.8
CH$_3$C(O)	cyclo-C$_3$H$_5$	93.6	95.2,[26] 95.5,[22] 92.5±2.5[14]		79.1
CH$_3$C(O)	C(CH$_3$)$_3$	81.7	79.4,[16] 78.5[14]		67.5
CH$_3$C(O)	CH$_2$CH=CH$_2$	68.8	70.6,[15] 71.1±1[14]		57.1
CH$_3$C(O)	CH$_2$Ph	71.9	71.4,[16] 70.1±1.4[14]		59.7
CH$_3$C(O)	CH=CH$_2$	95.5	96.4±2.8,[15] 96.4±3[14]		80.7
CH$_3$C(O)	Ph	98.0	98.8±0.8,[16] 99.8±2.1[14]		83.2
NH$_2$C(O)	CH$_3$	87.5	88.2±1,[25] 86.5[17]		79.2
NH$_2$C(O)	CH$_2$CH$_3$	86.7	86.7±1,[25] 84.7[17]		76.0
NH$_2$C(O)	CH(CH$_3$)$_2$	86.3	85.9±1,[25] 83.9[17]		73.7
NH$_2$C(O)	CH=CH$_2$	99.2	99.0±1.1,[25] 97.0±1.1[17]		85.6
NH$_2$C(O)	Ph	101.8	101.5±2.2[14]		88.1
CH$_3$O	CH$_3$	81.5	84.0,[31] 84.1,[15] 82.9±1[14]	82.6	
CH$_3$O	CH$_2$CH$_3$	83.9	85.0,[18] 85.1,[15] 84.2[14]	80.5	
CH$_3$O	CH(CH$_3$)$_2$	85.7	85.8,[18] 86.3[14]	78.5	
CH$_3$O	C(CH$_3$)$_3$	86.8	84.0,[18] 84.6,[15] 83.2[14]	76.9	
CH$_3$O [19]	CH$_2$Ph	70.8	72.7,[15] 71.6±1[14]	68.4	
CH$_3$O	SiH$_3$	113.8	111.9[31]		
CH$_3$O	PH$_2$	75.6	78.2[31]		
CH$_3$CH$_2$O	CH$_3$	83.4	83.5,[15] 83.3[14]	81.9	
CH$_3$CH$_2$O	CH$_2$CH$_3$	86.0	85.5,[15] 85.6[14]		
HC(O)O	CH$_3$	88.2	87.1±4.2,[16] 86.1±4.2[15]		
HC(O)O	CH$_2$CH$_3$	91.0	93.9,[22] 93.7[17] 92.6±3[15]		
HC(O)O	Ph	103.9	106.1±3,[16] 103.5±3.1[15]		
CH$_3$C(O)O	CH$_3$	84.3	88.1,[22] 86.1,[17] 90.1±3[15]		
CH$_3$C(O)O	CH$_2$CH$_3$	87.0	90.0,[22] 88.0,[17] 91.9±3,[15] 89.9[25]		
CH$_3$C(O)O	CH(CH$_3$)$_2$	89.0	93.3,[22] 91.6,[17] 95±3.1[15]		
CH$_3$C(O)O	C(CH$_3$)$_3$	90.2	91.5,[22] 89.7,[17] 91.7±3[15]		
CH$_3$C(O)O	Ph	99.8	101.3,[25] 102.7±3[15]		
CH$_3$	OH	90.5	92.2,[31] 92.1,[18] 92.4[14]	95.2	
CH$_3$CH$_2$	OH	93.2	94.2,[31] 94.0[18] 94.0[14]	93.3	
(CH$_3$)$_2$CH	OH	95.2	95.5,[31] 95.5,[18] 96.5[14]	91.6	
cyclo-C$_3$H$_5$ [32]	OH	99.5	103.3,[22] 100.6±2.5[14]		
(CH$_3$)$_3$C	OH	96.4	96.3,[31] 95.5,[18] 95.2,[15] 95.0[14]	90.0	
CH$_2$=CHCH$_2$	OH	77.1	80.1,[18] 79.5±1,[15] 79.8[14]	77.9	
HC≡CCH$_2$	OH	76.1	77.5[33]		
PhCH$_2$	OH	79.8	82.6,[18] 79.9,[15] 81.4[14]	80.9	
HOC(O)CH$_2$ [34]	OH	81.7	88.4±3.9[15]		

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[30] $\Delta_f H°$[HOCH$_2$CO$_2$H] = −139.3 ± 2.4 kcal mol$^{−1}$ from Dorofeeva, O.; Novikov, V. P.; Neumann, D. B. *J. Phys. Chem. Ref. Data* **2001**, *30*, 475–513.

[31] D value reported by the high level W1w calculation of Chan, B.; Radom, L. *J. Phys. Chem. A* **2012**, *116*, 4975–4986.

[32] Using $\Delta_f H°$[cyclo-C$_3$H$_5$OH] = −24.2 from the G3 calculation of Bond, D. *J. Org. Chem.* **2007**, *72*, 7313–7328.

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R· [10]	·R´	D[R–R´]$_{calc}$	D[R–R´]$_{lit}$ [11]	D[R–R´] [12]	D[R–R´] [13]
CH$_3$O	OH	43.2	43.8,[31] 45.4,[15] 44.7[14]	51.5	
CH$_3$CH$_2$O	OH	42.3	42.7±1.5[15]	50.7	
CH$_3$C(O)O	OH	41.8	40.6[15]		
HS	OH	68.9	70.1,[31] 70.1±4[15]	73.2	
CH$_3$S	OH	72.4	72.5,[31] 72.6±3[15]	71.4	
H$_2$N [19]	OH	59.7	63.7,[31] 63.4±2.2[15]	78.1	
CH$_3$NH	OH	59.3	63.2[31]		
(CH$_3$)$_2$N	OH	57.9	62.2[31]		
F	OH	47.2	48.3,[31] 51.8[14]	52.9	
PH$_2$	OH	85.6	89.9[31]		
Cl	OH	55.1	55.8,[31] 56.1[14]	66.5	
SiH$_3$	OH	125.6	124.3,[31] 124.0[35]		
Br [36]	OH	53.4	55.7,[25] 55.1[14]	65.4	
CH$_3$	NH$_2$	82.9	84.8,[31] 85.2,[18] 85.9[14]	87.3	
CH$_3$CH$_2$	NH$_2$	84.2	85.5,[31] 84.8,[16] 86.7,[15] 87.7[14]		
(CH$_3$)$_2$CH	NH$_2$	85.3	86.3,[31] 86.0,[16] 85.5,[15] 87.7[14]		
cyclo-C$_3$H$_5$ [24a]	NH$_2$	92.2	93.8,[22] 90.8±2.5[15]		
(CH$_3$)$_3$C	NH$_2$	85.9	86.2,[31] 85.7,[16] 85.0±1.5,[15] 85.3[14]		
PhCH$_2$	NH$_2$	71.8	71.7,[16] 73.3±1.5,[15] 74.0[14]		
CH$_3$O [19]	NH$_2$	53.0	55.6,[31] 55.6±2.2[14]	66.2	
HS	NH$_2$	64.0	66.8[31]	67.7	
CH$_3$S	NH$_2$	65.5	68.9[31]		
CH$_3$NH	NH$_2$	61.6	64.8[31]		
(CH$_3$)$_2$N	NH$_2$	60.0	60.7[31]		
PH$_2$	NH$_2$	73.5	76.8[31]		
SiH$_3$	NH$_2$	104.7	103.4[31]		
F [19]	NH$_2$	67.4	69.7,[31] 68.5±2.2,[15] 69.5±2.2[14]	82.6	
Cl [19]	NH$_2$	60.3	61.2,[31] 60.5,[15] 61.5[14]		
CH$_3$	F	109.9	110.6,[31] 110.0±2,[15] 109.8[14]	114.4	
CH$_3$CH$_2$	F	114.1	113.4,[31] 111.7±2[15]	114.0	
(CH$_3$)$_2$CH	F	117.2	115.4,[31] 117.0,[37] 110.6,[18] 115.5±2.2[15]	113.0	
cyclo-C$_3$H$_5$ [38]	F	118.6	120.1±2.5[14]		
(CH$_3$)$_3$C	F	118.7	116.9,[31] 117.0,[37] 118.2±2[15]	111.7	
CH$_2$=CHCH$_2$ [19]	F	97.1	96.9,[15] 96.9[14]	97.0	
PhCH$_2$	F	99.7	98.7,[18] 98.9,[15] 98.7±1[14]	100.0	
CH$_2$=CH	F	121.7	123.3,[18] 123.7±3,[15] 122.4±1[14]	123.5	
Ph	F	125.8	127.1,[18] 125.6±2,[15] 127.7±2[14]	124.7	
HC≡C	F	125.6	124.6,[15] 122.0±2[14]		
HC≡C [24b]	F	125.6	129.1,[15] 126.5±2[14]		
N≡C	F	113.9	115.4,[15] 114.4[14]	123.3	
HC(O)	F	115.7	119.2,[15] 119.4[14]	109.6	
CH$_3$C(O)	F	119.3	122.2,[18] 120.7[14]	111.7	
H$_2$B [40]	F	170.1	171.4,[39] 169.7±1.5[40]		
O$_2$N	F	37.1	46.0,[25] 52.9[14]	54.9	
CH$_3$O	F	44.1	44.7[31]	43.2	

[34] Enthalpy of formation –139 ± 3 kcal mol^{-1} from reference 25.

[35] McMillen, D. F.; Golden, D. M. *Annu. Rev. Phys. Chem.* **1982**, *33*, 493–532.

[36] Using $\Delta_f H°$[BrOH] = –19.1 kcal mol^{-1} from reference 19 and $\Delta_f H°$[Br·] and $\Delta_f H°$[·OH] from reference 14.

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R· [10]	·R′	$D[R\text{–}R']_{calc}$	$D[R\text{–}R']_{lit}$ [11]	$D[R\text{–}R']$ [12]	$D[R\text{–}R']$ [13]
CH$_3$HN	F	68.0	70.7[31]		
(CH$_3$)$_2$N	F	66.9	71.1[31]		
PH$_2$	F	109.9	111.9[31]		
HS	F	85.4	82.9,[31] 83.8[25]	86.4	
H$_3$Si	F	158.9	152.2,[31] 156.9,[41] 156.9[15]		
F	F	36.7	39.6,[31] 38.0[14]	23.3	
Cl	F	59.6	60.9,[31] 61.3,[25] 60.0[14]	59.7	
CH$_2$=CH	Cl	94.6	95.2,[15] 94.7±1.2[14]		
Ph	Cl	97.9	96.2±1,[15] 97±2[14]		
HC≡C	Cl	109.5	110.1±2.4,[25] 113.5±1,[15] 110.9±2[14]		
N≡C	Cl	102.7	101.2±1.2,[25] 101.0±2,[15] 100.0[14]		
HC(O) [24a]	Cl	82.9	83.3,[15] 83.4[14]		
CH$_3$C(O)	Cl	84.5	86.6±1,[15] 87.1±1[14]		
CH$_3$O [19]	Cl	48.9	48.5,[31] 48.0,[15] 47.1±1[14]	56.6	
CH$_3$NH	Cl	59.2	59.4[31]		
(CH$_3$)$_2$N	Cl	57.6	57.3[31]		
O$_2$N	Cl	34.2	34.2,[15] 34.0[14]		
S(O$_2$)CH$_3$ [24a]	Cl	67.2	66.0,[42] 67.8[43]		
PH$_2$	Cl	74.3	78.2[31]		
HS	Cl	63.2	64.0[31]	60.4	
CH$_3$S	Cl	65.2	64.0[31]		
Br	Cl	51.7	52.2,[25] 52.2[14]		
CH$_2$=CH	BH$_2$	117.9	118.6±1.5[44]		
HC≡C [24b]	BH$_2$	151.4	149.1,[44] 148.2±2[45]		
CH$_3$C(O)	BH$_2$	95.2	92.8±1.5[44]		
SiH$_3$	BH$_2$	89.7	87.4[46]		
CH$_3$	NO$_2$	60.4	60.9,[25] 62.2,[15] 62.1[14]	61.6	
CH$_3$CH$_2$	NO$_2$	62.1	61.6±0.4,[16] 61.0,[15] 60.8[14]		
(CH$_3$)$_2$CH	NO$_2$	63.4	63.9,[16] 62.0,[15] 63.1[14]		
cyclo-C$_3$H$_5$ [20]	NO$_2$	69.6	73.2,[26] 73.6,[22] 70.6±2.5[14]		
(CH$_3$)$_3$C	NO$_2$	64.2	62.8,[16] 61.9,[15] 61.2[14]		
CH$_2$=CHCH$_2$ [19]	NO$_2$	46.5	48.3±1[14]		
PhCH$_2$	NO$_2$	49.4	50.5,[16] 50.3±1.5,[15] 50.1±1.2[14]		
CH$_3$	Br	69.6	72.1,[18] 69.9[14]	75.1	
CH$_3$CH$_2$	Br	70.4	72.4,[16] 70.3,[15] 70.3[14]		
(CH$_3$)$_2$CH	Br	71.1	73.9,[16] 71.5±1.5,[15] 71.6[14]		
(CH$_3$)$_3$C	Br	71.6	72.6,[16] 69.9±1.5,[15] 69.4,[14]		
CH$_2$=CHCH$_2$	Br	55.4	59±1,[16] 55.5±1.2,[15] 56.2[14]		
HC≡CCH$_2$ [47]	Br	57.5	58.6,[15] 55.6[14]		
PhCH$_2$	Br	58.3	63±1,[16] 59.0,[48] 57.2±1.5,[15] 56.2[14]		

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[42] Theoretical CCSD(T) calculations to the CBS limit. Resende, S. M.; Ornellas, F. R. *Chem. Phys. Lett.* **2003**, *367*, 489–494.

[43] Theoretical G3(MP2) calculations. Frank, A. J.; Turecek, F. *J. Phys. Chem. A* **1999**, *103*, 5348–5361.

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[45] $\Delta_f H°[BH_2]$ = 78.4 kcal mol^{-1} is from Feller, D.; Dixon, B. A.; Peterson, K. A. *J. Phys. Chem. A* **1998**, *102*, 7053–7059. Coupled cluster theoretical calculations. $\Delta_f H°[HC≡C]$ = 135.6 from reference 15 was used for obtaining $D[R\text{–}R']_{lit}$.

[46] Theoretical doubly polarized triple ζ STO basis set. Bickelhaupt, F. M.; Ziegler, T.; Schleyer, P. v. R. *Organometallics* **1996**, *15*, 1477–1487.

[47] Using $\Delta_f H°[HC≡CCH_2Br]$ = 52.2 from Ritter, E. R.; Bozzelli, J. W. *Int. J. Chem. Kinet*. **1991**, *23*, 767–778.

[48] Tsang, W. *J. Phys. Chem.* **1984**, *88*, 2812–2817.

R·[10]	·R′	D[R–R′]$_{calc}$	D[R–R′]$_{lit}$[11]	D[R–R′][12]	D[R–R′][13]
CH$_2$=CH	Br	81.4	80.8,[16] 79.3,[15] 78.8±2[14]		
HC≡C	Br	99.9	98.2±2.1,[15] 95.2±2.5[14]		
Ph	Br	84.4	84±1,[16] 81.0±1.5,[15] 83.1±2.5[14]		
CH$_3$C(O)	Br	68.9	71.7,[16] 70.6[14]		
PhC(O)	Br	69.3	68.1±1.5,[17] 64.4±2.5,[49] 66.0±3[15]		
PH$_2$ [24a]	Br	58.5	65.2,[50] 63.1[51]		
CH$_3$	SH	73.1	74.5,[31] 74.7,[18] 73.8[14]	72.3	
CH$_3$CH$_2$	SH	73.0	73.8,[31] 73.6,[15] 73.0[14]	70.5	
(CH$_3$)$_2$CH	SH	73.1	73.6,[31] 73.4,[15] 73.7[14]	68.8	
(CH$_3$)$_3$C	SH	73.3	73.0,[31] 72.0,[15] 70.3[14]	67.2	
CH$_2$=CHCH$_2$ [19]	SH	58.5	59.2±2[14]	55.0	
PhCH$_2$	SH	61.5	61.3±1.5,[15] 60.2±1[14]	58.0	
Ph	SH	87.6	86.9,[18] 86.2±1.5,[15] 87.4±2[14]	83.4	
CH$_2$=CH	SH	84.8	83±3[52]		
HC≡C	SH	107.2	108.4,[15] 105.5±2[14]		
CH$_3$C(O) [25]	SH	69.7	73.6±2,[25] 73.1±2[14]	69.0	
CH$_3$O	SH	60.5	61.2[31]	62.0	
CH$_3$	SCH$_3$	72.0	73.6,[18] 73.9[15]	69.2	
CH$_3$CH$_2$	SCH$_3$	71.6	72.6±1.6[15]		
(CH$_3$)$_2$CH	SCH$_3$	71.5	72.2[15]		
(CH$_3$)$_3$C	SCH$_3$	71.5	70.2[15]		
HC≡C [24b]	SCH$_3$	107.5	109.0,[15] 105.6[14]		
Ph	SCH$_3$	86.4	89.2±2,[52] 85.5±1[15]		
CH$_2$=CHCH$_2$	SCH$_3$	57.2	58.7[15]		
PhCH$_2$	SCH$_3$	60.3	60.5[15]		
CH$_2$=CHCH$_2$	S(O$_2$)CH$_3$	56.7	55[52]		
Ph	S(O$_2$)CH$_3$	86.0	83,[52] 90.2±2,[43] 88.4±2[45]		
CH$_2$=CH	PH$_2$	84.7	81.9±1.5,[44] 84.8[53]		
HC≡C [24b]	PH$_2$	112.3	109.9±1.5,[44] 116.9[53]		
SiH$_3$	PH$_2$	69.4	71.5,[31] 71.4±1.5,[44] 71.6,[54] 79.2[15]		
CH$_3$NH	PH$_2$	70.3	71.3[31]		
(CH$_3$)$_2$N	PH$_2$	68.2	63.0[31]		
CH$_3$ [19]	SiH$_3$	92.6	89.0,[31] 89.6±1.6[15]		
CH$_3$CH$_2$	SiH$_3$	89.9	87.8[55]		
(CH$_3$)$_2$CH	SiH$_3$	88.1	87.2[55]		
CH$_2$=CH	SiH$_3$	104.2	100.2,[55] 101-107[55]		
CH$_3$NH	SiH$_3$	100.6	96.8[31]		
(CH$_3$)$_2$N	SiH$_3$	98.2	91.2[31]		
(CH$_3$)$_2$N [56]	CH$_2$Ph	67.2	65.0±2,[17] 68.1±1[15]		

[49] Using $\Delta_f H°$[PhC(O)·] = 26.1 ± 2.5 from Solly, R. K.; Benson, S.W. *J. Am. Chem. Soc.* **1971**, *93*, 1592–1595.

[50] Using the experimental value of $\Delta_f H°$[·PH$_2$] = 34.0 from Berkowitz, J.; Curtiss, L. A.; Gibson, S. T.; Greene, J. P.; Hillhouse, G. L.; Pople, J. A. *J. Chem. Phys.* **1986**, *84*, 375–384.)

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[54] Theoretical calculations at the MP2/6-31G level. Baboul, A. G.; Schlegel, H. B. *J. Am. Chem. Soc.* **1996**, *118*, 8444–8451.

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R·[10]	·R´	D[R–R´]$_{calc}$	D[R–R´]$_{lit}$[11]	D[R–R´][12]	D[R–R´][13]
CH$_3$C(O)	SH	69.7	not found		
CH$_3$C(O)O	NH$_2$	52.0	not found		
H$_2$NC(O)	SH	72.6	not found		
H$_2$NC(O)	CH$_2$Ph	75.7	not found		
Ph	S(O)CH$_3$	63.5	not found		
cyclo-C$_3$H$_5$-CH$_2$	C≡CH	123.0	not found		
cyclo-C$_3$H$_5$	CH$_2$CH=CH$_2$	83.4	not found		

Table S3 Total Energies at Various Levels of Theory, Thermal Correction, Zero Point Vibrational Energies, High Level Corrections, Entropies and Enthalpies (units are Hartrees unless otherwise noted).[57]

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
r.H	-0.50027	-0.49823	-0.49982	-0.49823	0.00236	0.00000	-0.00189	0.00000	114.60640	-0.49935
r.CH3	-39.83829	-39.66850	-39.73045	-39.69103	0.00405	0.02924	-0.03221	0.00000	195.33720	-39.75190
r.Cl	-460.13624	-459.55290	-459.63877	-459.57046	0.00236	0.00000	-0.03020	-0.00134	158.83930	-459.68551
r.CH3	-39.83829	-39.66850	-39.73045	-39.69103	0.00405	0.02924	-0.03221	0.00000	195.33720	-39.75190
r.CH2CH3	-79.15787	-78.83551	-78.94867	-78.87477	0.00490	0.05849	-0.06045	0.00000	255.49450	-78.98498
r.CH_CH3_2	-118.47816	-118.00532	-118.16947	-118.06103	0.00607	0.08690	-0.08869	0.00000	292.39510	-118.22089
r.CH_CH2_2	-117.21345	-116.77786	-116.92210	-116.82583	0.00438	0.06584	-0.07927	0.00000	257.19810	-116.97912
r.C_CH3_3	-157.79832	-157.17694	-157.39216	-157.24870	0.00733	0.11499	-0.11693	0.00000	315.18600	-157.45852
r.CH=CH2	-77.90121	-77.61167	-77.70619	-77.64918	0.00404	0.03601	-0.05103	0.00000	233.57700	-77.75469
r.CH=CHCH3	-117.22015	-116.78090	-116.92668	-116.83403	0.00507	0.06500	-0.07927	0.00000	269.99710	-116.98902
r.CH=C_CH3_2	-156.53929	-155.95208	-156.14965	-156.02057	0.00632	0.09309	-0.10751	0.00000	301.62440	-156.22623
r.Ph	-231.56128	-230.78241	-231.02550	-230.85634	0.00532	0.08592	-0.13575	0.00000	287.89980	-231.14395
r.CCH	-76.60444	-76.36083	-76.43322	-76.39078	0.00411	0.01218	-0.04162	0.00000	217.28910	-76.48850
r.CN	-92.71175	-92.46146	-92.53732	-92.48587	0.00330	0.00483	-0.04162	0.00000	202.50370	-92.59522
r.CH2OH	-115.05203	-114.69645	-114.84781	-114.72395	0.00422	0.03679	-0.06045	0.00000	239.29550	-114.89475
r.CH2F	-139.06427	-138.67917	-138.85005	-138.70244	0.00397	0.02443	-0.06045	0.00000	235.28780	-138.90536
r.CH2Cl	-499.43832	-498.69814	-498.84360	-498.73291	0.00459	0.02224	-0.06045	0.00000	257.70870	-498.91198

[57] Red value indictates ONIOM values where COPh core was taken from $COCH_3$, and SCH_2Ph core was taken from SCH_3.

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
r.CHO	-113.85017	-113.53452	-113.65577	-113.55322	0.00380	0.01282	-0.05103	0.00000	224.39090	-113.70887
r.COCH3	-153.17983	-152.71201	-152.88497	-152.74720	0.00491	0.04256	-0.07927	0.00000	269.00900	-152.95196
r.COOH	-189.08783	-188.58832	-188.79490	-188.61159	0.00413	0.02011	-0.07927	0.00000	251.61430	-188.87320
r.COPh	-344.92063	-343.84871	-344.20356	-343.93201	0.00728	0.09588	-0.18282	0.00000	339.20830	-344.36652
r.CONH2	-169.23206	-168.75266	-168.94205	-168.78072	0.00470	0.03222	-0.07927	0.00000	261.02440	-169.01246
r.CONHCH3	-208.54322	-207.91254	-208.15036	-207.95741	0.00587	0.06099	-0.10751	0.00000	300.79290	-208.23588
r.CON_CH3_2	-247.85494	-247.07471	-247.36115	-247.13582	0.00704	0.08877	-0.13575	0.00000	324.15740	-247.46220
r.CON_CH2CH3_2	-326.48666	-325.41203	-325.80154	-325.50521	0.00951	0.14511	-0.19223	0.00000	385.77900	-325.93233
r.COOCH3	-228.39717	-227.74458	-227.99717	-227.78513	0.00550	0.04857	-0.10751	0.00000	290.80630	-228.09116
r.COOCH2CH3	-267.71720	-266.91599	-267.21984	-266.97269	0.00670	0.07661	-0.13575	0.00000	322.52060	-267.32898
r.COOC_CH3_3	-346.35214	-345.26010	-345.66658	-345.34832	0.00918	0.13142	-0.19223	0.00000	366.48610	-345.80642
r.F	-99.71554	-99.48729	-99.59883	-99.49886	0.00236	0.00000	-0.03020	-0.00061	151.23030	-99.63884
r.Cl	-460.13624	-459.55290	-459.63877	-459.57046	0.00236	0.00000	-0.03020	-0.00134	158.83930	-459.68551
r.Br	-2573.83974	-2572.32667	-2572.74345	-2572.19601	0.00236	0.00000	-0.03020	-0.00560	168.99070	-2572.64624
r.OH	-75.72345	-75.52105	-75.61461	-75.53712	0.00330	0.00814	-0.03221	0.00000	178.29190	-75.65144
r.OCH3	-115.05046	-114.68575	-114.82548	-114.72111	0.00395	0.03606	-0.06045	0.00000	236.74820	-114.88127
r.OCH2CH3	-154.37049	-153.85615	-154.04665	-153.90809	0.00515	0.06401	-0.08869	0.00000	273.48550	-154.11811
r.OCHO	-189.07897	-188.58122	-188.78218	-188.59775	0.00399	0.01939	-0.07927	0.00000	245.30800	-188.85462
r.OCOCH3	-228.41136	-227.76284	-228.01548	-227.79546	0.00550	0.04706	-0.10751	0.00000	298.36450	-228.10305
r.NH2	-55.87262	-55.69078	-55.76632	-55.71156	0.00378	0.01861	-0.03221	0.00000	194.75530	-55.79691
r.NO2	-205.07221	-204.56594	-204.77694	-204.57474	0.00388	0.00865	-0.07927	0.00000	240.10230	-204.85248
r.NHCH3	-95.19086	-94.85328	-94.97721	-94.89142	0.00438	0.04813	-0.06045	0.00000	244.67580	-95.02329
r.N_CH3_2	-134.50949	-134.01953	-134.19265	-134.07445	0.00574	0.07610	-0.08869	0.00000	282.96140	-134.25442
r.NHCHO	-169.20001	-168.71127	-168.89466	-168.75082	0.00453	0.03006	-0.07927	0.00000	259.88580	-168.97889

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
r.NHCOCH3	-208.53211	-207.89381	-208.12834	-207.94831	0.00576	0.05825	-0.10751	0.00000	298.53360	-208.22634
r.SH	-398.74002	-398.16216	-398.25169	-398.18460	0.00330	0.00596	-0.03221	0.00000	192.14650	-398.29708
r.SCH3	-438.05972	-437.33123	-437.46922	-437.36941	0.00413	0.03519	-0.06045	0.00000	250.21660	-437.52852
r.SCH2Ph	-669.10963	-667.63195	-668.00594	-667.73392	0.00807	0.11601	-0.19223	0.00000	368.62310	-668.17607
r.SOCH3	-513.27328	-512.35242	-512.59283	-512.40230	0.00512	0.03962	-0.08869	0.00000	282.57460	-512.68666
r.SO2CH3	-588.46015	-587.37552	-587.71050	-587.41124	0.00570	0.04442	-0.11693	0.00000	298.55040	-587.81303
r.BH2	-25.93471	-25.80417	-25.83874	-25.82154	0.00381	0.01430	-0.02280	0.00000	194.22410	-25.86079
r.PH2	-342.50422	-341.93532	-342.01816	-341.96156	0.00380	0.01322	-0.03221	0.00000	212.60110	-342.05959
r.SiH3	-291.23226	-290.67427	-290.74995	-290.69859	0.00396	0.02089	-0.03221	0.00000	216.89840	-290.78163
r.CH2-CH=CH2	-117.26035	-116.82120	-116.96999	-116.87040	0.00477	0.06505	-0.07927	0.00000	257.63340	-117.02864
r.CH2-CH_CH2_2	-156.54436	-155.96111	-156.15944	-156.02441	0.00595	0.09309	-0.10751	0.00000	294.22650	-156.23122
r.CH2-CCH	-116.00128	-115.59762	-115.72713	-115.63993	0.00509	0.04021	-0.06986	0.00000	255.12220	-115.79399
r.CH2-CN	-132.09467	-131.68718	-131.81919	-131.72198	0.00456	0.03061	-0.06986	0.00000	247.97320	-131.88869
r.CH2-Ph	-270.91514	-269.98389	-270.28287	-270.07441	0.00662	0.11272	-0.16399	0.00000	313.60160	-270.41804
r.CH2-NH2	-95.19561	-94.86098	-94.99290	-94.89435	0.00431	0.04954	-0.06045	0.00000	241.75720	-95.03288
r.CH2-N_CH3_2	-173.81714	-173.18124	-173.41233	-173.24759	0.00654	0.10540	-0.11693	0.00000	304.53400	-173.48367
r.CH2-Br	-2613.12361	-2611.45326	-2611.92916	-2611.33974	0.00445	0.02194	-0.06045	0.00000	263.52990	-2611.84970
r.CH2-SH	-438.03412	-437.30110	-437.44931	-437.34150	0.00474	0.03129	-0.06045	0.00000	258.74710	-437.51412
r.CH2-SCH3	-477.35164	-476.47042	-476.66797	-476.52632	0.00598	0.06087	-0.08869	0.00000	295.61020	-476.74571
r.CH2-NO2	-244.33932	-243.67248	-243.93951	-243.70554	0.00522	0.03464	-0.10751	0.00000	279.29760	-244.04021
r.CH2-SiH3	-330.53971	-329.82771	-329.96052	-329.87024	0.00545	0.04633	-0.06045	0.00000	279.69730	-330.01172
r.CH2-COOH	-228.41666	-227.76446	-228.02474	-227.80521	0.00517	0.04742	-0.10751	0.00000	281.66780	-228.12041
r.CH2-COCH3	-192.49502	-191.87306	-192.09805	-191.92755	0.00603	0.06931	-0.10751	0.00000	304.02860	-192.18471
r.CH2-OCHO	-228.39410	-227.73858	-227.99441	-227.78033	0.00563	0.04650	-0.10751	0.00000	288.73830	-228.09155

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
r.CH2-OCOCH3	-267.72026	-266.91586	-267.22321	-266.97368	0.00721	0.07389	-0.13575	0.00000	329.21990	-267.33569
r.CH2-CONH2	-208.54679	-207.91462	-208.15793	-207.96142	0.00569	0.05897	-0.10751	0.00000	289.19710	-208.24758
r.CH2-SOCH3	-552.51499	-551.45076	-551.74977	-551.51041	0.00674	0.06431	-0.11693	0.00000	314.27590	-551.85529
r.CH2-SO2CH3	-627.72443	-6.26E+02	-6.27E+02	-626.54633	0.00737	0.069639	-0.14516		330.0708	-627.01302
n.H-CH3	-40.51838	-40.33253	-40.40413	-40.35591	0.00381	0.04434	-0.03765	0.00000	186.08070	-40.41701
n.H-CH2CH3	-79.83042	-79.49468	-79.61744	-79.53449	0.00441	0.07378	-0.06589	0.00000	227.41460	-79.64495
n.H-CH_CH3_2	-119.14424	-118.66023	-118.83467	-118.71621	0.00546	0.10209	-0.09413	0.00000	268.07880	-118.87724
n.H-CH_CH2_2	-117.89520	-117.44850	-117.60374	-117.49637	0.00430	0.08015	-0.08472	0.00000	236.83470	-117.65187
n.H-C_CH3_3	-158.45881	-157.82851	-158.05505	-157.90032	0.00663	0.12981	-0.12237	0.00000	292.38800	-158.11278
n.H-CH=CH2	-78.58746	-78.28498	-78.39082	-78.32186	0.00399	0.05023	-0.05648	0.00000	218.91460	-78.42996
n.H-CH=CHCH3	-117.90756	-117.45546	-117.61276	-117.50788	0.00502	0.07852	-0.08472	0.00000	264.35670	-117.66635
n.H-CH=C_CH3_2	-157.22729	-156.62724	-156.83637	-156.69496	0.00624	0.10642	-0.11296	0.00000	289.30120	-156.90440
n.H-Ph	-232.24865	-231.45773	-231.71309	-231.53072	0.00533	0.09878	-0.14120	0.00000	268.03870	-231.82315
n.H-CCH	-77.32565	-77.06649	-77.15444	-77.09341	0.00388	0.02612	-0.04707	0.00000	201.64490	-77.19843
n.H-CN	-93.42262	-93.15810	-93.24878	-93.17795	0.00348	0.01615	-0.04707	0.00000	201.25910	-93.29607
n.H-CH2OH	-115.71441	-115.34608	-115.50784	-115.37463	0.00423	0.05048	-0.06589	0.00000	237.34000	-115.54757
n.H-CH2F	-139.73392	-139.33575	-139.51790	-139.36018	0.00385	0.03874	-0.06589	0.00000	222.52590	-139.56562
n.H-CH2Cl	-500.10853	-499.35433	-499.50942	-499.38972	0.00396	0.03738	-0.06589	0.00000	234.19160	-499.56937
n.H-CHO	-114.50047	-114.16740	-114.30010	-114.19031	0.00381	0.02630	-0.05648	0.00000	218.55900	-114.34937
n.H-COCH3	-153.83012	-153.34662	-153.53058	-153.38521	0.00484	0.05474	-0.08472	0.00000	262.39280	-153.59430
n.H-COOH	-189.75546	-189.24162	-189.46050	-189.26667	0.00410	0.03327	-0.08472	0.00000	248.16430	-189.53289
n.H-COPh	-345.57344	-344.48614	-344.85256	-344.57231	0.00724	0.10806	-0.18826	0.00000	332.34440	-345.01170
n.H-CONH2	-169.88884	-169.39433	-169.59627	-169.42517	0.00494	0.04439	-0.08472	0.00000	265.54310	-169.66249
n.H-CONHCH3	-209.20043	-208.55487	-208.80517	-208.60231	0.00589	0.07316	-0.11296	0.00000	293.76770	-208.88651

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.H-CON_CH3_2	-248.51225	-247.71735	-248.01631	-247.78083	0.00703	0.10104	-0.14120	0.00000	318.06470	-248.11291
n.H-CON_CH2CH3_2	-327.14326	-326.05440	-326.45646	-326.14993	0.00952	0.15738	-0.19767	0.00000	379.00470	-326.58276
n.H-COOCH3	-229.06301	-228.39640	-228.66166	-228.43865	0.00548	0.06129	-0.11296	0.00000	284.33290	-228.75011
n.H-COOCH2CH3	-268.38210	-267.56703	-267.88353	-267.62546	0.00669	0.08929	-0.14120	0.00000	315.90620	-267.98719
n.H-COOC_CH3_3	-347.01420	-345.90884	-346.32791	-345.99873	0.00918	0.14412	-0.19767	0.00000	360.31020	-346.46217
n.H-F	-100.42017	-100.18217	-100.32428	-100.18832	0.00330	0.00888	-0.03765	0.00000	173.78320	-100.35590
n.H-Cl	-460.79570	-460.19230	-460.30252	-460.21158	0.00330	0.00656	-0.03765	0.00000	186.66860	-460.34960
n.H-Br	-2574.48183	-2572.94897	-2573.38526	-2572.82045	0.00330	0.00584	-0.03765	0.00000	198.53830	-2573.28525
n.H-OH	-76.40895	-76.19684	-76.31475	-76.20784	0.00378	0.02076	-0.03765	0.00000	188.85250	-76.33886
n.H-OCH3	-115.71441	-115.34608	-115.50783	-115.37463	0.00423	0.05047	-0.06589	0.00000	237.25380	-115.54757
n.H-OCH2CH3	-155.03380	-154.51687	-154.72995	-154.56154	0.00521	0.07875	-0.09413	0.00000	269.15540	-154.78479
n.H-OCHO	-189.75546	-189.24161	-189.46049	-189.26667	0.00410	0.03326	-0.08472	0.00000	248.16390	-189.53290
n.H-OCOCH3	-229.08179	-228.41875	-228.68915	-228.45989	0.00549	0.06085	-0.11296	0.00000	287.19840	-228.77690
n.H-NH2	-56.54795	-56.35418	-56.44804	-56.37208	0.00380	0.03387	-0.03765	0.00000	192.35690	-56.46592
n.H-NO2	-205.68695	-205.16040	-205.38818	-205.17772	0.00390	0.02158	-0.08472	0.00000	238.21670	-205.46473
n.H-NHCH3	-95.85321	-95.50649	-95.64776	-95.54125	0.00433	0.06318	-0.06589	0.00000	239.67250	-95.68090
n.H-N_CH3_2	-135.16286	-134.66519	-134.85461	-134.71637	0.00531	0.09121	-0.09413	0.00000	270.54800	-134.90340
n.H-NHCHO	-169.88884	-169.39433	-169.59627	-169.42517	0.00494	0.04439	-0.08472	0.00000	265.50860	-169.66250
n.H-NHCOCH3	-209.21220	-208.56873	-208.82241	-208.61564	0.00630	0.07220	-0.11296	0.00000	308.87110	-208.90378
n.H-SH	-399.38543	-398.78830	-398.89669	-398.81344	0.00379	0.01485	-0.03765	0.00000	205.69550	-398.94085
n.H-SCH3	-438.69834	-437.95246	-438.10879	-437.99325	0.00453	0.04549	-0.06589	0.00000	253.19950	-438.16545
n.H-SCH2Ph	-669.74903	-668.25438	-668.64674	-668.35866	0.00845	0.12599	-0.19767	0.00000	364.53590	-668.81425
n.H-SOCH3	-513.85836	-512.92961	-513.18937	-512.97352	0.00507	0.04982	-0.09413	0.00000	274.88050	-513.27252
n.H-SO2CH3	-589.06795	-587.96725	-588.32767	-588.00864	0.00557	0.05600	-0.12237	0.00000	290.71070	-588.42986

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.H-BH2	-26.61300	-26.46424	-26.50821	-26.48464	0.00383	0.02599	-0.02824	0.00000	188.29560	-26.52704
n.H-PH2	-343.14028	-342.55150	-342.64931	-342.58067	0.00384	0.02377	-0.03765	0.00000	210.02530	-342.68852
n.H-SiH3	-291.88369	-291.30711	-291.39627	-291.33423	0.00401	0.03073	-0.03765	0.00000	204.54420	-291.42630
n.CH3-CH=CH2	-117.90756	-117.45546	-117.61275	-117.50788	0.00502	0.07852	-0.08472	0.00000	264.35010	-117.66634
n.CH3-CH_CH2_2	-157.21201	-156.61742	-156.82429	-156.68110	0.00557	0.10793	-0.11296	0.00000	282.52240	-156.88743
n.CH3-CCH	-116.65327	-116.24149	-116.38100	-116.28374	0.00494	0.05463	-0.07530	0.00000	247.69280	-116.43898
n.CH3-CN	-132.75493	-132.33746	-132.48010	-132.37279	0.00454	0.04475	-0.07530	0.00000	242.28840	-132.54143
n.CH3-Ph	-271.56664	-270.62839	-270.93538	-270.71647	0.00718	0.12580	-0.16943	0.00000	335.42470	-271.05992
n.CH3-NH2	-95.85321	-95.50649	-95.64776	-95.54125	0.00433	0.06318	-0.06589	0.00000	239.66170	-95.68090
n.CH3-N_CH3_2	-174.47440	-173.82834	-174.06692	-173.89543	0.00636	0.11878	-0.12237	0.00000	287.04120	-174.13124
n.CH3-Br	-2613.79557	-2612.11200	-2612.59711	-2611.99877	0.00404	0.03675	-0.06589	0.00000	245.84520	-2612.50898
n.CH3-SH	-438.69834	-437.95246	-438.10879	-437.99325	0.00454	0.04548	-0.06589	0.00000	253.26170	-438.16545
n.CH3-SCH3	-478.01381	-477.12074	-477.32564	-477.17686	0.00583	0.07484	-0.09413	0.00000	283.79430	-477.39520
n.CH3-NO2	-245.00933	-244.33135	-244.60822	-244.36529	0.00533	0.04918	-0.11296	0.00000	296.49140	-244.70060
n.CH3-SiH3	-331.21087	-330.48519	-330.62917	-330.52786	0.00514	0.06024	-0.06589	0.00000	255.38040	-330.67234
n.CH3-COOH	-229.08179	-228.41875	-228.68915	-228.45989	0.00549	0.06085	-0.11296	0.00000	287.33100	-228.77690
n.CH3-COCH3	-193.15569	-192.52362	-192.75895	-192.57801	0.00634	0.08248	-0.11296	0.00000	299.45770	-192.83749
n.CH3-OCHO	-229.06301	-228.39640	-228.66166	-228.43865	0.00548	0.06129	-0.11296	0.00000	284.34920	-228.75010
n.CH3-OCOCH3	-268.38848	-267.57298	-267.88986	-267.63136	0.00713	0.08853	-0.14120	0.00000	325.41280	-267.99379
n.CH3-CONH2	-209.21220	-208.56875	-208.82241	-208.61566	0.00628	0.07222	-0.11296	0.00000	307.18250	-208.90379
n.CH3-SOCH3	-553.18693	-552.11174	-552.42079	-552.17071	0.00661	0.07831	-0.12237	0.00000	307.86360	-552.51721
n.CH3-SO2CH3	-628.40082	-627.15372	-627.56263	-627.21070	0.00715	0.08401	-0.15061	0.00000	315.50470	-627.67906
n.CH3-CH3	-79.83042	-79.49469	-79.61745	-79.53449	0.00441	0.07378	-0.06589	0.00000	227.44250	-79.64495
n.CH3-CH2CH3	-119.14424	-118.66023	-118.83469	-118.71621	0.00545	0.10211	-0.09413	0.00000	268.05180	-118.87723

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.CH3-CH_CH3_2	-158.45881	-157.82853	-158.05507	-157.90033	0.00663	0.12982	-0.12237	0.00000	292.30840	-158.11278
n.CH3-CH_CH2_2	-157.21201	-156.61742	-156.82429	-156.68110	0.00557	0.10793	-0.11296	0.00000	282.52240	-156.88743
n.CH3-C_CH3_3	-197.77298	-196.99876	-197.27771	-197.08594	0.00786	0.15720	-0.15061	0.00000	304.74260	-197.35043
n.CH3-CH=CH2	-117.90756	-117.45546	-117.61275	-117.50788	0.00502	0.07852	-0.08472	0.00000	264.35010	-117.66634
n.CH3-CH=CHCH3	-157.22691	-156.62579	-156.83407	-156.69375	0.00641	0.10639	-0.11296	0.00000	291.84240	-156.90219
n.CH3-CH=C_CH3_2	-196.54358	-195.79482	-196.05528	-195.87811	0.00780	0.13420	-0.14120	0.00000	330.48630	-196.13778
n.CH3-Ph	-271.56664	-270.62839	-270.93538	-270.71647	0.00718	0.12580	-0.16943	0.00000	335.42470	-271.05992
n.CH3-CCH	-116.65327	-116.24149	-116.38100	-116.28374	0.00494	0.05463	-0.07530	0.00000	247.69280	-116.43898
n.CH3-CN	-132.75493	-132.33746	-132.48010	-132.37279	0.00454	0.04475	-0.07530	0.00000	242.28840	-132.54143
n.CH3-CH2OH	-155.03380	-154.51687	-154.72996	-154.56154	0.00521	0.07875	-0.09413	0.00000	269.25140	-154.78479
n.CH3-CH2F	-179.05642	-178.50862	-178.74088	-178.54932	0.00477	0.06719	-0.09413	0.00000	263.30480	-178.80375
n.CH3-CH2Cl	-539.42626	-538.52362	-538.73034	-538.57499	0.00497	0.06582	-0.09413	0.00000	274.65960	-538.80505
n.CH3-CHO	-153.83012	-153.34663	-153.53058	-153.38522	0.00484	0.05474	-0.08472	0.00000	262.35150	-153.59430
n.CH3-COCH3	-193.15569	-192.52362	-192.75895	-192.57801	0.00634	0.08248	-0.11296	0.00000	299.45770	-192.83749
n.CH3-COOH	-229.08179	-228.41875	-228.68915	-228.45989	0.00549	0.06085	-0.11296	0.00000	287.33100	-228.77690
n.CH3-COPh	-384.89599	-383.66137	-384.07952	-383.76334	0.00876	0.13575	-0.21650	0.00000	364.91780	-384.25348
n.CH3-CONH2	-209.21220	-208.56875	-208.82241	-208.61566	0.00628	0.07222	-0.11296	0.00000	307.18250	-208.90379
n.CH3-CONHCH3	-248.52356	-247.72933	-248.03131	-247.79281	0.00750	0.10058	-0.14120	0.00000	333.83500	-248.12789
n.CH3-CON_CH3_2	-287.83021	-286.88756	-287.23843	-286.96721	0.00866	0.12846	-0.16943	0.00000	357.01760	-287.35040
n.CH3-CON_CH2CH3_2	-366.46181	-365.22595	-365.68006	-365.33762	0.01094	0.18502	-0.22591	0.00000	405.10050	-365.82169
n.CH3-COOCH3	-268.38848	-267.57298	-267.88987	-267.63136	0.00713	0.08853	-0.14120	0.00000	325.41890	-267.99379
n.CH3-COOCH2CH3	-307.70744	-306.74359	-307.11166	-306.81817	0.00838	0.11648	-0.16943	0.00000	356.88860	-307.23081
n.CH3-COOC_CH3_3	-386.33898	-385.08519	-385.55584	-385.19123	0.01091	0.17125	-0.22591	0.00000	400.60390	-385.70562
n.CH3-F	-139.73392	-139.33575	-139.51790	-139.36017	0.00385	0.03874	-0.06589	0.00000	222.52450	-139.56562

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.CH3-Cl	-500.10853	-499.35432	-499.50941	-499.38972	0.00396	0.03738	-0.06589	0.00000	234.19930	-499.56936
n.CH3-Br	-2613.79557	-2612.11200	-2612.59711	-2611.99877	0.00404	0.03675	-0.06589	0.00000	245.84520	-2612.50898
n.CH3-OH	-115.71441	-115.34608	-115.50784	-115.37463	0.00423	0.05047	-0.06589	0.00000	237.33120	-115.54758
n.CH3-OCH3	-155.02505	-154.50332	-154.70972	-154.54895	0.00523	0.07876	-0.09413	0.00000	263.58320	-154.76549
n.CH3-OCH2CH3	-194.34430	-193.67435	-193.93208	-193.73609	0.00646	0.10681	-0.12237	0.00000	301.19910	-194.00293
n.CH3-OCHO	-229.06301	-228.39640	-228.66166	-228.43865	0.00548	0.06129	-0.11296	0.00000	284.34920	-228.75010
n.CH3-OCOCH3	-268.38848	-267.57298	-267.88986	-267.63136	0.00713	0.08853	-0.14120	0.00000	325.41280	-267.99379
n.CH3-NH2	-95.85321	-95.50649	-95.64776	-95.54125	0.00433	0.06318	-0.06589	0.00000	239.66170	-95.68090
n.CH3-NO2	-245.00933	-244.33135	-244.60822	-244.36529	0.00533	0.04918	-0.11296	0.00000	296.49140	-244.70060
n.CH3-NHCH3	-135.16286	-134.66519	-134.85461	-134.71637	0.00531	0.09121	-0.09413	0.00000	270.54590	-134.90340
n.CH3-N_CH3_2	-174.47440	-173.82834	-174.06692	-173.89543	0.00636	0.11878	-0.12237	0.00000	287.04120	-174.13124
n.CH3-NHCHO	-209.20043	-208.55487	-208.80517	-208.60231	0.00589	0.07316	-0.11296	0.00000	293.79870	-208.88651
n.CH3-NHCOCH3	-248.52356	-247.72933	-248.03131	-247.79281	0.00750	0.10058	-0.14120	0.00000	333.83730	-248.12789
n.CH3-SH	-438.69834	-437.95246	-438.10879	-437.99325	0.00454	0.04548	-0.06589	0.00000	253.26170	-438.16545
n.CH3-SCH3	-478.01381	-477.12074	-477.32564	-477.17686	0.00583	0.07484	-0.09413	0.00000	283.79430	-477.39520
n.CH3-SCH2Ph	-709.06456	-707.42422	-707.86554	-707.54341	0.00994	0.15526	-0.22591	0.00000	398.14440	-708.04544
n.CH3-SOCH3	-553.18693	-552.11174	-552.42079	-552.17071	0.00661	0.07831	-0.12237	0.00000	307.86360	-552.51721
n.CH3-SO2CH3	-628.40082	-627.15372	-627.56263	-627.21070	0.00715	0.08401	-0.15061	0.00000	315.50470	-627.67906
n.CH3-BH2	-65.94666	-65.64636	-65.74488	-65.68326	0.00485	0.05500	-0.05648	0.00000	248.73050	-65.77841
n.CH3-PH2	-382.45777	-381.72097	-381.87066	-381.76549	0.00472	0.05382	-0.06589	0.00000	257.63620	-381.92253
n.CH3-SiH3	-331.21087	-330.48519	-330.62917	-330.52786	0.00514	0.06024	-0.06589	0.00000	255.38040	-330.67234
n.CH2_CH3_-CH=CH2	-157.22036	-156.62026	-156.82978	-156.68872	0.00608	0.10703	-0.11296	0.00000	293.10550	-156.89808
n.CH2_CH3_-CH_CH2_2	-196.52593	-195.78352	-196.04229	-195.86320	0.00683	0.13611	-0.14120	0.00000	313.63130	-196.12022
n.CH2_CH3_-CCH	-155.96688	-155.40705	-155.59802	-155.46516	0.00598	0.08327	-0.10354	0.00000	289.15560	-155.67041

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.CH2_CH3_-CN	-172.06867	-171.50275	-171.69700	-171.55406	0.00561	0.07336	-0.10354	0.00000	284.34700	-171.77288
n.CH2_CH3_-Ph	-310.88023	-309.79502	-310.15383	-309.89867	0.00827	0.15432	-0.19767	0.00000	356.33900	-310.29256
n.CH2_CH3_-NH2	-135.17073	-134.67545	-134.86766	-134.72638	0.00529	0.09148	-0.09413	0.00000	270.60100	-134.91595
n.CH2_CH3_-N_CH3_2	-213.78720	-212.99347	-213.28346	-213.07670	0.00771	0.14683	-0.15061	0.00000	327.69760	-213.36275
n.CH2_CH3_-Br	-2653.11274	-2651.28094	-2651.81755	-2651.18338	0.00510	0.06520	-0.09413	0.00000	286.46290	-2651.74382
n.CH2_CH3_-SH	-478.01289	-477.11920	-477.32729	-477.17587	0.00564	0.07392	-0.09413	0.00000	285.47030	-477.39852
n.CH2_CH3_-SCH3	-517.32822	-516.28751	-516.54429	-516.35947	0.00713	0.10316	-0.12237	0.00000	322.43750	-516.62833
n.CH2_CH3_-NO2	-284.32809	-283.50154	-283.82909	-283.55166	0.00638	0.07753	-0.14120	0.00000	315.12570	-283.93650
n.CH2_CH3_-SiH3	-370.52075	-369.64669	-369.84199	-369.70566	0.00634	0.08876	-0.09413	0.00000	297.70010	-369.89999
n.CH2_CH3_-COOH	-268.39662	-267.58514	-267.90697	-267.64246	0.00668	0.08916	-0.14120	0.00000	317.07480	-268.00965
n.CH2_CH3_-COCH3	-232.47056	-231.69046	-231.97702	-231.76096	0.00756	0.11081	-0.14120	0.00000	337.54630	-232.07035
n.CH2_CH3_-OCHO	-268.38210	-267.56702	-267.88353	-267.62546	0.00669	0.08928	-0.14120	0.00000	316.00360	-267.98719
n.CH2_CH3_-OCOCH3	-307.70744	-306.74359	-307.11166	-306.81817	0.00838	0.11648	-0.16943	0.00000	357.01750	-307.23081
n.CH2_CH3_-CONH2	-248.52685	-247.73539	-248.04008	-247.79851	0.00730	0.10072	-0.14120	0.00000	329.01430	-248.13636
n.CH2_CH3_-SOCH3	-592.51383	-591.28892	-591.62911	-591.36708	0.00808	0.10748	-0.15061	0.00000	346.47970	-591.74233
n.CH2_CH3_-SO2CH3	-667.71677	-666.32196	-666.78212	-666.39502	0.00852	0.11233	-0.17885	0.00000	353.51640	-666.91317
n.Cl-CH3	-500.10853	-499.35432	-499.50941	-499.38972	0.00396	0.03738	-0.06589	0.00000	234.19720	-499.56937
n.Cl-CH2CH3	-539.42626	-538.52362	-538.73034	-538.57500	0.00497	0.06581	-0.09413	0.00000	274.69290	-538.80506
n.Cl-CH_CH3_2	-578.74360	-577.69454	-577.95320	-577.76164	0.00620	0.09351	-0.12237	0.00000	302.38830	-578.04296
n.Cl-CH_CH2_2	-577.49014	-576.47773	-576.71559	-576.53684	0.00510	0.07134	-0.11296	0.00000	283.08490	-576.81121
n.Cl-C_CH3_3	-618.05960	-616.86639	-617.17719	-616.94887	0.00750	0.12081	-0.15061	0.00000	317.41640	-617.28196
n.Cl-CH=CH2	-538.18539	-537.31633	-537.50505	-537.36398	0.00448	0.04202	-0.08472	0.00000	263.57390	-537.59093
n.Cl-CH=CHCH3	-577.50527	-576.48711	-576.72684	-576.55030	0.00594	0.06995	-0.11296	0.00000	296.88280	-576.82710
n.Cl-CH=C_CH3_2	-616.82480	-615.65938	-615.95135	-615.73773	0.00731	0.09775	-0.14120	0.00000	328.91140	-616.06585

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.Cl-Ph	-691.84497	-690.49045	-690.82887	-690.57353	0.00645	0.08944	-0.16943	0.00000	313.11930	-690.98550
n.Cl-CCH	-536.91326	-536.08626	-536.25866	-536.12379	0.00456	0.01845	-0.07530	0.00000	242.96280	-536.34849
n.Cl-CN	-553.00829	-552.17531	-552.35109	-552.20599	0.00404	0.00860	-0.07530	0.00000	235.59390	-552.44443
n.Cl-CH2OH	-575.31848	-574.38129	-574.62606	-574.42127	0.00462	0.04273	-0.09413	0.00000	268.74190	-574.71281
n.Cl-CH2F	-599.33194	-598.36536	-598.63043	-598.40131	0.00429	0.03069	-0.09413	0.00000	264.50250	-598.72553
n.Cl-CH2Cl	-959.69635	-958.37554	-958.61630	-958.42234	0.00452	0.02906	-0.09413	0.00000	270.21460	-958.72367
n.Cl-CHO	-574.11700	-573.21557	-573.43210	-573.24831	0.00420	0.01888	-0.08472	0.00000	259.15660	-573.52649
n.Cl-COCH3	-613.44592	-612.39573	-612.66345	-612.44380	0.00558	0.04667	-0.11296	0.00000	294.14010	-612.77223
n.Cl-COOH	-649.35491	-648.27432	-648.57698	-648.30978	0.00475	0.02445	-0.11296	0.00000	278.94000	-648.69620
n.Cl-COPh	-805.18497	-803.53241	-803.98256	-803.62793	0.00831	0.09935	-0.21650	0.00000	364.47400	-804.18693
n.Cl-CONH2	-629.49699	-628.43582	-628.72082	-628.47648	0.00552	0.03601	-0.11296	0.00000	292.33560	-628.83290
n.Cl-CONHCH3	-668.80892	-667.59727	-667.93072	-667.65444	0.00694	0.06427	-0.14120	0.00000	331.09820	-668.05786
n.Cl-CON_CH3_2	-708.11481	-706.75457	-707.13775	-706.82776	0.00837	0.09189	-0.16943	0.00000	363.82510	-707.28012
n.Cl-CON_CH2CH3_2	-786.74799	-785.09457	-785.58085	-785.19965	0.01052	0.14863	-0.22591	0.00000	404.12330	-785.75271
n.Cl-COOCH3	-688.66391	-687.43091	-687.77982	-687.48349	0.00639	0.05225	-0.14120	0.00000	314.78870	-687.91495
n.Cl-COOCH2CH3	-727.98371	-726.60223	-727.00238	-726.67096	0.00768	0.08017	-0.16943	0.00000	346.46440	-727.15270
n.Cl-COOC_CH3_3	-806.61708	-804.94535	-805.44828	-805.04539	0.01028	0.13484	-0.22591	0.00000	392.40480	-805.62910
n.Cl-F	-559.94270	-559.12695	-559.33555	-559.14995	0.00339	0.00175	-0.06589	0.00000	217.92990	-559.41930
n.Cl-Cl	-920.34988	-919.17116	-919.36645	-919.20563	0.00351	0.00116	-0.06589	0.00000	223.33360	-919.46214
n.Cl-Br	-3034.05328	-3031.94557	-3032.46687	-3031.83151	0.00359	0.00095	-0.06589	0.00000	240.14860	-3032.41415
n.Cl-OH	-535.94355	-535.15678	-535.34786	-535.18353	0.00389	0.01278	-0.06589	0.00000	236.71580	-535.42383
n.Cl-OCH3	-575.25537	-574.31502	-574.55152	-574.35872	0.00481	0.04129	-0.09413	0.00000	270.91090	-574.64326
n.Cl-OCH2CH3	-614.57534	-613.48713	-613.77499	-613.54659	0.00612	0.06934	-0.12237	0.00000	302.98710	-613.88136
n.Cl-OCHO	-649.28433	-648.19836	-648.49349	-648.23823	0.00495	0.02313	-0.11296	0.00000	282.52430	-648.61823

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.Cl-OCOCH3	-688.61081	-687.37652	-687.72324	-687.43210	0.00672	0.05045	-0.14120	0.00000	328.20270	-687.86284
n.Cl-NH2	-516.10346	-515.33730	-515.50992	-515.36995	0.00394	0.02593	-0.06589	0.00000	240.89050	-515.57859
n.Cl-NO2	-665.26127	-664.16276	-664.46923	-664.18989	0.00464	0.01211	-0.11296	0.00000	272.20160	-664.59257
n.Cl-NHCH3	-555.41503	-554.49799	-554.71918	-554.54683	0.00488	0.05411	-0.09413	0.00000	272.50280	-554.80316
n.Cl-N_CH3_2	-594.72712	-593.66175	-593.93240	-593.72639	0.00602	0.08157	-0.12237	0.00000	298.52820	-594.03181
n.Cl-NHCHO	-629.43627	-628.37203	-628.65448	-628.41630	0.00532	0.03530	-0.11296	0.00000	288.66340	-628.77109
n.Cl-NHCOCH3	-668.76029	-667.54786	-667.88207	-667.60799	0.00696	0.06285	-0.14120	0.00000	328.21730	-668.01358
n.Cl-SH	-858.96602	-857.79628	-857.99219	-857.83463	0.00405	0.00913	-0.06589	0.00000	251.32370	-858.08324
n.Cl-SCH3	-898.28769	-896.96985	-897.21441	-897.02333	0.00529	0.03879	-0.09413	0.00000	288.47380	-897.31793
n.Cl-SCH2Ph	-1129.33799	-1127.27223	-1127.75358	-1127.38895	0.00950	0.11895	-0.22591	0.00000	398.18130	-1127.96777
n.Cl-SOCH3	-973.47969	-971.98079	-972.32648	-972.03444	0.00621	0.04246	-0.12237	0.00000	309.34250	-972.45383
n.Cl-SO2CH3	-1048.68068	-1047.01129	-1047.45901	-1047.06199	0.00675	0.04791	-0.15061	0.00000	321.52330	-1047.60565
n.Cl-BH2	-486.26958	-485.55547	-485.68250	-485.58700	0.00396	0.02094	-0.05648	0.00000	234.29550	-485.74561
n.Cl-PH2	-802.75438	-801.59632	-801.78332	-801.63667	0.00416	0.01821	-0.06589	0.00000	256.24520	-801.86721
n.Cl-SiH3	-751.53106	-750.38895	-750.56709	-750.42557	0.00437	0.02589	-0.06589	0.00000	250.73830	-750.63935
n.CH2Cl-CH=CH2	-577.49943	-576.48106	-576.72282	-576.54495	0.00568	0.07034	-0.11296	0.00000	295.72360	-576.82364
n.CH2Cl-CH_CH2_2	-616.80812	-615.64705	-615.93790	-615.72206	0.00641	0.09975	-0.14120	0.00000	314.83860	-616.04794
n.CH2Cl-CCH	-576.24109	-575.26256	-575.48539	-575.31616	0.00555	0.04652	-0.10354	0.00000	290.99630	-575.59047
n.CH2Cl-CN	-592.33654	-591.35252	-591.57892	-591.39943	0.00516	0.03651	-0.10354	0.00000	285.62770	-591.68770
n.CH2Cl-Ph	-731.16024	-729.65583	-730.04687	-729.75502	0.00787	0.11780	-0.19767	0.00000	356.91850	-730.21806
n.CH2Cl-NH2	-555.46175	-554.54520	-554.76926	-554.59108	0.00481	0.05545	-0.09413	0.00000	271.73660	-554.84901
n.CH2Cl-N_CH3_2	-634.08232	-632.86641	-633.18935	-632.94463	0.00747	0.11069	-0.15061	0.00000	332.14610	-633.30001
n.CH2Cl-Br	-3073.38223	-3071.13200	-3071.70290	-3071.03001	0.00467	0.02842	-0.09413	0.00000	287.81790	-3071.66195
n.CH2Cl-SH	-898.28464	-896.97236	-897.21461	-897.02486	0.00534	0.03695	-0.09413	0.00000	291.29960	-897.31894

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.CH2Cl-SCH3	-937.60123	-936.14195	-936.43249	-936.20966	0.00674	0.06636	-0.12237	0.00000	326.19420	-936.54948
n.CH2Cl-NO2	-704.59422	-703.35027	-703.71084	-703.39516	0.00590	0.04062	-0.14120	0.00000	311.35860	-703.85040
n.CH2Cl-SiH3	-790.79867	-789.50579	-789.73400	-789.56058	0.00585	0.05236	-0.09413	0.00000	297.82070	-789.82471
n.CH2Cl-COOH	-688.66732	-687.43831	-687.79199	-687.49089	0.00620	0.05240	-0.14120	0.00000	316.28250	-687.92716
n.CH2Cl-COCH3	-652.74368	-651.54574	-651.86444	-651.61145	0.00710	0.07412	-0.14120	0.00000	336.85520	-651.99012
n.CH2Cl-OCHO	-688.65323	-687.42037	-687.76967	-687.47424	0.00635	0.05239	-0.14120	0.00000	330.49780	-687.90600
n.CH2Cl-OCOCH3	-727.97998	-726.59820	-726.99910	-726.66817	0.00805	0.07960	-0.16943	0.00000	371.43470	-727.15086
n.CH2Cl-CONH2	-668.80536	-667.59477	-667.93245	-667.65309	0.00670	0.06432	-0.14120	0.00000	323.68350	-668.06094
n.CH2Cl-SOCH3	-1012.78849	-1011.14379	-1011.51870	-1011.21751	0.00767	0.07063	-0.15061	0.00000	348.61110	-1011.66473
n.CH2Cl-SO2CH3	-1087.98132	-1086.16835	-1086.66263	-1086.23670	0.00817	0.07531	-0.17885	0.00000	356.63700	-1086.82634
n.CH3-CH3	-79.83042	-79.49469	-79.61745	-79.53449	0.00441	0.07378	-0.06589	0.00000	227.44080	-79.64495
n.CH2CH3-CH2CH3	-158.45804	-157.82588	-158.05211	-157.89803	0.00671	0.13024	-0.12237	0.00000	299.75110	-158.10967
n.CH_CH3_2-CH_CH3_2	-237.08251	-236.15892	-236.49036	-236.26262	0.00921	0.18582	-0.17885	0.00000	354.62550	-236.57788
n.CH_CH2_2-CH_CH2_2	-234.59323	-233.73965	-234.03133	-233.82693	0.00707	0.14176	-0.16002	0.00000	317.98050	-234.12980
n.C_CH3_3-C_CH3_3	-315.70136	-314.49187	-314.93013	-314.62611	0.01144	0.24129	-0.23533	0.00000	386.11440	-315.04697
n.CH=CH2-CH=CH2	-155.99214	-155.42260	-155.61408	-155.48697	0.00559	0.08382	-0.10354	0.00000	276.29900	-155.69258
n.CH=CHCH3-CH=CHCH3	-234.63203	-233.76475	-234.05826	-233.85973	0.00855	0.13932	-0.16002	0.00000	343.19900	-234.16540
n.CH=C_CH3_2-CH=C_CH3_2	-313.26566	-312.10436	-312.50217	-312.22949	0.01146	0.19477	-0.21650	0.00000	407.87400	-312.63757
n.Ph-Ph	-463.30607	-461.76885	-462.25954	-461.90285	0.00982	0.17843	-0.27298	0.00000	379.05810	-462.47826
n.CCH-CCH	-153.48164	-152.99222	-153.14581	-153.03456	0.00512	0.03736	-0.08472	0.00000	244.06510	-153.23039
n.CN-CN	-185.65461	-185.15555	-185.31699	-185.18410	0.00468	0.01619	-0.08472	0.00000	239.38980	-185.40938
n.CH2OH-CH2OH	-230.23572	-229.53753	-229.84015	-229.58725	0.00635	0.08344	-0.12237	0.00000	293.79440	-229.92246
n.CH2F-CH2F	-278.27799	-277.51785	-277.85834	-277.55971	0.00537	0.06041	-0.12237	0.00000	280.22280	-277.95679
n.CH2Cl-CH2Cl	-999.01901	-997.55023	-997.84127	-997.61310	0.00585	0.05752	-0.12237	0.00000	301.04150	-997.96315

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.CHO-CHO	-227.81863	-227.18828	-227.43175	-227.22594	0.00514	0.03645	-0.10354	0.00000	270.72210	-227.53137
n.COCH3-COCH3	-306.47602	-305.54807	-305.89403	-305.61689	0.00813	0.09196	-0.16002	0.00000	343.27220	-306.02279
n.COOH-COOH	-378.31344	-377.32174	-377.73819	-377.36348	0.00650	0.04809	-0.16002	0.00000	315.91820	-377.88537
n.COPh-COPh	-689.95296	-687.81996	-688.53210	-687.88879	0.01372	0.19758	-0.36711	0.00000	478.19130	-688.75674
n.CONH2-CONH2	-338.60130	-337.65025	-338.03130	-337.70311	0.00715	0.07234	-0.16002	0.00000	317.88560	-338.16468
n.CONHCH3-CONHCH3	-417.22645	-415.97453	-416.45213	-416.06031	0.01018	0.12862	-0.21650	0.00000	389.10300	-416.61561
n.CON_CH3_2-CON_CH3_2	-495.82668	-494.27891	-494.85627	-494.39731	0.01333	0.18316	-0.27298	0.00000	455.06910	-495.05116
n.CON_CH2CH3_2-CON_CH2CH3_2	-653.09093	-650.95760	-651.74113	-651.13983	0.01802	0.29622	-0.38593	0.00000	560.70330	-651.99505
n.COOCH3-COOCH3	-456.92956	-455.63312	-456.14304	-455.70920	0.00986	0.10344	-0.21650	0.00000	389.33170	-456.32232
n.COOCH2CH3-COOCH2CH3	-535.56819	-533.97509	-534.58755	-534.08358	0.01245	0.15925	-0.27298	0.00000	451.89730	-534.79732
n.COOC_CH3_3-COOC_CH3_3	-692.83212	-690.65963	-691.47756	-690.83116	0.01772	0.26862	-0.38593	0.00000	545.37670	-691.74868
n.F-F	-199.49825	-199.03468	-199.26020	-199.05049	0.00333	0.00238	-0.06589	0.00000	202.17180	-199.33619
n.Cl-Cl	-920.34988	-919.17116	-919.36645	-919.20563	0.00351	0.00116	-0.06589	0.00000	223.33360	-919.46214
n.Br-Br	-5147.75475	-5144.71907	-5145.56616	-5144.45592	0.00370	0.00071	-0.06589	0.00000	245.40450	-5145.36448
n.OH-OH	-151.53321	-151.13003	-151.32273	-151.15107	0.00420	0.02574	-0.06589	0.00000	227.90640	-151.37973
n.OCH3-OCH3	-230.16112	-229.45056	-229.73432	-229.50555	0.00646	0.08192	-0.12237	0.00000	304.74600	-229.82328
n.OCH2CH3-OCH2CH3	-308.79922	-307.79246	-308.17892	-307.87940	0.00902	0.13810	-0.17885	0.00000	362.55180	-308.29760
n.OCHO-OCHO	-378.21400	-377.21236	-377.61555	-377.26068	0.00665	0.04581	-0.16002	0.00000	314.86290	-377.77142
n.OCOCH3-OCOCH3	-456.86912	-455.57041	-456.07675	-455.65046	0.01006	0.10056	-0.21650	0.00000	392.89780	-456.26267
n.NH2-NH2	-111.85645	-111.49786	-111.65556	-111.52866	0.00420	0.05245	-0.06589	0.00000	230.33230	-111.69559
n.NO2-NO2	-410.16824	-409.15266	-409.58124	-409.16804	0.00626	0.02305	-0.16002	0.00000	301.25970	-409.72733
n.NHCH3-NHCH3	-190.47601	-189.81657	-190.07027	-189.88072	0.00648	0.10818	-0.12237	0.00000	303.77400	-190.14213
n.N_CH3_2-N_CH3_2	-269.09044	-268.13650	-268.49197	-268.23227	0.00867	0.16357	-0.17885	0.00000	348.72950	-268.59435
n.NHCHO-NHCHO	-338.54074	-337.58533	-337.96107	-337.64173	0.00720	0.07161	-0.16002	0.00000	325.66330	-338.09869

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2 /GTMP2Large	URCCSD(T) /6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.NHCOCH3-NHCOCH3	-417.19087	-415.93921	-416.41803	-416.02783	0.01047	0.12652	-0.21650	0.00000	400.51180	-416.58617
n.SH-SH	-797.57178	-796.41099	-796.60666	-796.45372	0.00438	0.01791	-0.06589	0.00000	252.25270	-796.69299
n.SCH3-SCH3	-876.20751	-874.75241	-875.04572	-874.82530	0.00746	0.07643	-0.12237	0.00000	328.74400	-875.15709
n.SCH2Ph-SCH2Ph	-1338.30976	-1335.36322	-1336.13075	-1335.43611	0.01588	0.23695	-0.38593	0.00000	541.35810	-1336.33675
n.SOCH3-SOCH3	-1026.55785	-1024.73751	-1025.23191	-1024.81588	0.00964	0.08292	-0.17885	0.00000	384.22590	-1025.39656
n.SO2CH3-SO2CH3	-1176.96114	-1174.79731	-1175.49242	-1174.86943	0.01102	0.09321	-0.23533	0.00000	408.31260	-1175.69563
n.BH2-BH2	-52.04446	-51.77724	-51.84792	-51.81381	0.00474	0.03816	-0.04707	0.00000	231.15870	-51.88865
n.PH2-PH2	-685.09493	-683.95326	-684.13016	-684.00371	0.00521	0.03461	-0.06589	0.00000	272.43680	-684.20668
n.SiH3-SiH3	-582.58273	-581.46466	-581.62218	-581.51322	0.00597	0.04832	-0.06589	0.00000	273.36920	-581.68233
n.CH=CH2-H2CCH2-CH=CH2	-234.60965	-233.74565	-234.04175	-233.84269	0.00812	0.13993	-0.16002	0.00000	338.35310	-234.15076
n.CH_CH2_2-H2CCH2-CH_CH2_2	-313.22135	-312.07275	-312.46762	-312.19225	0.00966	0.19805	-0.21650	0.00000	385.07920	-312.59591
n.CCH-H2CCH2-CCH	-232.10310	-231.31921	-231.57826	-231.39533	0.00782	0.09248	-0.14120	0.00000	329.31100	-231.69527
n.CN-H2CCH2-CN	-264.30139	-263.50539	-263.77112	-263.56803	0.00711	0.07244	-0.14120	0.00000	320.49070	-263.89540
n.Ph-H2CCH2-Ph	-541.93036	-540.09693	-540.69200	-540.26402	0.01266	0.23432	-0.32946	0.00000	462.76440	-540.94156
n.NH2-H2CCH2-NH2	-190.51110	-189.85628	-190.11800	-189.91827	0.00641	0.10900	-0.12237	0.00000	293.73310	-190.18695
n.N_CH3_2-H2CCH2-N_CH3_2	-347.74148	-346.49019	-346.94713	-346.61694	0.01155	0.21937	-0.23533	0.00000	410.77920	-347.07829
n.Br-H2CCH2-Br	-5226.39297	-5223.06566	-5224.01693	-5222.83044	0.00622	0.05621	-0.12237	0.00000	324.46070	-5223.84164
n.SH-H2CCH2-SH	-876.19333	-874.74248	-875.03593	-874.81590	0.00738	0.07352	-0.12237	0.00000	328.96290	-875.15082
n.SCH3-H2CCH2-SCH3	-954.82472	-953.07994	-953.47080	-953.18392	0.01028	0.13216	-0.17885	0.00000	399.61320	-953.61119
n.NO2-H2CCH2-NO2	-488.81719	-487.50039	-488.03220	-487.56045	0.00871	0.08065	-0.21650	0.00000	381.01270	-488.21939
n.SiH3-H2CCH2-SiH3	-661.21144	-659.79969	-660.06747	-659.87773	0.00852	0.10352	-0.12237	0.00000	346.40110	-660.15584
n.COOH-H2CCH2-COOH	-456.96216	-455.67485	-456.19565	-455.74970	0.00933	0.10404	-0.21650	0.00000	398.95100	-456.37364
n.COCH3-H2CCH2-COCH3	-385.11137	-383.88709	-384.33717	-383.98825	0.01094	0.14755	-0.21650	0.00000	417.80280	-384.49633
n.OCHO-H2CCH2-OCHO	-456.92863	-455.63422	-456.14414	-455.71173	0.00938	0.10429	-0.21650	0.00000	385.59310	-456.32447

mol	B3LYP/6-31G*	ROMP2/6-31G*	ROMP2/GTMP2Large	URCCSD(T)/6-31G*	Temperature Correction	Zero Point Vibrational Energy	High Level Correction	Spin Orbital Correction	Entropy (J/mol K)	G3(MP2)-RAD Enthalpy
n.OCOCH3-H2CCH2-OCOCH3	-535.58037	-533.98836	-534.60147	-534.09813	0.01287	0.15859	-0.27298	0.00000	467.13630	-534.81276
n.CONH2-H2CCH2-CONH2	-417.22535	-415.97828	-416.46429	-416.06468	0.01021	0.12769	-0.21650	0.00000	395.64010	-416.62928
n.SOCH3-H2CCH2-SOCH3	-1105.19840	-1103.08543	-1103.64302	-1103.20172	0.01218	0.14077	-0.23533	0.00000	449.47340	-1103.84167
n.SO2CH3-H2CCH2-SO2CH3	-1255.60018	-1253.14761	-1253.94522	-1253.25368	0.01315	0.15027	-0.29180	0.00000	459.77160	-1254.17967
r.COPh ONIOM	-344.92063	-343.84871	-344.20356	-343.88389	0.00728	0.09588	-0.18282	0.00000	339.20830	-344.31841
r.SCH2Ph ONIOM	-669.10963	-667.63195	-668.00594	-667.67013	0.00807	0.11601	-0.19223	0.00000	368.62310	-668.11227

Table S4 B3-LYP/6-31G(d) Optimized Geometries of All Species

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r.H
 1\1\GINC-LC127\FOpt\UB3LYP\Gen\H1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.H.freq\\
 0,2\H,-0.001,0.,0.\\Version=IA32L-G03RevC.02\State=2-A1G\HF=-0.5002728
 \S2=0.75\S2-1=0.\S2A=0.75\RMSD=8.343e-12\RMSF=0.000e+00\Dipole=0.,0.,0
 .\PG=OH [O(H1)]\\@

r.BH2
 1\1\GINC-LC72\FOpt\UB3LYP\Gen\B1H2(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.BH2.fre
 q\\0,2\B,0.0493936865,0.0434439027,0.1345738972\H,0.8573047997,-0.4630
 297747,-0.5820039413\H,-1.1042732321,0.2458102613,-0.0908655445\\Versi
 on=IA32L-G03RevC.02\State=2-A'\HF=-25.9347113\S2=0.750873\S2-1=0.\S2A=
 0.75\RMSD=3.990e-09\RMSF=2.360e-05\Dipole=-0.0477883,-0.0420326,-0.130
 2018\PG=CS [SG(B1H2)]\\@

r.CH3
 1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1H3(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
 N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH3.fr
 eq\\0,2\C,-0.0001249111,0.0000332268,-0.000028932\H,0.7849181686,0.644
 7974652,-0.3753921373\H,0.1534759631,-0.5641961968,0.911541984\H,-0.93
 76446653,-0.0808006292,-0.5359762544\\Version=IA32L-G03RevC.02\State=2
 -A\HF=-39.8382917\S2=0.753767\S2-1=0.\S2A=0.750007\RMSD=3.352e-09\RMSF
 =1.010e-04\Dipole=0.0001085,-0.0001092,-0.0000499\PG=C01 [X(C1H3)]\\@

r.NH2
 1\1\GINC-LC127\FOpt\UB3LYP\Gen\H2N1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
 N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.NH2.fr
 eq\\0,2\N,0.0888723112,-0.0801519968,0.0808448842\H,-0.9433242776,-0.1
 123523509,0.0225778534\H,0.3212180989,0.6734163287,-0.5884920426\\Vers
 ion=IA32L-G03RevC.02\State=2-B1\HF=-55.8726204\S2=0.752803\S2-1=0.\S2A
 =0.750004\RMSD=2.062e-09\RMSF=2.185e-05\Dipole=-0.4871377,0.4393389,-0
 .4431368\PG=C02V [C2(N1),SGV(H2)]\\@

r.OH
 1\1\GINC-LC127\FOpt\UB3LYP\Gen\H1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
 N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OH.fre
 q\\0,2\O,-0.050878519,-0.0905506976,-0.0337549811\H,0.4070281516,0.724
 4055807,0.2700398489\\Version=IA32L-G03RevC.02\HF=-75.7234538\S2=0.751
 967\S2-1=0.\S2A=0.750002\RMSD=2.933e-09\RMSF=1.982e-07\Dipole=0.322109
 5,0.5732722,0.2137012\PG=C*V [C*(H1O1)]\\@

r.F
 1\1\GINC-LC127\FOpt\UB3LYP\Gen\F1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.F.freq\\
 0,2\F,0.400808,0.577206,0.269857\\Version=IA32L-G03RevC.02\HF=-99.7155
 355\S2=0.750978\S2-1=0.\S2A=0.75\RMSD=2.800e-09\RMSF=0.000e+00\Dipole=
 0.,0.,0.\PG=OH [O(F1)]\\@

r.SiH3
 1\1\GINC-LC12\FOpt\UB3LYP\Gen\H3Si1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
 N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SiH3.f
 req\\0,2\Si,0.0383639103,-0.0664481773,-0.0271383241\H,-1.3588970721,-
 0.0984536663,-0.5407000742\H,0.0571193176,-0.0988848971,1.4613765601\H
 ,0.7646830105,1.127613045,-0.5407399492\\Version=IA32L-G03RevC.02\Stat
 e=2-A\HF=-291.232263\S2=0.751364\S2-1=0.\S2A=0.750001\RMSD=3.603e-09\R
 MSF=1.375e-05\Dipole=0.0077902,-0.0134929,-0.0054515\PG=C01 [X(H3Si1)]
 \\@

r.PH2
 1\1\GINC-LC16\FOpt\UB3LYP\Gen\H2P1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.PH2.fre
 q\\0,2\P,0.0343870474,0.01354731,0.1113374407\H,-1.0499535111,-0.67268
 40638,-0.5209148094\H,0.5341477995,0.4694744141,-1.1491468017\\Version
 =IA32L-G03RevC.02\State=2-A"\HF=-342.5042163\S2=0.753627\S2-1=0.\S2A=0
 .750005\RMSD=9.038e-09\RMSF=1.202e-05\Dipole=-0.1003871,-0.0395491,-0.
 3250307\PG=CS [SG(H2P1)]\\@

r.SH
 1\1\GINC-LC59\FOpt\UB3LYP\Gen\H1S1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SH.freq
 \\0,2\S,-0.0393355621,0.0689744181,0.0071146406\H,0.6293689937,-1.1035
 906894,-0.1138342498\\Version=IA32L-G03RevC.02\HF=-398.7400218\S2=0.75
```

2432\S2-1=0.\S2A=0.750002\RMSD=3.287e-09\RMSF=5.241e-05\Dipole=0.20576
31,-0.3608031,-0.0372165\PG=C*V [C*(H1S1)]\\@

r.Cl
1\1\GINC-LC51\FOpt\UB3LYP\Gen\Cl1(2)\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.Cl.freq\
\0,2\Cl,1.274,0.,0.\\Version=IA32L-G03RevC.02\HF=-460.1362423\S2=0.751
721\S2-1=0.\S2A=0.750001\RMSD=7.828e-10\RMSF=0.000e+00\Dipole=0.,0.,0.
\PG=OH [O(Cl1)]\\@

r.Br
1\1\GINC-LC76\FOpt\UB3LYP\Gen\Br1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.Br.freq\
\0,2\Br,0.227076,0.324848,0.153903\\Version=IA32L-G03RevC.02\HF=-2573.
8397406\S2=0.751467\S2-1=0.\S2A=0.75\RMSD=5.590e-09\RMSF=0.000e+00\Dip
ole=0.,0.,0.\PG=OH [O(Br1)]\\@

r.N_CH3_2
1\1\GINC-LC76\FOpt\UB3LYP\Gen\C2H6N1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.N_CH3
_2.freq\\0,2\C,0.8514615911,0.2358642064,0.8192677711\H,1.9402502567,0
.3435285235,0.8208846498\H,0.5755864521,-0.5630148677,1.5308482389\H,0
.4047418761,1.1668718705,1.2120138296\N,0.3786292823,-0.0542652751,-0.
5120166866\C,-1.055160241,-0.2069280693,-0.5437239237\H,-1.391214696,-
1.0206187859,0.1238402503\H,-1.3913430366,-0.4292190724,-1.5608882086\
H,-1.5662339292,0.7086924353,-0.1958450383\\Version=IA32L-G03RevC.02\S
tate=2-A\HF=-134.5094891\S2=0.75361\S2-1=0.\S2A=0.75001\RMSD=5.980e-09
\RMSF=5.647e-05\Dipole=-0.4100606,0.0593468,0.554335\PG=C01 [X(C2H6N1)
]\\@

r.NHCH3
1\1\GINC-LC151\FOpt\UB3LYP\Gen\C1H4N1(2)\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.NHCH
3.freq\\0,2\N,0.8170000572,-0.0036460428,0.0775085711\C,-0.6240650919,
-0.0763279944,0.0105357862\H,-0.9978236155,-0.8646317389,0.6715040864\
H,-0.975525978,-0.2847577049,-1.015484086\H,-1.0954713631,0.8782858001
,0.3040260168\H,1.0942111077,0.7545939095,-0.5658207319\\Version=IA32L
-G03RevC.02\State=2-A\HF=-95.1908608\S2=0.753275\S2-1=0.\S2A=0.750008\
RMSD=8.132e-10\RMSF=3.441e-05\Dipole=-0.5339046,0.4096999,-0.4097511\P
G=C01 [X(C1H4N1)]\\@

r.NHCHO
1\1\GINC-LC12\FOpt\UB3LYP\Gen\C1H2N1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.NHC
HO.freq\\0,2\N,-0.7135839196,-0.3901674214,0.8219894711\H,-1.711084485
2,-0.5801629906,0.6429000757\C,-0.150540372,0.0559181041,-0.3427285568
\O,1.0482583833,0.3533304829,-0.3862438881\H,-0.7766529121,0.149182452
8,-1.2505039278\\Version=IA32L-G03RevC.02\State=2-A\HF=-169.2000091\S2
=0.778\S2-1=0.\S2A=0.750117\RMSD=2.890e-09\RMSF=6.916e-05\Dipole=-1.16
73332,-0.1574232,-0.451787\PG=C01 [X(C1H2N1O1)]\\@

r.NHCOCH3
1\1\GINC-AC8\FOpt\UB3LYP\Gen\C2H4N1O1(2)\CYL509\19-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\test.f
req\\0,2\H,-1.6629109093,-1.1577580506,-0.353187704\C,-1.3934086206,-0
.174971035,0.0476696025\C,0.093647795,0.0446201244,-0.0521855925\O,0.6
055828432,1.1220416729,-0.3879364746\H,-1.6965547819,-0.1566160268,1.1
007507225\H,-1.9235501534,0.6111830158,-0.4933109812\N,0.9144579976,-0
.9485609752,0.4153095735\H,1.8357120691,-0.8511100319,-0.0308313156\\V
ersion=IA64L-G03RevC.02\State=2-A\HF=-208.5321137\S2=0.76798\S2-1=0.\S
2A=0.75007\RMSD=7.050e-09\RMSF=1.361e-05\Dipole=-0.3748795,-0.4604407,
-0.1892604\PG=C01 [X(C2H4N1O1)]\\@

r.NO2
1\1\GINC-LC16\FOpt\UB3LYP\Gen\N1O2(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.NO2.fre
q\\0,2\N,0.1376665018,-0.2430965251,-0.1721682798\O,0.9348648835,0.569
9789982,0.2163813033\O,-1.0553230726,-0.3572695388,-0.0657340585\\Vers
ion=IA32L-G03RevC.02\State=2-A1\HF=-205.0722069\S2=0.753298\S2-1=0.\S2
A=0.750007\RMSD=2.786e-09\RMSF=1.544e-05\Dipole=0.0530556,-0.0936875,-
0.0663523\PG=C02V [C2(N1),SGV(O2)]\\@

r.OCF3
1\1\GINC-LC44\FOpt\UB3LYP\Gen\C1F3O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OCF3.
freq\\0,2\O,-1.0374085479,0.5593487278,-0.7408641945\C,-0.0241929362,0
.0013112985,-0.0320561289\F,1.1325954914,0.012590764,-0.7038680751\F,-

0.2815298353,-1.2658318007,0.3110825532\F,0.0872038996,0.7551679686,1.
0727022252\\Version=IA32L-G03RevC.02\State=2-A\HF=-412.7726789\S2=0.75
2399\S2-1=0.\S2A=0.750004\RMSD=4.446e-09\RMSF=6.922e-05\Dipole=0.03750
27,-0.0183365,0.0291574\PG=C01 [X(C1F3O1)]\\@

r.OCH2CH3
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C2H5O1(2)\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OCH2C
H3.freq\\0,2\O,-0.5815105059,-0.0040949456,-1.1730345777\C,-0.47743497
13,-0.0080315087,0.1938198643\C,0.9491299715,0.0185764459,0.742601877\
H,-1.0115280091,-0.9252062308,0.5244523317\H,-1.0955854549,0.813382911
7,0.6081376667\H,0.9490069881,-0.020837353,1.8382807649\H,1.4594893433
,0.9365308909,0.4324661902\H,1.5205311786,-0.8343802774,0.3624092202\\
Version=IA64L-G03RevC.02\State=2-A\HF=-154.3704938\S2=0.753018\S2-1=0.
\S2A=0.750007\RMSD=3.836e-09\RMSF=1.443e-05\Dipole=0.051118,-0.0331855
,0.7711156\PG=C01 [X(C2H5O1)]\\@

r.OCH3
1\1\GINC-LC72\FOpt\UB3LYP\Gen\C1H3O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OCH3.
freq\\0,2\O,-0.7401800878,0.0044987004,-0.2863968812\C,0.5430046856,-0
.0032913313,0.189874558\H,1.1047084642,-0.9156166856,-0.0725884565\H,0
.4431127973,-0.0032134174,1.296084607\H,1.1155111269,0.9025884872,-0.0
716562485\\Version=IA32L-G03RevC.02\State=2-A\HF=-115.0504607\S2=0.752
915\S2-1=0.\S2A=0.750006\RMSD=2.210e-09\RMSF=1.851e-04\Dipole=0.693121
9,-0.0042534,0.3592879\PG=C01 [X(C1H3O1)]\\@

r.OCHO
1\1\GINC-LC76\FOpt\UB3LYP\Gen\C1H1O2(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OCHO.
freq\\0,2\O,-0.9875690251,0.4363425415,0.0004305887\C,0.2652673298,0.3
433534606,0.002578765\O,0.6714394061,-0.8456354069,-0.0035019841\H,0.9
374329736,1.2142221597,0.0090985726\\Version=IA32L-G03RevC.02\State=2-
A\HF=-189.0789655\S2=0.755961\S2-1=0.\S2A=0.750019\RMSD=5.360e-09\RMSF
=1.263e-04\Dipole=0.5505261,0.7128088,0.005349\PG=C01 [X(C1H1O2)]\\@

r.OCOCH3
1\1\GINC-AC8\FOpt\UB3LYP\Gen\C2H3O2(2)\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.OCOCH3
.freq\\0,2\O,-0.3555142374,-0.2619269769,-1.2474695946\C,-0.0975675853
,-0.0106712683,-0.0383312764\C,1.2838487647,0.0217180176,0.5360060333\
O,-1.1440722065,0.2376904663,0.621084662\H,1.2553563471,-0.2397765432,
1.5973203364\H,1.6899845565,1.0350302623,0.4376936024\H,1.933663571,-0
.6676421299,-0.009983019\\Version=IA64L-G03RevC.02\State=2-A\HF=-228.4
113647\S2=0.755832\S2-1=0.\S2A=0.750018\RMSD=1.480e-09\RMSF=4.918e-06\
Dipole=1.1430117,0.0403125,0.4716707\PG=C01 [X(C2H3O2)]\\@

r.Si_CH3_3
1\1\GINC-LC59\FOpt\UB3LYP\Gen\C3H9Si1(2)\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.Si_C
H3_3.freq\\0,2\H,0.9245956779,-1.601942021,-1.2760281951\C,0.901951082
5,-1.5623059598,-0.1773961143\H,1.9380925215,-1.587126337,0.1780153873
\H,0.4055908155,-2.4720205258,0.178364213\Si,0.0000075511,0.0000077486
,0.4251456083\C,-1.8039882018,0.0000231856,-0.1773617565\C,0.902023573
9,1.5622746977,-0.1774288428\H,-1.849667786,0.0001779706,-1.2759968359
\H,-2.3436400594,0.8847545845,0.178365742\H,-2.3435233196,-0.884886480
4,0.1781019868\H,1.9379377382,1.5874276323,0.1786136991\H,0.4052467373
,2.4720057212,0.1777086195\H,0.9253432312,1.6015494339,-1.2760628518\\
Version=IA32L-G03RevC.02\State=2-A\HF=-409.2109419\S2=0.751147\S2-1=0.
\S2A=0.750001\RMSD=2.601e-09\RMSF=9.102e-05\Dipole=0.0000112,-0.000013
3,-0.2627105\PG=C01 [X(C3H9Si1)]\\@

r.P_CH3_2
1\1\GINC-LC76\FOpt\UB3LYP\Gen\C2H6P1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.P_CH3
_2.freq\\0,2\C,-0.29648447,1.3709391052,0.539869766\H,0.3714549665,2.1
500549861,0.9194063283\H,-1.0094727095,1.1112087426,1.3330016321\H,-0.
8672404183,1.7854421443,-0.3011600439\P,0.7017807761,-0.1174276828,0.0
125207179\C,-0.7075846044,-1.2029425107,-0.557754767\H,-0.3168272134,-
2.1592512578,-0.9183025077\H,-1.2690138418,-0.7299394486,-1.3738251976
\H,-1.4111979788,-1.4040794911,0.2603790258\\Version=IA32L-G03RevC.02\
State=2-A\HF=-421.1466401\S2=0.753989\S2-1=0.\S2A=0.750006\RMSD=3.712e
-09\RMSF=8.282e-06\Dipole=-0.6084818,0.1018271,-0.0108811\PG=C01 [X(C2
H6P1)]\\@

r.SC_CH3_2CN
1\1\GINC-LC48\FOpt\UB3LYP\Gen\C4H6N1S1(2)\CYL509\19-Jun-2008\0\\#B3LYP

/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SC_
CH3_2CN.freq\\0,2\S,1.6051906045,-0.3470482178,-0.2605504015\C,-0.1911
878503,-0.1757260052,0.1337985611\C,-0.3631818145,-0.2565377242,1.6689
015547\C,-0.9580341427,-1.3211558788,-0.5678856709\C,-0.6910103887,1.1
220236604,-0.3508712694\H,-0.0071131492,-1.2258554118,2.0280111935\H,0
.191455218,0.5376683047,2.1761382573\H,-1.4242820797,-0.1482360937,1.9
208843565\H,-0.8265475341,-1.2849961005,-1.6528167836\H,-2.0279719606,
-1.2283914577,-0.3491939011\H,-0.5989493353,-2.2848595187,-0.196907132
4\N,-1.1098793793,2.1394024926,-0.7229955171\\Version=IA32L-G03RevC.02
\State=2-A\HF=-608.9213547\S2=0.752708\S2-1=0.\S2A=0.750003\RMSD=1.427
e-09\RMSF=1.554e-05\Dipole=-0.1086183,-1.333372,0.6631612\PG=C01 [X(C4
H6N1S1)]\\@

r.SCH2COOCH3
1\1\GINC-LC96\FOpt\UB3LYP\Gen\C3H5O2S1(2)\CYL509\19-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SCH
2COOCH3.freq\\0,2\S,-2.0294359063,-0.6962534572,-0.4570065699\C,-0.845
4809447,-0.3639412981,0.8853159927\C,0.3767998907,0.4063602133,0.42408
12496\O,0.5223624977,1.6016429309,0.5488998809\O,1.2726590463,-0.41475
57502,-0.1577507279\C,2.4413211834,0.2307978553,-0.6932302517\H,-1.359
043997,0.2084057505,1.6642981961\H,-0.5589707547,-1.3353838311,1.30680
61378\H,2.984610208,0.7555110787,0.0968979429\H,2.1582906216,0.9470899
613,-1.4688303624\H,3.0500752937,-0.5699657129,-1.1132619631\\Version=
IA32L-G03RevC.02\State=2-A\HF=-665.928579\S2=0.752589\S2-1=0.\S2A=0.75
0003\RMSD=2.743e-09\RMSF=1.174e-05\Dipole=0.5813038,-0.5280112,0.18019
77\PG=C01 [X(C3H5O2S1)]\\@

r.SCH2Ph
1\1\GINC-LC71\FOpt\UB3LYP\Gen\C7H7S1(2)\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SCH2P
h.freq\\0,2\S,2.7485761877,-0.1941908606,-0.2487728861\C,1.3954036734,
-0.1685523798,0.9865421682\C,0.0029829314,-0.0315707773,0.4206602397\H
,1.6096785558,0.6210502487,1.7146530166\H,1.5125846551,-1.1215487923,1
.524170838\C,-0.6696716624,1.1933365492,0.4975156409\C,-0.6399403993,-
1.1176700718,-0.1880267542\C,-1.9583827097,1.3327658277,-0.021994291\C
,-1.9265339203,-0.9820175266,-0.7055828584\C,-2.5903672488,0.245194201
9,-0.6244014523\H,-3.5937379032,0.3507000121,-1.02795999\H,-2.41323604
18,-1.8346024161,-1.1717744647\H,-2.4665077135,2.2910537122,0.04585805
57\H,-0.1246623001,-2.0726849832,-0.261392132\H,-0.1822822404,2.044251
048,0.9685346972\\Version=IA32L-G03RevC.02\State=2-A\HF=-669.1096289\S
2=0.752624\S2-1=0.\S2A=0.750003\RMSD=7.466e-09\RMSF=2.331e-05\Dipole=-
0.5754054,-0.0248041,0.4197679\PG=C01 [X(C7H7S1)]\\@

r.SCH3
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1H3S1(2)\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SCH3
.freq\\0,2\S,0.1912298327,-0.6710754324,0.\C,-0.2951055369,1.075991173
5,0.\H,-1.3936899616,1.0993485756,0.\H,0.0523229297,1.5909556511,0.899
6434741\H,0.0523229297,1.5909556511,-0.8996434741\\Version=IA32L-G03Re
vC.02\State=2-A'\HF=-438.0597202\S2=0.75249\S2-1=0.\S2A=0.750003\RMSD=
6.765e-09\RMSF=1.654e-04\Dipole=-0.2246521,0.669623,0.\PG=CS [SG(C1H1S
1),X(H2)]\\@

r.SO2CH3
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1H3O2S1(2)\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SO
2CH3.freq\\0,2\C,-0.2954959735,-1.3420842587,-0.7983595115\S,0.2326687
273,0.2612981493,-0.0649391413\O,-0.9430014243,1.1683229006,-0.1741701
86\O,0.8479339146,-0.0726640613,1.2491170284\H,0.5687233955,-2.0070507
332,-0.8138501784\H,-0.6745094858,-1.1455814424,-1.8018687998\H,-1.083
3976273,-1.7409033758,-0.1546724317\\Version=IA32L-G03RevC.02\State=2-
A'\HF=-588.4601498\S2=0.754937\S2-1=0.\S2A=0.750017\RMSD=2.558e-09\RMS
F=7.621e-05\Dipole=0.0359156,-1.0719063,-0.9798053\PG=CS [SG(C1H1S1),X
(H2O2)]\\@

r.SOCH3
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1H3O1S1(2)\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.SO
CH3.freq\\0,2\S,0.3684078351,0.3247742359,0.2610150498\O,0.961350937,-
1.0013442073,-0.2274326576\C,-1.394342227,0.3114495676,-0.2307279877\H
,-1.9021932723,-0.5347251635,0.2403832735\H,-1.4725281588,0.2293401826
,-1.3184308435\H,-1.8445580647,1.2510534597,0.1056359611\\Version=IA32
L-G03RevC.02\State=2-A\HF=-513.2732772\S2=0.753678\S2-1=0.\S2A=0.75001
\RMSD=7.187e-09\RMSF=2.656e-05\Dipole=-0.9343302,0.677628,0.0757606\PG
=C01 [X(C1H3O1S1)]\\@

r.Ph

1\1\GINC-LC59\FOpt\UB3LYP\Gen\C6H5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.Ph.freq
\\0,2\C,0.4686493048,0.2473621694,1.2960171962\C,-0.4433854235,-0.2340
349348,-1.2262080703\C,0.0668711912,1.3371237364,0.5544431838\C,0.4497
416955,-1.0644256939,0.8743621831\C,-0.0222108537,-1.300571853,-0.4271
930004\C,-0.4012666454,1.0770496135,-0.7439244114\H,0.105332673,2.3514
828048,0.9427407163\H,0.7805670558,-1.8839145085,1.5069530788\H,-0.058
2889309,-2.3179534885,-0.8103367118\H,-0.7309584999,1.9013556012,-1.37
24059535\H,-0.8070479132,-0.4259886237,-2.2319336174\\Version=IA32L-G0
3RevC.02\State=2-A\HF=-231.5612757\S2=0.757483\S2-1=0.\S2A=0.750031\RM
SD=6.002e-09\RMSF=4.454e-05\Dipole=-0.1032723,-0.0545231,-0.2856972\PG
=C01 [X(C6H5)]\\@

r.C6H4CN
1\1\GINC-LC70\FOpt\UB3LYP\Gen\C7H4N1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C6H4C
N.freq\\0,2\C,0.7673021909,0.39154957,2.0037227229\C,-0.1899639786,-0.
0968706776,-0.4957966663\C,0.5253763777,1.4862256345,1.2016083182\C,0.
5690318221,-0.9276983308,1.6565838928\C,0.0765757227,-1.1734287229,0.3
699016108\C,0.0331189222,1.2295104981,-0.0830036271\H,0.7029364611,2.5
045018824,1.5351926468\H,0.779840244,-1.7478926952,2.3366821721\H,-0.1
018626033,-2.1904919092,0.0335060251\H,-0.1785061777,2.0475225437,-0.7
652727957\C,-0.6945704424,-0.3543810586,-1.8135660853\N,-1.1033759445,
-0.5632973283,-2.882401292\\Version=IA32L-G03RevC.02\State=2-A\HF=-323
.8038793\S2=0.758193\S2-1=0.\S2A=0.750035\RMSD=9.794e-09\RMSF=5.844e-0
5\Dipole=0.5152828,0.263108,1.3462804\PG=C01 [X(C7H4N1)]\\@

r.C6H4NO2
1\1\GINC-LC28\FOpt\UB3LYP\Gen\C6H4N1O2(2)\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C6H
4NO2.freq\\0,2\C,0.8423455548,0.4438773677,2.3239737584\C,-0.060680135
,-0.0319786492,-0.1674349267\C,0.4408328338,1.5374554721,1.5854040733\
C,0.8247344282,-0.8705629465,1.9061852666\C,0.3546975339,-1.114442957,
0.6104575957\C,-0.0280838133,1.2865487237,0.2906124606\H,0.4800712012,
2.5505581666,1.9743676403\H,1.1558874429,-1.6884915827,2.5390674062\H,
0.3064930829,-2.1165902107,0.2011552962\H,-0.3635892028,2.0864933642,-
0.3587532802\N,-0.5544356247,-0.2921640773,-1.5296694879\O,-0.91639287
18,0.6736072812,-2.2010804805\O,-0.5762185738,-1.4601321639,-1.9168370
212\\Version=IA32L-G03RevC.02\State=2-A'\HF=-436.0618911\S2=0.757995\S
2-1=0.\S2A=0.750033\RMSD=3.510e-09\RMSF=5.522e-05\Dipole=0.4919479,0.2
592226,1.3571653\PG=CS [SG(C2N1),X(C4H4O2)]\\@

r.C6H4OCH3
1\1\GINC-LC62\FOpt\UB3LYP\Gen\C7H7O1(2)\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C6H4O
CH3.freq\\0,2\C,-0.5291598867,-0.0459680097,-1.3081257437\C,-0.4565266
707,-0.0079245834,0.0944726819\C,0.7865039415,0.0371831215,0.739444609
5\C,1.9669799145,0.0442787005,-0.0256213525\C,1.8412398156,0.005916285
8,-1.3938529884\C,0.639382341,-0.0391506786,-2.0736713175\O,-1.6624413
701,-0.0186742004,0.7403187931\C,-1.6654257371,0.0177078027,2.15731784
13\H,0.5859768767,-0.0685180229,-3.1586774883\H,2.9343742222,0.0791806
344,0.4685529561\H,0.8553229486,0.0668345501,1.8213949297\H,-1.5091882
623,-0.0804634842,-1.7753786966\H,-1.1542229158,-0.8547810925,2.586262
8225\H,-2.7154959059,0.0013175944,2.4552468033\H,-1.1951983124,0.93356
75913,2.5402659447\\Version=IA32L-G03RevC.02\State=2-A\HF=-346.0822455
\S2=0.757767\S2-1=0.\S2A=0.750031\RMSD=6.963e-09\RMSF=2.983e-05\Dipole
=-0.1582765,0.0133277,0.6584874\PG=C01 [X(C7H7O1)]\\@

r.C6H4OH
1\1\GINC-LC47\FOpt\UB3LYP\Gen\C6H5O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C6H4O
H.freq\\0,2\C,-0.7692550969,-0.0695296385,-0.9668909504\C,-0.757394864
3,-0.0030274228,0.4326938551\C,0.4526008795,0.0675932237,1.1335569033\
C,1.6690814168,0.0722038484,0.433130571\C,1.6054063309,0.0053196361,-0
.9404376934\C,0.4387764942,-0.0655105574,-1.6741733904\O,-1.9727938137
,-0.0108413304,1.0648640249\H,0.4390647807,-0.1167991856,-2.7596557949
\H,2.6115703669,0.1268409766,0.9713037987\H,0.4499991026,0.1189311155,2
.221812505\H,-1.7238421045,-0.12346674,-1.4821940241\H,-1.8297325976,0
.0389299007,2.0225455444\\Version=IA32L-G03RevC.02\State=2-A\HF=-306.7
756848\S2=0.757826\S2-1=0.\S2A=0.750032\RMSD=6.712e-09\RMSF=7.863e-05\
Dipole=0.0084734,0.0289293,0.6055328\PG=C01 [X(C6H5O1)]\\@

r.CF2CF3
1\1\GINC-LC44\FOpt\UB3LYP\Gen\C2F5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CF2CF3.
freq\\0,2\F,-1.058801049,-0.1560716874,-1.5327684975\C,-0.9101785668,-
0.0969758518,-0.2146179586\C,0.5297144684,-0.1640791176,0.2494478574\F

,-1.6090653113,0.8939542943,0.3264080753\F,1.1140619093,-1.2590952955,
-0.2562223607\F,0.5682034652,-0.2174583457,1.5880684205\F,1.2392437179
,0.9127076805,-0.1487055702\\Version=IA32L-G03RevC.02\State=2-A\HF=-57
5.3382183\S2=0.752116\S2-1=0.\S2A=0.750003\RMSD=7.310e-09\RMSF=1.167e-
04\Dipole=-0.1560107,-0.0570794,-0.013942\PG=C01 [X(C2F5)]\\@

r.CF2H
1\1\GINC-LC12\FOpt\UB3LYP\Gen\C1H1F2(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CF2H.
freq\\0,2\C,0.4425343829,0.0302880093,0.249555976\H,1.4802643232,0.083
0753671,-0.0898369768\F,-0.2927950402,1.0866539224,-0.1013104961\F,-0.
1667016955,-1.1160765249,-0.0550782683\\Version=IA32L-G03RevC.02\State
=2-A\HF=-238.3054839\S2=0.751708\S2-1=0.\S2A=0.750002\RMSD=4.787e-09\R
MSF=1.429e-04\Dipole=0.4791133,0.0253287,-0.0499901\PG=C01 [X(C1H1F2)]
\\@

r.CF3
1\1\GINC-LC26\FOpt\UB3LYP\Gen\C1F3(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CF3.fre
q\\0,2\F,-0.1944535666,-0.2884494772,-1.2180862584\C,-0.1612913351,-0.
2653273437,0.1083653597\F,1.0844490802,-0.3398081684,0.5596877822\F,-0
.7824679568,0.8051425414,0.586154903\\Version=IA32L-G03RevC.02\State=2
-A\HF=-337.5510254\S2=0.751413\S2-1=0.\S2A=0.750001\RMSD=9.193e-09\RMS
F=9.499e-05\Dipole=-0.0431848,-0.069927,0.0290461\PG=C01 [X(C1F3)]\\@

r.CCl2H
1\1\GINC-LC3\FOpt\UB3LYP\Gen\C1H1Cl2(2)\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CCl2H
.freq\\0,2\C,0.3176873661,-0.5486581303,-0.2903275764\Cl,1.2041353662,
0.8829354238,0.0596229372\Cl,-1.3667344449,-0.6019829647,0.0556903264\
H,0.8580601405,-1.4842430227,-0.2183600215\\Version=IA32L-G03RevC.02\S
tate=2-A\HF=-959.0341043\S2=0.753601\S2-1=0.\S2A=0.75001\RMSD=5.620e-0
9\RMSF=9.271e-05\Dipole=0.2062396,-0.3552698,0.0497585\PG=C01 [X(C1H1C
l2)]\\@

r.CCl3
1\1\GINC-LC43\FOpt\UB3LYP\Gen\C1Cl3(2)\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CCl3.f
req\\0,2\C,0.000566088,0.0014529732,-0.2751347933\Cl,0.8518835577,1.47
46328133,0.0408143902\Cl,-1.7032237261,0.0000267132,0.0312148423\Cl,0.
8511403727,-1.4751723405,0.0250771651\\Version=IA32L-G03RevC.02\State=
2-A\HF=-1418.6234706\S2=0.753363\S2-1=0.\S2A=0.750009\RMSD=5.446e-09\R
MSF=9.472e-05\Dipole=0.0012152,-0.0007275,0.0832673\PG=C01 [X(C1Cl3)]\
\@

r.CH2Cl
1\1\GINC-LC26\FOpt\UB3LYP\Gen\C1H2Cl1(2)\CYL509\19-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2C
l.freq\\0,2\C,-0.5552872493,-0.9607618405,-0.1898386006\Cl,0.290968502
9,0.5034279735,0.0918118323\H,-1.6346986437,-0.9185879146,-0.211348424
3\H,0.0199575905,-1.8751165919,-0.2104211208\\Version=IA32L-G03RevC.02
\State=2-A\HF=-499.4383231\S2=0.754071\S2-1=0.\S2A=0.750011\RMSD=2.654
e-09\RMSF=1.460e-04\Dipole=-0.2374433,-0.4107761,-0.0307624\PG=C01 [X(
C1H2Cl1)]\\@

r.CH2F
1\1\GINC-LC72\FOpt\UB3LYP\Gen\C1H2F1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2F.
freq\\0,2\C,-0.6565177966,-0.0146459942,0.037439143\F,0.6860015872,-0.
0061899471,0.0158219644\H,-1.1174533115,0.9598026872,0.1638762458\H,-1
.1174541938,-0.8162171979,-0.5309087835\\Version=IA32L-G03RevC.02\Stat
e=2-A'\HF=-139.0642653\S2=0.753037\S2-1=0.\S2A=0.750006\RMSD=3.281e-09
\RMSF=1.084e-05\Dipole=-0.4658412,0.0554493,-0.1417398\PG=CS [SG(C1F1)
,X(H2)]\\@

r.CH2OH
1\1\GINC-AC23\FOpt\UB3LYP\Gen\C1H3O1(2)\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2OH
.freq\\0,2\C,0.0932134602,-0.0784053246,-0.6800020648\O,-0.1730410428,
0.0063499153,0.6612610064\H,0.9700017808,0.4366242434,-1.0693165209\H,
-0.8070545997,-0.1345359672,-1.2807850436\H,0.6621003996,0.1175443489,
1.1400259021\\Version=IA64L-G03RevC.02\State=2-A\HF=-115.0520323\S2=0.
75293\S2-1=0.\S2A=0.750006\RMSD=9.206e-09\RMSF=1.937e-05\Dipole=0.5591
389,0.2338011,0.0526082\PG=C01 [X(C1H3O1)]\\@

r.CH2Ph
1\1\GINC-LC70\FOpt\UB3LYP\Gen\C7H7(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN

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 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2Ph.f
 req\\0,2\C,-0.9038700985,2.2253244416,0.\C,-0.3747685394,0.9220585177,
 0.\C,-0.0948447982,0.2334880424,1.2181342437\C,-0.0948447982,0.2334880
 424,-1.2181342437\C,0.4267109965,-1.0504733246,1.211984871\C,0.4267109
 965,-1.0504733246,-1.211984871\C,0.6923325203,-1.7045265783,0.\H,1.101
 1980438,-2.710923037,0.\H,0.6310298927,-1.5533536155,2.153841864\H,0.6
 310298927,-1.5533536155,-2.153841864\H,-0.2986888051,0.7356552408,2.16
 07807669\H,-0.2986888051,0.7356552408,-2.1607807669\H,-1.1152189461,2.
 7465024431,-0.9280751648\H,-1.1152189461,2.7465024431,0.9280751648\\Ve
 rsion=IA32L-G03RevC.02\State=2-A'\HF=-270.9151377\S2=0.783691\S2-1=0.\
 S2A=0.75077\RMSD=5.267e-09\RMSF=1.161e-05\Dipole=0.019999,-0.0486899,0
 .\PG=CS [SG(C3H1),X(C4H6)]]\\@

r.CH_CH2_2
 1\1\GINC-LC16\FOpt\UB3LYP\Gen\C3H5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH_CH2_
 2.freq\\0,2\C,-0.3657777832,0.0491714814,-0.7661253671\C,-0.355933366,
 0.0578474124,0.7701456647\C,0.8894644781,-0.0340165939,-0.0055075354\H
 ,1.6808269278,-0.7740247736,-0.006399583\H,-0.610404943,1.0003226974,1
 .2561765428\H,-0.7168671373,-0.8178624981,1.3110067344\H,-0.6265253344
 ,0.9861158437,-1.259468461\H,-0.7335494864,-0.832565069,-1.292391806\\
 Version=IA32L-G03RevC.02\State=2-A\HF=-117.2134542\S2=0.75302\S2-1=0.\
 S2A=0.750007\RMSD=6.542e-09\RMSF=1.656e-05\Dipole=-0.150749,-0.1698864
 ,0.0019254\PG=C01 [X(C3H5)]]\\@

r.CH2CH=CH2
 1\1\GINC-LC12\FOpt\UB3LYP\Gen\C3H5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2CH=C
 H2.freq\\0,2\C,-0.2645231763,-1.1341600991,0.4419390685\C,0.4252008181
 ,0.0246749205,0.1214133628\H,0.2136539909,-1.9530124871,0.9690285688\H
 ,-1.3101105551,-1.2582842059,0.1725510053\H,1.4727940998,0.0845933834,
 0.4185591966\C,-0.1119869738,1.1124396502,-0.5490212892\H,0.4808465197
 ,1.9931225865,-0.7725262183\H,-1.1493280628,1.1158538934,-0.8735994056
 \\Version=IA32L-G03RevC.02\State=2-A\HF=-117.2603508\S2=0.781808\S2-1=
 0.\S2A=0.750195\RMSD=3.743e-09\RMSF=4.993e-05\Dipole=0.0292469,0.00140
 67,0.0075648\PG=C01 [X(C3H5)]]\\@

r.CH2CH3
 1\1\GINC-LC16\FOpt\UB3LYP\Gen\C2H5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH2CH3.
 freq\\0,2\C,-0.0455131941,0.260306509,-0.7503963798\H,0.7395018641,0.8
 796409361,-1.1726717325\C,0.0479238853,-0.2451741012,0.6476201971\H,-0
 .965226821,0.1616711279,-1.3183217185\H,1.083669566,-0.4681046169,0.93
 2318145\H,-0.5472679413,-1.1552123892,0.7928837298\H,-0.3251408148,0.4
 912104953,1.3824486727\\Version=IA32L-G03RevC.02\State=2-A\HF=-79.1578
 681\S2=0.75392\S2-1=0.\S2A=0.75001\RMSD=3.021e-09\RMSF=5.063e-05\Dipol
 e=-0.014963,0.0157321,0.0975537\PG=C01 [X(C2H5)]]\\@

r.CH_CH3_2
 1\1\GINC-LC110\FOpt\UB3LYP\Gen\C3H7(2)\CYL509\19-Jun-2008\0\\#B3LYP/GE
 N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH_CH3
 _2.freq\\0,2\C,-0.2162320945,1.29800782,0.0238493546\H,0.095425968,1.4
 588146208,1.0657130288\H,-1.3173105881,1.4026313646,0.0142909333\H,0.1
 842468585,2.1199801523,-0.5804295077\C,0.2287570903,-0.0341833847,-0.4
 816740217\H,0.4292655613,-0.1443344599,-1.5451390217\C,0.0759395501,-1
 .2678962095,0.344705016\H,0.6650536962,-2.102406208,-0.0524257545\H,-0
 .9739487426,-1.6128179001,0.3913412585\H,0.3864799711,-1.0974369249,1.
 3853669698\\Version=IA32L-G03RevC.02\State=2-A\HF=-118.4781563\S2=0.75
 4003\S2-1=0.\S2A=0.750011\RMSD=4.749e-09\RMSF=2.408e-05\Dipole=-0.0786
 124,-0.0075381,0.0113041\PG=C01 [X(C3H7)]]\\@

r.C_CH3_3
 1\1\GINC-LC72\FOpt\UB3LYP\Gen\C4H9(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
  6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C_CH3_3
 .freq\\0,2\C,-0.4761514448,-0.8802852695,1.1028950364\C,-0.0584937749,
 -0.0876611733,-0.0971363407\C,-0.8538443646,1.1228711351,-0.477638624\
 H,-0.1416081747,-0.4141620331,2.0494808823\H,-0.0512810452,-1.89225378
 57,1.0899412285\H,-1.5679803011,-0.9694501551,1.1715528248\C,1.3478869
 39,-0.2157668808,-0.5955425176\H,2.0595117077,0.3879476014,-0.00028283
 7\H,1.4444078078,0.1277129028,-1.6335510993\H,1.7045483028,-1.25256702
 4,-0.5446274882\H,-0.5976041842,2.0037070478,0.1417835708\H,-1.9314580
 67,0.9582259752,-0.3495865973\H,-0.6749201751,1.415892601,-1.520175809
 5\\Version=IA32L-G03RevC.02\State=2-A\HF=-157.7983171\S2=0.75402\S2-1=
 0.\S2A=0.750012\RMSD=2.677e-09\RMSF=3.767e-05\Dipole=0.0309079,0.04630
 42,0.0513057\PG=C01 [X(C4H9)]]\\@

r.CCH
```

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C2H1(2)\CYL509\19-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CCH.fre
q\\0,2\C,-0.0407153711,0.,-0.7382974252\C,-0.0138154385,0.,0.487923726
\H,0.3271848578,0.,1.5022421953\\Version=IA64L-G03RevC.02\State=2-A'\H
F=-76.6044421\S2=0.760284\S2-1=0.\S2A=0.750057\RMSD=5.153e-09\RMSF=1.7
58e-05\Dipole=-0.0221188,0.,0.4374653\PG=CS [SG(C2H1)]\\@
```

r.CH=C_CH3_2
```
1\1\GINC-LC12\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH=C_CH
3_2.freq\\0,2\C,-0.8763524765,0.1795241122,1.2105504061\C,-0.089357429
2,0.0283843999,0.1647550344\H,-1.9366259632,0.0901963,1.4166458117\C,1
.4072888403,0.2433501721,0.2389002817\C,-0.6352933629,-0.3749840957,-1
.1964155674\H,-0.1738603298,-1.3129282579,-1.5339578062\H,-0.397884755
3,0.3895088368,-1.9485998544\H,-1.7200329303,-0.5134992916,-1.17906240
5\H,1.7221068546,1.0297145876,-0.460597643\H,1.9458175478,-0.670611518
3,-0.046474751\H,1.7227661452,0.529951812,1.2453057193\\Version=IA32L-
G03RevC.02\State=2-A\HF=-156.539289\S2=0.760752\S2-1=0.\S2A=0.750038\R
MSD=8.278e-09\RMSF=7.669e-05\Dipole=0.0001386,-0.0861941,-0.3539402\PG
=C01 [X(C4H7)]\\@
```

r.CH=CH2
```
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C2H3(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH=CH2
.freq\\0,2\C,-0.4265319626,0.0823941787,0.5803580311\C,0.4141879408,-0
.0517351908,-0.4157589109\H,-1.498408357,0.0416494899,0.7320823737\H,1
.4924159219,0.0420708124,-0.2829251253\H,0.0800565659,-0.2676742297,-1
.4367519695\\Version=IA32L-G03RevC.02\State=2-A\HF=-77.901208\S2=0.761
317\S2-1=0.\S2A=0.750045\RMSD=8.710e-09\RMSF=4.007e-05\Dipole=-0.11088
22,-0.0489191,-0.2171438\PG=C01 [X(C2H3)]\\@
```

r.CH=CHCH3
```
1\1\GINC-LC151\FOpt\UB3LYP\Gen\C3H5(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CH=CHC
H3.freq\\0,2\C,-0.3336521623,0.373491049,1.2828178946\C,0.4230898746,-
0.041194908,0.2925376811\H,-1.3676790921,0.6669505877,1.4232794941\H,1
.4759852017,-0.26421146,0.4863277898\C,-0.0353999224,-0.2474479255,-1.
1382211059\H,0.5433522273,0.3840962203,-1.8245460412\H,-1.0954876652,-
0.006539678,-1.2603517363\H,0.1196025894,-1.2892049633,-1.4475163251\\
Version=IA32L-G03RevC.02\State=2-A\HF=-117.2201501\S2=0.761001\S2-1=0.
\S2A=0.750041\RMSD=7.518e-09\RMSF=6.789e-05\Dipole=-0.084881,-0.058416
6,-0.3545664\PG=C01 [X(C3H5)]\\@
```

r.CHO
```
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1H1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CHO.
freq\\0,2\C,-0.3286695621,0.0964558989,0.4833633419\O,0.4277002641,-0.
0754280776,-0.4095007795\H,-1.4495847398,0.0246892274,0.3758261851\\Ve
rsion=IA32L-G03RevC.02\State=2-A'\HF=-113.8501703\S2=0.75249\S2-1=0.\S
2A=0.750004\RMSD=1.453e-09\RMSF=3.787e-05\Dipole=-0.5899704,0.0123958,
0.1632454\PG=CS [SG(C1H1O1)]\\@
```

r.CN
```
1\1\GINC-LC127\FOpt\UB3LYP\Gen\C1N1(2)\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CN.fre
q\\0,2\C,0.214006281,0.1078562891,0.5849150897\N,-0.1834339551,-0.0924
482478,-0.5013557912\\Version=IA32L-G03RevC.02\State=2-SG\HF=-92.71174
8\S2=0.757409\S2-1=0.\S2A=0.750041\RMSD=1.889e-09\RMSF=2.534e-07\Dipol
e=0.1688805,0.0851135,0.4615788\PG=C*V [C*(C1N1)]\\@
```

r.COCH3
```
1\1\GINC-LC59\FOpt\UB3LYP\Gen\C2H3O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COCH3
.freq\\0,2\C,-0.1940847561,-0.0446039805,-0.4645483715\C,1.1346913106,
0.2069974042,0.2255941761\O,-1.2558682586,-0.2228541177,0.0397654652\H
,1.5344847125,1.1662531725,-0.1192845023\H,1.0252339454,0.2110314368,1
.3167514775\H,1.8435880839,-0.5688122096,-0.0818655245\\Version=IA32L-
G03RevC.02\State=2-A\HF=-153.1798341\S2=0.752253\S2-1=0.\S2A=0.750003\
RMSD=9.654e-09\RMSF=2.206e-04\Dipole=0.9289623,0.1684694,0.1383348\PG=
C01 [X(C2H3O1)]\\@
```

r.CON_CH2CH3_2
```
1\1\GINC-LC122\FOpt\UB3LYP\Gen\C5H10N1O1(2)\CYL509\19-Jun-2008\0\\#B3L
YP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.C
ON_CH2CH3_2.freq\\0,2\C,-0.4793628753,0.8237681964,-1.168068435\O,0.03
91606483,0.7901009231,-2.2590564722\N,-0.1697445837,0.1343237861,-0.05
75330296\C,-0.9361494673,0.3418671135,1.1733832091\C,0.9734563799,-0.8
```

003845046,-0.0593379635\H,-0.2317586517,0.4447813126,2.0087861498\C,-1
.9419044383,-0.7763910479,1.4581808779\H,-1.4562451213,1.2981437409,1.
0688777336\H,1.0228797645,-1.2488061293,-1.0555205435\H,0.7545182211,-
1.601369898,0.6551464094\C,2.2974874573,-0.1139355581,0.2805747964\H,-
2.6751277831,-0.8479507834,0.6481814563\H,-2.4771397341,-0.5753900085,
2.3932616547\H,-1.4489643721,-1.7498885378,1.5581893806\H,2.5253918168
,0.659769215,-0.4590293067\H,3.1156660504,-0.8435056463,0.2777569002\H
,2.2645443715,0.3535976515,1.2711382406\\Version=IA32L-G03RevC.02\Stat
e=2-A\HF=-326.4866578\S2=0.752952\S2-1=0.\S2A=0.750006\RMSD=4.241e-09\
RMSF=5.256e-06\Dipole=0.085896,-0.5720211,1.3893733\PG=C01 [X(C5H10N1O
1)]\\@

r.CON_CH3_2
1\1\GINC-LC66\FOpt\UB3LYP\Gen\C3H6N1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CON
_CH3_2.freq\\0,2\H,-1.0479004513,1.260455923,-1.4628339029\C,-1.202662
4572,0.6436220032,-0.568728375\N,0.080983733,0.3099125583,0.0519033925
\H,-1.7007924313,-0.2848242157,-0.8502378519\H,-1.8360344834,1.1990612
672,0.1342554248\C,0.4810510391,-0.96451537,0.2002715985\O,-0.07419254
94,-1.9892324039,-0.1131762763\C,0.9200428578,1.4054976101,0.508119659
9\H,1.1878677683,2.0655912436,-0.3273309122\H,1.8322751935,0.992332080
1,0.9424118919\H,0.4006500306,2.0042295656,1.2678445129\\Version=IA32L
-G03RevC.02\State=2-A\HF=-247.8549435\S2=0.752894\S2-1=0.\S2A=0.750005
\RMSD=7.219e-09\RMSF=3.116e-05\Dipole=-0.1213329,1.4718151,-0.0032331\
PG=C01 [X(C3H6N1O1)]\\@

r.CONH2
1\1\GINC-LC16\FOpt\UB3LYP\Gen\C1H2N1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CON
H2.freq\\0,2\C,-0.1513347668,-0.0421615458,-0.4177950103\N,1.054633045
2,0.2435106579,0.1051945167\O,-1.1897048077,-0.269684954,0.1448713288\
H,1.200705654,0.2940591331,1.1110958911\H,1.8425420914,0.4118151689,-0
.4996580766\\Version=IA32L-G03RevC.02\State=2-A\HF=-169.2320635\S2=0.7
52721\S2-1=0.\S2A=0.750005\RMSD=5.767e-09\RMSF=6.439e-05\Dipole=1.3793
847,0.3175095,0.1776135\PG=C01 [X(C1H2N1O1)]\\@

r.CONHCH3
1\1\GINC-LC28\FOpt\UB3LYP\Gen\C2H4N1O1(2)\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.CON
HCH3.freq\\0,2\C,0.1144247923,0.9047663218,0.4273241357\O,1.2625478581
,1.0015309641,0.0718961904\N,-0.7596681607,-0.0948457288,0.2193050792\
H,-1.685834544,0.0175282437,0.6043468691\C,-0.4506072501,-1.3195591745
,-0.5230766246\H,0.5867659667,-1.2510575147,-0.8536235905\H,-1.1001315
745,-1.4218538147,-1.3997009094\H,-0.5664108409,-2.2041874099,0.113187
4872\\Version=IA32L-G03RevC.02\State=2-A\HF=-208.5432196\S2=0.752832\S
2-1=0.\S2A=0.750005\RMSD=5.890e-09\RMSF=1.823e-04\Dipole=-1.1607922,-0
.9191297,-0.06532\PG=C01 [X(C2H4N1O1)]\\@

r.COOC_CH3_3
1\1\GINC-LC128\FOpt\UB3LYP\Gen\C5H9O2(2)\CYL509\19-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COOC
_CH3_3.freq\\0,2\C,-1.5092090913,0.6784513471,-0.7873163187\O,-0.96707
63966,1.0657508578,-1.7851688676\O,-1.0655972646,0.0649417145,0.284524
3331\C,0.400624979,-0.2924518118,0.4370234819\C,0.787810876,-1.2544357
397,-0.6841118252\C,0.4269761424,-0.9707198082,1.8033786739\C,1.220961
4806,0.9956322427,0.4244832249\H,1.448636638,-1.2854406719,2.042969865
4\H,-0.218675877,-1.8542744196,1.8101808221\H,0.0835124305,-0.28451309
7,2.5835931341\H,1.8216550085,-1.5877708611,-0.5372417426\H,0.71795522
5,-0.7747335921,-1.6631077164\H,0.1405185305,-2.1373864248,-0.67488895
62\H,2.2734434299,0.7591118649,0.619050912\H,0.8754132327,1.6801279817
,1.2059794593\H,1.1559443507,1.5004812612,-0.5421229218\\Version=IA32L
-G03RevC.02\State=2-A\HF=-346.3521359\S2=0.752826\S2-1=0.\S2A=0.750006
\RMSD=5.170e-09\RMSF=1.326e-06\Dipole=0.8544575,-0.5194661,0.720447\PG
=C01 [X(C5H9O2)]\\@

r.COOCH2CH3
1\1\GINC-LC16\FOpt\UB3LYP\Gen\C3H5O2(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COOCH
2CH3.freq\\0,2\C,-1.0280715273,0.6868234398,-0.8778312379\O,-0.4226029
607,0.8021788564,-1.9041561381\O,-0.6623822174,0.1596373011,0.27419380
09\C,0.7077578966,-0.3824282387,0.3358823976\H,1.3983186632,0.43154138
74,0.0967364183\H,0.7958619253,-1.1519354868,-0.4365864965\C,0.9145096
738,-0.9308717334,1.7306970191\H,1.9255103204,-1.34463645,1.8171269124
\H,0.1962046355,-1.7272437689,1.9482421459\H,0.7988096219,-0.143395747
9,2.4816906451\\Version=IA32L-G03RevC.02\State=2-A\HF=-267.7171998\S2=
0.752762\S2-1=0.\S2A=0.750005\RMSD=8.285e-09\RMSF=9.210e-05\Dipole=0.6
568212,-0.5146351,0.7859486\PG=C01 [X(C3H5O2)]\\@

r.COOCH3
1\1\GINC-LC12\FOpt\UB3LYP\Gen\C2H3O2(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COOCH
3.freq\\0,2\C,-0.0658396903,0.9632185431,0.1043021553\O,1.1165593199,1
.0304549898,-0.0639053277\O,-0.8672295797,-0.0860350467,0.1197637564\C
,-0.2243187711,-1.3790684433,-0.1022308665\H,0.2569725394,-1.386876101
1,-1.0827567121\H,-1.0274634533,-2.1131663757,-0.0560106508\H,0.516803
7605,-1.5602176667,0.6794722005\\Version=IA32L-G03RevC.02\State=2-A\HF
=-228.3971658\S2=0.752762\S2-1=0.\S2A=0.750005\RMSD=8.345e-09\RMSF=7.5
36e-05\Dipole=-0.2484656,-0.9862332,-0.0600959\PG=C01 [X(C2H3O2)]\\@

r.COOH
1\1\GINC-LC16\FOpt\UB3LYP\Gen\C1H1O2(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COOH.
freq\\0,2\C,0.1443704555,0.0112838123,-0.4234353726\O,1.1357236016,0.2
12983425,0.207353603\O,-1.1033814297,-0.2002432979,-0.0113029437\H,-1.
1249601083,-0.1696238913,0.9722069615\\Version=IA32L-G03RevC.02\State=
2-A\HF=-189.087828\S2=0.75265\S2-1=0.\S2A=0.750005\RMSD=2.012e-09\RMSF
=1.144e-05\Dipole=-0.5651641,-0.0841771,0.5180243\PG=C01 [X(C1H1O2)]\\
@

r.COPh
1\1\GINC-LC39\FOpt\UB3LYP\Gen\C7H5O1(2)\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.COPh.
freq\\0,2\C,-1.8403781164,-0.0057886264,-0.1347289117\C,-1.7906316385,
-0.0027585223,1.2642706593\C,-0.5624480256,0.0022902487,1.9297772263\C
,0.6226447087,0.0043279523,1.1958654789\C,0.5772707739,0.0013087381,-0
.2039897875\C,-0.6603910706,-0.0037720787,-0.8714236988\C,1.8478962757
,0.0035422102,-0.9666194165\O,1.9957781292,0.0015428815,-2.1526484935\
H,-0.6731622761,-0.0060462784,-1.9572835874\H,1.5890454053,0.008243136
3,1.6918510562\H,-0.5309384066,0.0046208125,3.0155475891\H,-2.80022803
59,-0.0097123473,-0.6441284412\H,-2.7147191635,-0.0043478895,1.8362920
306\\Version=IA32L-G03RevC.02\State=2-A\HF=-344.9206262\S2=0.752759\S2
-1=0.\S2A=0.750005\RMSD=7.038e-09\RMSF=2.921e-05\Dipole=-1.0118542,-0.
0011421,0.9166601\PG=C01 [X(C7H5O1)]\\@

n.Cl-H
1\1\GINC-LC12\FOpt\RB3LYP\Gen\Cl1H1\CYL509\18-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-H.freq\\
0,1\H,0.,0.,-1.218293883\Cl,0.,0.,0.0716643461\\Version=IA32L-G03RevC.
02\State=1-SG\HF=-460.7956962\RMSD=4.893e-09\RMSF=1.474e-04\Dipole=0.,
0.,-0.5777023\PG=C*V [C*(H1Cl1)]\\@

n.Cl-BH2
1\1\GINC-LC151\FOpt\RB3LYP\Gen\B1Cl1H2\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-BH2.f
req\\0,1\B,-0.3827015236,-0.3035725217,-1.0901717235\H,0.3988628694,-0
.7941660515,-1.8403229115\H,-1.5230263514,-0.0996641981,-1.3591030218\
Cl,0.1786865353,0.1418642858,0.5088402677\\Version=IA32L-G03RevC.02\St
ate=1-A\HF=-486.2695796\RMSD=7.581e-10\RMSF=1.326e-04\Dipole=-0.093961
9,-0.0741037,-0.2682509\PG=C01 [X(B1Cl1H2)]\\@

n.Cl-CH3
1\1\GINC-LC16\FOpt\RB3LYP\Gen\C1H3Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH3.fr
eq\\0,1\C,-0.4164721234,0.8670162752,0.6102446889\H,0.2069901666,1.744
0435256,0.4554077563\H,-0.3959009409,0.5895945921,1.6642921207\H,-1.44
00100604,1.0574673134,0.28697768\Cl,0.2248090338,-0.5054825346,-0.3557
81099\\Version=IA32L-G03RevC.02\State=1-A\HF=-500.1085335\RMSD=8.778e-
10\RMSF=2.110e-05\Dipole=-0.2996044,0.6237196,0.4390018\PG=C01 [X(C1H3
Cl1)]\\@

n.Cl-NH2
1\1\GINC-LC16\FOpt\RB3LYP\Gen\Cl1H2N1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-NH2.fr
eq\\0,1\N,-0.2821441708,-0.36432139,-1.0518300809\H,-1.3042682887,-0.3
544361516,-1.0132942601\H,-0.0273692249,0.4397021262,-1.6305693883\Cl,
0.1945086299,0.1449990444,0.588627895\\Version=IA32L-G03RevC.02\State=
1-A\HF=-516.1034594\RMSD=2.733e-09\RMSF=2.037e-05\Dipole=-0.5482626,0.
48576,-0.5090194\PG=C01 [X(Cl1H2N1)]\\@

n.Cl-OH
1\1\GINC-LC59\FOpt\RB3LYP\Gen\Cl1H1O1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-OH.fre
q\\0,1\O,-0.0306717013,-0.0609721259,1.1200440755\H,0.4327781063,0.764

2448717,1.3568964516\Cl,-0.0110237939,-0.0162628156,-0.6068970033\\Ver
sion=IA32L-G03RevC.02\State=1-A'\HF=-535.9435469\RMSD=2.596e-09\RMSF=3
.277e-05\Dipole=0.330794,0.5892945,0.1183436\PG=CS [SG(Cl1H1O1)]\\@

n.Cl-F
1\1\GINC-LC72\FOpt\RB3LYP\Gen\Cl1F1\CYL509\18-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-F.freq\\
0,1\F,-0.3900625968,0.83418578,0.5792980721\Cl,0.2065037277,-0.4416277
659,-0.3066873735\\Version=IA32L-G03RevC.02\State=1-SG\HF=-559.9426959
\RMSD=2.861e-09\RMSF=5.253e-06\Dipole=0.1379362,-0.2949897,-0.2048549\
PG=C*V [C*(F1Cl1)]\\@

n.Cl-SiH3
1\1\GINC-LC16\FOpt\RB3LYP\Gen\Cl1H3Si1\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SiH3.
freq\\0,1\Si,-0.470305113,0.8145805985,0.3325533065\H,-1.8632373568,0.
7953537957,-0.1716712089\H,-0.4591816422,0.79538166,1.8138979646\H,0.2
427939825,2.0112787296,-0.1717065902\Cl,0.5096409763,-0.8827142685,-0.
3603686151\\Version=IA32L-G03RevC.02\State=1-A\HF=-751.5310613\RMSD=9.
340e-09\RMSF=3.476e-05\Dipole=-0.3313391,0.5738695,0.2342843\PG=C01 [X
(Cl1H3Si1)]\\@

n.Cl-PH2
1\1\GINC-LC26\FOpt\RB3LYP\Gen\Cl1H2P1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-PH2.fr
eq\\0,1\P,0.5414682579,-0.8672821444,-0.2114391155\H,-0.5499583506,-1.
541591596,-0.8333519665\H,1.03723242,-0.3972058768,-1.4628091928\Cl,-0
.5064292904,0.8792958611,0.3216322289\\Version=IA32L-G03RevC.02\State=
1-A'\HF=-802.7543782\RMSD=9.137e-09\RMSF=4.982e-05\Dipole=0.4958102,-0
.5981522,0.1627251\PG=CS [SG(Cl1P1),X(H2)]\\@

n.Cl-SH
1\1\GINC-LC16\FOpt\RB3LYP\Gen\Cl1H1S1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SH.fre
q\\0,1\S,-0.3356676403,-0.1948418572,-0.959996599\H,0.3389432637,-1.36
26466354,-1.0623182318\Cl,0.295984646,0.2635362559,0.9660155186\\Versi
on=IA32L-G03RevC.02\State=1-A'\HF=-858.966025\RMSD=2.932e-09\RMSF=5.06
3e-05\Dipole=0.1053498,-0.4640021,-0.3829107\PG=CS [SG(Cl1H1S1)]\\@

n.Cl-Cl
1\1\GINC-LC26\FOpt\RB3LYP\Gen\Cl2\CYL509\18-Jun-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-Cl.freq\\0
,1\Cl,-0.3684993338,0.7807665613,0.5447329659\Cl,0.3684993338,-0.78076
65613,-0.5447329659\\Version=IA32L-G03RevC.02\State=1-SGG\HF=-920.3498
788\RMSD=2.076e-09\RMSF=1.560e-05\Dipole=0.,0.,0.\PG=D*H [C*(Cl1.Cl1)]
\\@

n.Cl-Br
1\1\GINC-LC72\FOpt\RB3LYP\Gen\Br1Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-Br.freq
\\0,1\Br,-0.2585782904,0.54584833,0.381539602\Cl,0.5323670684,-1.12380
53853,-0.78552271\\Version=IA32L-G03RevC.02\State=1-SG\HF=-3034.053283
5\RMSD=4.797e-09\RMSF=1.510e-05\Dipole=-0.0837655,0.1768256,0.1235984\
PG=C*V [C*(Cl1Br1)]\\@

n.Cl-N_CH3_2
1\1\GINC-LC12\FOpt\RB3LYP\Gen\C2H6Cl1N1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-N_CH
3_2.freq\\0,1\C,0.5016714625,-0.2287401969,1.4945133078\H,1.5898780933
,-0.1404486972,1.4783867732\H,0.2278740825,-1.0568161288,2.1589931785\
H,0.0649442097,0.7037375042,1.8859520597\N,0.0234759416,-0.5873876656,
0.1579342878\C,-1.436986567,-0.6788390492,0.1086739502\H,-1.7222222984
,-1.5095370328,0.765019061\H,-1.7510058628,-0.9161510691,-0.909817751\
H,-1.9498621922,0.2359763206,0.4456310457\Cl,0.5287031178,0.7200251905
,-0.9734604665\\Version=IA32L-G03RevC.02\State=1-A\HF=-594.7271162\RMS
D=5.141e-09\RMSF=7.244e-05\Dipole=-0.4756374,-0.1485047,0.7136088\PG=C
01 [X(C2H6Cl1N1)]\\@

n.Cl-NHCH3
1\1\GINC-LC59\FOpt\RB3LYP\Gen\C1H4Cl1N1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-NHCH
3.freq\\0,1\N,0.1270086456,-0.2621570608,-0.7869053091\C,-1.338993904,
-0.2955704141,-0.8043385426\H,-1.6832998538,-1.1016834072,-0.152209458
2\H,-1.6253303366,-0.5362381606,-1.8355185193\H,-1.8251999914,0.642996
0693,-0.5032341652\H,0.4397795801,0.5157968289,-1.3707457812\Cl,0.6964
090298,0.2404500341,0.8350633143\\Version=IA32L-G03RevC.02\State=1-A\H
F=-555.415025\RMSD=5.280e-09\RMSF=8.449e-05\Dipole=-0.5955458,0.361937

7,-0.5812815\PG=C01 [X(C1H4Cl1N1)]\\@

n.Cl-NHCHO
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C1H2Cl1N1O1\CYL509\19-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\Cl-NH
CHO.freq\\0,1\N,0.114940128,0.2964322551,0.764273058\H,0.0738050268,0.
2169436239,1.774341997\C,1.3237863736,0.1675624592,0.1170432201\O,1.49
45540146,-0.0775824395,-1.0525818406\H,2.1395493327,0.3783454181,0.838
6062998\Cl,-1.3480638596,-0.179707651,-0.0143802529\\Version=IA64L-G03
RevC.02\State=1-A\HF=-629.4362657\RMSD=9.606e-09\RMSF=6.355e-05\Dipole
=-0.0649956,0.0829931,1.4380648\PG=C01 [X(C1H2Cl1N1O1)]\\@

n.Cl-NHCOCH3
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H4Cl1N1O1\CYL509\19-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-NH
COCH3.freq\\0,1\N,-0.3084811702,0.1889755559,0.6121148748\H,-0.3241676
48,-0.0257997425,1.6020575066\C,0.885849814,0.1074341677,-0.093357946\
O,0.9512165348,-0.049829119,-1.2929017269\C,2.1043601736,0.2993120974,
0.8018693595\H,2.7243739381,1.0878961531,0.3673312738\H,2.6894071142,-
0.6260712742,0.7977032164\H,1.8630347407,0.5666320805,1.8347025287\Cl,
-1.7849571857,-0.2569018086,-0.1643796068\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-668.7602912\RMSD=9.346e-09\RMSF=5.901e-06\Dipole=0.3373765
,-0.0329167,1.5076321\PG=C01 [X(C2H4Cl1N1O1)]\\@

n.Cl-NO2
1\1\GINC-LC151\FOpt\RB3LYP\Gen\Cl1N1O2\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-NO2.f
req\\0,1\N,-0.2584847511,0.4518559448,0.338338934\O,0.5263458434,1.257
7458324,0.7398892986\O,-1.4414154676,0.3409462941,0.4609531148\Cl,0.53
70558971,-0.9383840368,-0.7044183438\\Version=IA32L-G03RevC.02\State=1
-A'\HF=-665.2612662\RMSD=2.689e-09\RMSF=1.943e-04\Dipole=-0.0071821,0.
0127071,0.0089009\PG=CS [SG(Cl1N1),X(O2)]\\@

n.Cl-OCF3
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C1Cl1F3O1\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-OCF
3.freq\\0,1\O,-0.6496883501,0.6496096483,-0.086955667\C,0.3858659343,0
.0673308163,0.6223878088\F,1.539692179,0.0840147003,-0.0512648862\F,0.
1228132138,-1.1969160466,0.9657290521\F,0.4989422464,0.8127157888,1.71
87572687\Cl,-0.9747480916,-0.1705407098,-1.5728043781\\Version=IA32L-G
03RevC.02\State=1-A\HF=-872.982\RMSD=5.741e-09\RMSF=8.194e-05\Dipole=-
0.0395573,-0.1495572,-0.2434746\PG=C01 [X(C1Cl1F3O1)]\\@

n.Cl-OCH2CH3
1\1\GINC-LC59\FOpt\RB3LYP\Gen\C2H5Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-OCH2
CH3.freq\\0,1\O,-0.1294171351,-0.5005459444,0.2085343611\C,0.955335465
5,0.2510214268,-0.3560917674\C,2.1391607292,-0.7052144028,-0.361899945
4\H,1.1594062403,1.1376960439,0.2575897368\H,0.6991346206,0.5777751483
,-1.3719833257\H,3.0130437575,-0.1960281142,-0.7837011921\H,1.92336772
38,-1.5882151366,-0.9706360967\H,2.3822919458,-1.0299367807,0.65410141
56\Cl,-1.5711108456,0.4604843677,0.2855473441\\Version=IA32L-G03RevC.0
2\State=1-A\HF=-614.5753377\RMSD=9.056e-09\RMSF=7.422e-05\Dipole=0.685
282,0.2902889,-0.2933008\PG=C01 [X(C2H5Cl1O1)]\\@

n.Cl-OCH3
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C1H3Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-OCH
3.freq\\0,1\O,-0.3842474583,0.0019032047,0.7208859789\C,0.9508694052,-
0.0062515014,1.2213622844\H,1.4956926939,-0.907717308,0.9176237315\H,0
.8123191525,-0.0059840929,2.307786868\H,1.5063236324,0.8890129797,0.91
85385769\Cl,-0.3791513085,0.0027630466,-1.0140712184\\Version=IA32L-G0
3RevC.02\State=1-A\HF=-575.2553665\RMSD=6.697e-09\RMSF=1.061e-04\Dipol
e=0.686273,-0.0042129,0.299697\PG=C01 [X(C1H3Cl1O1)]\\@

n.Cl-OCHO
1\1\GINC-LC72\FOpt\RB3LYP\Gen\C1H1Cl1O2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-OCHO
.freq\\0,1\O,-0.140241342,0.8952340153,0.0049300918\C,1.1793646045,0.5
541630118,0.0057787858\O,1.6635084347,-0.5371442989,0.0004543809\H,1.7
155257931,1.5184483367,0.0125914183\Cl,-1.233991186,-0.4534202434,-0.0
053141126\\Version=IA32L-G03RevC.02\State=1-A\HF=-649.2843252\RMSD=2.7
39e-09\RMSF=9.046e-05\Dipole=-0.0314645,0.5654301,0.0032338\PG=C01 [X(
C1H1Cl1O2)]\\@

n.Cl-OCOCH3
1\1\GINC-AC8\FOpt\RB3LYP\Gen\C2H3Cl1O2\CYL509\19-Jun-2008\0\\#B3LYP/GE

N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\Cl-OCOCH
3.freq\\0,1\O,0.4409912053,-0.0869050675,-0.5966651722\C,0.4051393163,
0.0035813349,0.7791390399\C,1.837983963,-0.0367204899,1.2707665702\O,-
0.5873324305,0.1170353025,1.4408823436\H,1.8314557782,-0.3426958119,2.
3181212148\H,2.269333584,0.9672244986,1.1939639314\H,2.4498278209,-0.7
180612218,0.6758788922\Cl,-1.1081545328,0.0030191521,-1.3671255924\\Ve
rsion=IA64L-G03RevC.02\State=1-A\HF=-688.610813\RMSD=4.141e-09\RMSF=3.
450e-06\Dipole=0.8860813,-0.0245882,0.0349299\PG=C01 [X(C2H3Cl1O2)]\\@

n.Cl-Si_CH3_3
1\1\GINC-LC110\FOpt\RB3LYP\Gen\C3H9Cl1Si1\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-Si
_CH3_3.freq\\0,1\H,0.9254450426,-1.6009521311,-1.996586285\C,0.8977102
95,-1.5546672641,-0.9002380598\H,1.9309117197,-1.5728886969,-0.5369913
507\H,0.3960832926,-2.4586613145,-0.538370107\Si,0.0000349386,-0.00001
83755,-0.3373416031\C,-1.7950806861,-0.0001397324,-0.9004975675\C,0.89
75627999,1.5546579716,-0.9003772793\H,-1.8488708049,-0.0011601053,-1.9
968532459\H,-2.3271656665,0.8863615992,-0.5388569688\H,-2.327539103,-0
.8857379978,-0.5371986009\H,1.9315414744,1.5718129186,-0.5393045526\H,
0.3972664013,2.4585430042,-0.5363988466\H,0.92295042,1.6022377776,-1.9
967265781\Cl,-0.0001333158,0.0000939031,1.7733380246\\Version=IA32L-G0
3RevC.02\State=1-A\HF=-869.5225589\RMSD=9.742e-09\RMSF=9.389e-05\Dipol
e=0.0000807,-0.0000381,-1.0620148\PG=C01 [X(C3H9Cl1Si1)]\\@

n.Cl-P_CH3_2
1\1\GINC-LC72\FOpt\RB3LYP\Gen\C2H6Cl1P1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-P_CH
3_2.freq\\0,1\C,-0.8387939308,1.2455405192,1.0387415975\H,-0.147688863
,2.0418899693,1.3293731953\H,-1.5033209034,1.0444838298,1.8885720563\H
,-1.4370031795,1.5809212903,0.1856255851\P,0.1170491195,-0.3081084642,
0.6786788235\C,-1.250067892,-1.3295663652,-0.0593811166\H,-0.831657569
1,-2.2405275888,-0.4968091827\H,-1.815476148,-0.7888316126,-0.82492834
29\H,-1.9292079459,-1.6220645733,0.7514490898\Cl,1.0848111032,0.300582
9838,-1.111154567\\Version=IA32L-G03RevC.02\State=1-A\HF=-881.4043866\
RMSD=7.575e-09\RMSF=7.244e-06\Dipole=-1.0020748,-0.0523785,0.4981351\P
G=C01 [X(C2H6Cl1P1)]\\@

n.Cl-SC_CH3_2CN
1\1\GINC-LC71\FOpt\RB3LYP\Gen\C4H6Cl1N1S1\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SC
_CH3_2CN.freq\\0,1\S,0.9656761643,-0.6553321111,-0.5027883309\C,-0.809
7759878,-0.442763587,0.0360690644\C,-0.9613315559,-0.5211653999,1.5635
915497\C,-1.530887414,-1.6147536912,-0.6691100561\C,-1.3289991283,0.83
67319092,-0.466090007\H,-0.5916399347,-1.4869419723,1.9197369247\H,-0.
4024961288,0.276712972,2.0581996741\H,-2.0182474301,-0.4205719983,1.83
40479401\H,-1.4227050006,-1.5611360919,-1.7560477669\H,-2.5976855937,-
1.5721668748,-0.4280431747\H,-1.132768809,-2.5694361571,-0.3115719933\
N,-1.7650456579,1.8436581361,-0.8460530759\Cl,1.9327063758,0.90382068,
0.462582348\\Version=IA32L-G03RevC.02\State=1-A\HF=-1069.1484007\RMSD=
3.701e-09\RMSF=2.636e-05\Dipole=-0.3440992,-1.5037463,0.5361926\PG=C01
 [X(C4H6Cl1N1S1)]\\@

n.Cl-SCH2COOCH3
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C3H5Cl1O2S1\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-S
CH2COOCH3.freq\\0,1\S,-1.4015696671,-0.9819200911,-0.2199366779\C,-0.2
041527548,-0.6241337872,1.1170336563\C,1.0446327094,0.1127814154,0.661
7955149\O,1.2880063424,1.2655940844,0.9360015831\O,1.8367864952,-0.682
4962645,-0.0797356668\C,3.02392025,-0.056292839,-0.599528507\H,-0.6887
221162,-0.0551841146,1.9118083352\H,0.0580994146,-1.6237505467,1.48464
01079\H,3.6528230898,0.3070990744,0.2172503735\H,2.7578268743,0.782645
5691,-1.2474176938\H,3.5376304224,-0.8326053316,-1.1663580457\Cl,-2.06
336982,0.9337415007,-0.6827569145\\Version=IA32L-G03RevC.02\State=1-A\
HF=-1126.1542574\RMSD=8.230e-09\RMSF=6.458e-06\Dipole=0.7531552,-0.803
893,0.1805638\PG=C01 [X(C3H5Cl1O2S1)]\\@

n.Cl-SCH2Ph
1\1\GINC-LC110\FOpt\RB3LYP\Gen\C7H7Cl1S1\CYL509\18-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SCH
2Ph.freq\\0,1\S,2.1967961102,-0.5997966237,-0.0355397719\C,0.835642030
1,-0.4900722469,1.2073883309\C,-0.5558019152,-0.3495110492,0.651664421
6\H,1.0782829143,0.3151790694,1.905923806\H,0.9632827724,-1.44212182,1
.740982468\C,-1.2183988176,0.881833261,0.7144931647\C,-1.2102448748,-1
.4422491787,0.0661167143\C,-2.5103311691,1.0203048135,0.2034126662\C,-
2.499779035,-1.306572461,-0.4428269783\C,-3.1538204398,-0.073152939,-0
.3755693619\H,-4.1600019621,0.0324220859,-0.7720197997\H,-2.9964259295
,-2.1630455882,-0.8907589372\H,-3.0116764933,1.9827556346,0.2588052491

\H,-0.7025425161,-2.4022587262,0.0052028468\H,-0.7199475735,1.73621538
74,1.1654396776\Cl,2.1339233149,1.2996540434,-0.8819419238\\Version=IA
32L-G03RevC.02\State=1-A\HF=-1129.3379859\RMSD=5.157e-09\RMSF=1.656e-0
6\Dipole=-0.7053664,-0.3429044,0.6033392\PG=C01 [X(C7H7Cl1S1)]\\@

n.Cl-SCH3
1\1\GINC-LC59\FOpt\RB3LYP\Gen\C1H3Cl1S1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SCH3
.freq\\0,1\S,-0.7281953161,-0.4735518792,0.\C,-1.2073153893,1.28253490
89,0.\H,-2.3035441949,1.2754501871,0.\H,-0.8503784796,1.7903735723,0.8
986530272\H,-0.8503784796,1.7903735723,-0.8986530272\Cl,1.3470187381,-
0.2926221599,0.\\Version=IA32L-G03RevC.02\State=1-A'\HF=-898.2876887\R
MSD=6.826e-09\RMSF=1.331e-05\Dipole=-0.6644961,0.662857,0.\PG=CS [SG(C
1H1Cl1S1),X(H2)]\\@

n.Cl-SO2CH3
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C1H3Cl1O2S1\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-S
O2CH3.freq\\0,1\C,-0.7656694303,-1.5799296416,-0.4141172583\S,-0.30564
48451,-0.0202842117,0.3669092592\O,-1.4098322382,0.921013559,0.2459973
106\O,0.344685464,-0.2947390567,1.6403439919\H,0.1097414166,-2.2296734
886,-0.4314625801\H,-1.1327041028,-1.3687494932,-1.4188563149\H,-1.556
3107262,-2.0061007186,0.2091678685\Cl,1.2108695123,0.6116737011,-0.990
3190583\\Version=IA32L-G03RevC.02\State=1-A'\HF=-1048.6806789\RMSD=7.2
83e-09\RMSF=1.058e-04\Dipole=-0.3796788,-1.3385614,-0.6893596\PG=CS [S
G(C1H1Cl1S1),X(H2O2)]\\@

n.Cl-SOCH3
1\1\GINC-LC26\FOpt\RB3LYP\Gen\C1H3Cl1O1S1\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-SO
CH3.freq\\0,1\S,0.0367937019,-0.4098030315,0.6000244831\O,0.5900369654
,-1.6568008189,0.0126800889\C,-1.7082152485,-0.328939404,0.0508223914\
H,-2.2243422627,-1.1582550543,0.5441609364\H,-1.7390386382,-0.45334588
74,-1.033444054\H,-2.1382199585,0.6295166293,0.349289885\Cl,0.64952337
63,1.3392338701,-0.5803984445\\Version=IA32L-G03RevC.02\State=1-A\HF=-
973.479694\RMSD=7.886e-09\RMSF=2.585e-05\Dipole=-1.271794,0.0331219,0.
5576637\PG=C01 [X(C1H3Cl1O1S1)]\\@

n.Cl-Ph
1\1\GINC-LC127\FOpt\RB3LYP\Gen\C6H5Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-Ph.fr
eq\\0,1\C,0.1711257296,0.0892743045,0.4653602463\C,-0.7708024629,-0.40
29106424,-2.102068708\C,-0.250125724,1.1591069597,-0.3236037629\C,0.12
95320106,-1.2222897003,-0.0063691764\C,-0.3450230101,-1.4610829278,-1.
2973316399\C,-0.7219795507,0.9033705181,-1.6123091338\H,-0.2083292859,
2.1707775378,0.0656004289\H,0.4626711869,-2.0380614367,0.6262752505\H,
-0.3800956411,-2.4806917822,-1.6712906581\H,-1.0517697172,1.7323724278
,-2.2325283958\H,-1.1391117003,-0.5953105213,-3.1055818694\Cl,0.767074
8938,0.4010648677,2.0926740168\\Version=IA32L-G03RevC.02\State=1-A\HF=
-691.8449668\RMSD=5.508e-09\RMSF=6.666e-05\Dipole=-0.2572257,-0.134454
5,-0.7014742\PG=C01 [X(C6H5Cl1)]\\@

n.Cl-C6H4CN
1\1\GINC-LC70\FOpt\RB3LYP\Gen\C7H4Cl1N1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C6H4
CN.freq\\0,1\C,0.4485154549,0.2266425478,1.1593950781\C,-0.5377288783,
-0.272078543,-1.3919994541\C,0.1839810904,1.2996145058,0.3061508439\C,
0.2272294502,-1.091799628,0.7568832455\C,-0.2663084844,-1.3395466819,-
0.5201221437\C,-0.309491637,1.048260928,-0.9701747913\H,0.362717366,2.
3160910878,0.6387002021\H,0.4391571739,-1.9106549581,1.4353543341\H,-0
.4430579987,-2.3591732156,-0.8464392127\H,-0.5195848329,1.8723858532,-
1.6440002437\C,-1.0464099746,-0.5291933615,-2.7072806905\N,-1.45878534
41,-0.7379229543,-3.7747832959\Cl,1.0690319748,0.5409066652,2.76722090
97\\Version=IA32L-G03RevC.02\State=1-A\HF=-784.0866954\RMSD=8.265e-09\
RMSF=5.863e-05\Dipole=0.3942316,0.1994426,1.020114\PG=C01 [X(C7H4Cl1N1
)]\\@

n.Cl-C6H4NO2
1\1\GINC-LC71\FOpt\RB3LYP\Gen\C6H4Cl1N1O2\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C6
H4NO2.freq\\0,1\C,0.5563305076,0.2912273526,1.5203653258\C,-0.37377547
41,-0.1957397624,-1.0220421939\C,0.1349821084,1.3636099033,0.729737359
3\C,0.5154914011,-1.023130266,1.0476840296\C,0.044965316,-1.2694838214
,-0.2386408785\C,-0.3355388102,1.117223941,-0.5565832318\H,0.175903047
9,2.3750461099,1.1179329151\H,0.8477668956,-1.8392121606,1.6793301724\
H,-0.0013608733,-2.2745832653,-0.6392461642\H,-0.6705139628,1.92267180
52,-1.198378361\N,-0.8710575992,-0.4560424749,-2.3809319403\O,-1.23380

14976,0.5108925166,-3.0500800279\O,-0.8933255025,-1.6247392531,-2.7655
844557\Cl,1.1475231644,0.6009943908,3.1381810839\\Version=IA32L-G03Rev
C.02\State=1-A'\HF=-896.344808\RMSD=5.571e-09\RMSF=7.562e-05\Dipole=0.
3899849,0.204198,1.0661366\PG=CS [SG(C2Cl1N1),X(C4H4O2)]]\\@

n.Cl-C6H4OCH3
1\1\GINC-LC28\FOpt\RB3LYP\Gen\C7H7Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C6H4
OCH3.freq\\0,1\C,-1.2976605839,-0.0492072971,-0.7572928382\C,-1.235297
8577,-0.011424642,0.6439888132\C,0.0109320164,0.0334850359,1.279237099
5\C,1.1825879986,0.0404042348,0.5162197226\C,1.1061325696,0.0026548389
,-0.8713651369\C,-0.1334652144,-0.0423113991,-1.5148794586\O,-2.437004
6088,-0.0220676926,1.2891414349\C,-2.4382184758,0.0143886019,2.7076823
095\H,-0.183213742,-0.0715574622,-2.5981439241\H,2.1494387358,0.075194
5146,1.0070834055\H,0.0886290408,0.0633120247,2.3598504122\H,-2.272445
772,-0.0837949675,-1.2333330756\H,-1.9265019369,-0.85848919,3.13431799
18\H,-3.4878617926,-0.0019792387,3.0061067031\H,-1.967490711,0.9305373
527,3.0883105516\Cl,2.5838482548,0.0114930746,-1.8293450947\\Version=I
A32L-G03RevC.02\State=1-A\HF=-806.3671032\RMSD=7.334e-09\RMSF=5.503e-0
5\Dipole=-0.6026446,0.0111623,0.9656502\PG=C01 [X(C7H7Cl1O1)]\\@

n.Cl-C6H4OH
1\1\GINC-LC44\FOpt\RB3LYP\Gen\C6H5Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C6H4
OH.freq\\0,1\C,-1.5823512004,-0.07160115,-0.4833312882\C,-1.5797141053
,-0.0052998306,0.9145833655\C,-0.3658589338,0.0647617891,1.6052984456\
C,0.84099128,0.0687370445,0.9049803657\C,0.827150986,0.0024387441,-0.4
859041659\C,-0.3798443682,-0.0677715849,-1.1838217382\O,-2.7921550308,
-0.0127560513,1.5450363254\H,-0.3775931846,-0.1190368901,-2.2673924367
\H,1.7833291435,0.1230400726,1.4394685399\H,-0.3572757673,0.1165034436
,2.6923974846\H,-2.5318006685,-0.125589847,-1.0061336227\H,-2.65254679
87,0.0369954,2.5033805839\Cl,2.3476991513,0.0072085976,-1.3736965329\\
Version=IA32L-G03RevC.02\State=1-A\HF=-767.0603187\RMSD=3.624e-09\RMSF
=6.121e-05\Dipole=-0.4382982,0.0279614,0.8745564\PG=C01 [X(C6H5Cl1O1)]
\\@

n.Cl-CF2CF3
1\1\GINC-LC59\FOpt\RB3LYP\Gen\C2Cl1F5\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CF2CF3
.freq\\0,1\F,-0.5728276051,0.2679812972,-1.6145628837\C,-0.5412811131,
0.2036482286,-0.275210256\C,0.9400521203,0.1712791328,0.1814494654\F,-
1.1171667253,1.3069533711,0.2248683269\F,1.5606292545,-0.8990640583,-0
.3232167387\F,1.0166181441,0.1393258212,1.5150708862\F,1.5507306539,1.
2776137048,-0.2627677504\Cl,-1.431439973,-1.2402856113,0.2769434224\\V
ersion=IA32L-G03RevC.02\State=1-A\HF=-1035.5993631\RMSD=9.540e-09\RMSF
=6.417e-05\Dipole=-0.007884,-0.0204572,0.0092248\PG=C01 [X(C2Cl1F5)]\\
@

n.Cl-CF2H
1\1\GINC-LC76\FOpt\RB3LYP\Gen\C1H1Cl1F2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CF2H
.freq\\0,1\C,-0.2264043689,0.0020482611,-0.5390477823\H,1.2433612143,0.
0521012142,-0.9299337626\F,-0.4945249046,1.0452970762,-0.9766682443\F,
-0.370488416,-1.1329598151,-0.9328594116\Cl,0.3049019093,0.0426219923,
1.2558805506\\Version=IA32L-G03RevC.02\State=1-A\HF=-698.5720444\RMSD=
1.173e-09\RMSF=7.763e-05\Dipole=0.4886227,0.0215162,-0.3133445\PG=C01
[X(C1H1Cl1F2)]\\@

n.Cl-CF3
1\1\GINC-LC110\FOpt\RB3LYP\Gen\C1Cl1F3\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CF3.f
req\\0,1\F,0.1722592582,0.3139247948,-1.4496980185\C,0.1773681396,0.29
16537566,-0.1192022055\F,1.4371327983,0.2632111054,0.3084875389\F,-0.4
090555199,1.3966179706,0.3345652232\Cl,-0.698072804,-1.1478651398,0.46
91188553\\Version=IA32L-G03RevC.02\State=1-A\HF=-797.8167605\RMSD=6.22
5e-09\RMSF=1.476e-04\Dipole=0.0054393,0.0089441,-0.003666\PG=C01 [X(C1
Cl1F3)]\\@

n.Cl-CCl2H
1\1\GINC-LC127\FOpt\RB3LYP\Gen\C1H1Cl3\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CCl2H
.freq\\0,1\C,0.4199260178,-0.0309708827,-0.1711876976\H,1.4236182571,-
0.104950287,-0.5782056519\Cl,-0.2900197018,1.4991440735,-0.7628023837\
Cl,-0.5036689543,-1.4459211927,-0.7542591211\Cl,0.5617372229,-0.036118
4347,1.6114927893\\Version=IA32L-G03RevC.02\State=1-A\HF=-1419.2791102
\RMSD=1.851e-09\RMSF=7.535e-05\Dipole=0.4632858,-0.0342364,-0.1900525\
PG=C01 [X(C1H1Cl3)]\\@

n.Cl-CCl3
1\1\GINC-LC72\FOpt\RB3LYP\Gen\C1Cl4\CYL509\18-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CCl3.fre
q\\0,1\C,-0.0000522091,-0.0000556381,-0.0009583141\Cl,1.6553946181,-0.
1745026194,-0.6643532442\Cl,-0.7199339022,1.5332643754,-0.5853051569\C
l,-1.0093131458,-1.3786546524,-0.541016181\Cl,0.0738708567,0.019912533
4,1.7910128107\\Version=IA32L-G03RevC.02\State=1-A\HF=-1878.8542564\RM
SD=9.434e-09\RMSF=1.638e-04\Dipole=-0.0002324,-0.000069,-0.0033128\PG=
C01 [X(C1Cl4)]\\@

n.Cl-CH2Cl
1\1\GINC-LC16\FOpt\RB3LYP\Gen\C1H2Cl2\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2Cl.
freq\\0,1\C,-0.6268549588,-0.0076008646,0.443252681\Cl,0.16471688,1.49
8302796,-0.1164724876\H,-0.6072385883,-0.0137301188,1.530628206\H,-1.6
455030669,-0.0137303657,0.0622981387\Cl,0.1890402616,-1.4940048153,-0.
1336711848\\Version=IA32L-G03RevC.02\State=1-A'\HF=-959.696347\RMSD=8.
701e-09\RMSF=2.209e-05\Dipole=-0.5951324,-0.0071222,0.4208215\PG=CS [S
G(C1Cl2),X(H2)]\\@

n.Cl-CH2F
1\1\GINC-LC16\FOpt\RB3LYP\Gen\C1H2Cl1F1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2F
.freq\\0,1\C,-0.1614674724,0.2917634803,-0.7458100554\F,1.1777800133,0
.3752410028,-0.9591982519\H,-0.6085016625,1.285740803,-0.801180749\H,-
0.6085024903,-0.4007849765,-1.460955304\Cl,-0.494953596,-0.3536885726,
0.9041047443\\Version=IA32L-G03RevC.02\State=1-A'\HF=-599.3319432\RMSD
=3.753e-09\RMSF=2.700e-05\Dipole=-0.445697,0.2246031,-0.5741333\PG=CS
[SG(C1Cl1F1),X(H2)]\\@

n.Cl-CH2OH
1\1\GINC-LC75\FOpt\RB3LYP\Gen\C1H3Cl1O1\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2O
H.freq\\0,1\C,0.3430136365,-0.7350494487,-0.19963828\O,0.3703192856,-1
.0998428119,1.1261309716\H,1.3299813414,-0.6631404796,-0.6655260639\H,
-0.2935178299,-1.4414599163,-0.7291850342\H,0.9881923429,-0.518656208,
1.5988014208\Cl,-0.4144289388,0.9313115171,-0.4714887303\\Version=IA32
L-G03RevC.02\State=1-A\HF=-575.3184757\RMSD=3.217e-09\RMSF=4.390e-05\D
ipole=0.7692375,-0.3615773,0.0551035\PG=C01 [X(C1H3Cl1O1)]\\@

n.Cl-CH2Ph
1\1\GINC-LC70\FOpt\RB3LYP\Gen\C7H7Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2Ph.
freq\\0,1\C,-0.331576553,1.6683662712,0.\C,0.3144322789,0.3156587289,0
.\C,0.6229526307,-0.3247405992,1.2071403329\C,0.6229526307,-0.32474059
92,-1.2071403329\C,1.2294474611,-1.5802564785,1.2083237332\C,1.2294474
611,-1.5802564785,-1.2083237332\C,1.5338197971,-2.2106037877,0.\H,2.00
83053848,-3.188189458,0.\H,1.4661285659,-2.0654852759,2.15131054\H,1.4
661285659,-2.0654852759,-2.15131054\H,0.3838121973,0.1635339976,2.1489
610999\H,0.3838121973,0.1635339976,-2.1489610999\H,-0.0760047633,2.245
086506,-0.8897729273\H,-0.0760047633,2.245086506,0.8897729273\Cl,-2.16
97077426,1.5718445094,0.\\Version=IA32L-G03RevC.02\State=1-A'\HF=-731.
1602439\RMSD=4.400e-09\RMSF=1.425e-05\Dipole=0.9499953,-0.1856628,0.\P
G=CS [SG(C3H1Cl1),X(C4H6)]\\@

n.Cl-CH_CH2_2
1\1\GINC-LC127\FOpt\RB3LYP\Gen\C3H5Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH_CH
2_2.freq\\0,1\C,-1.2114361605,-0.5891771517,-0.7470184134\C,-1.2018633
161,-0.5807336627,0.7687725444\C,0.0862147706,-0.6009201638,0.00280061
76\H,0.6898113077,-1.5016687568,0.0040069656\H,-1.4771610767,0.3457690
245,1.2630575159\H,-1.4812641822,-1.4819150375,1.3083521391\H,-1.49301
83203,0.3317819187,-1.2480773953\H,-1.4975688031,-1.4962932881,-1.2729
527356\Cl,1.130688783,0.8486654122,-0.0118655871\\Version=IA32L-G03Rev
C.02\State=1-A\HF=-577.4901384\RMSD=5.020e-09\RMSF=4.884e-05\Dipole=-0
.5659952,-0.5892213,0.0068554\PG=C01 [X(C3H5Cl1)]\\@

n.Cl-CH2CH=CH2
1\1\GINC-LC127\FOpt\RB3LYP\Gen\C3H5Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2CH
=CH2.freq\\0,1\C,-0.4291276112,-0.1497447262,0.6080142522\C,0.24549749
17,1.1564683207,0.3525511705\H,-0.3111147508,-0.4803302091,1.642660312
1\H,-1.4904284499,-0.1189276205,0.3560924202\H,1.3040776015,1.20535517
35,0.6019267836\C,-0.3835052514,2.2259116993,-0.1361384929\H,0.1313691
91,3.1707045089,-0.2849889666\H,-1.4379920227,2.1983719347,-0.40249825
11\Cl,0.3062882739,-1.4924109147,-0.4035149339\\Version=IA32L-G03RevC.

02\State=1-A\HF=-577.5013633\RMSD=3.579e-09\RMSF=2.881e-05\Dipole=-0.3
092136,0.7147278,0.4531096\PG=C01 [X(C3H5Cl1)]\\@

n.Cl-CH2CH3
1\1\GINC-LC76\FOpt\RB3LYP\Gen\C2H5Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH2CH3
.freq\\0,1\C,-0.3236564932,0.7463137653,0.1090261753\H,0.293999951,1.6
195168533,-0.1096040587\C,-0.298099223,0.3864073717,1.5847337187\H,-1.
3380983375,0.9320797529,-0.2489979078\H,0.722306486,0.1883837903,1.925
5278551\H,-0.9087719685,-0.49849383,1.786255342\H,-0.7008344104,1.2247
087435,2.1669308625\Cl,0.3330548575,-0.6036777725,-0.9225100857\\Versi
on=IA32L-G03RevC.02\State=1-A\HF=-539.4262582\RMSD=3.441e-09\RMSF=9.72
4e-05\Dipole=-0.3081495,0.6165999,0.5671897\PG=C01 [X(C2H5Cl1)]\\@

n.Cl-CH_CH3_2
1\1\GINC-LC12\FOpt\RB3LYP\Gen\C3H7Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH_CH3
_2.freq\\0,1\C,-1.1532027018,1.1871610258,0.2060363496\H,-0.8865952056
,1.3831866323,1.2496643427\H,-2.2437526262,1.0826106018,0.1421773784\H
,-0.8536024092,2.0491266222,-0.3963619915\C,-0.4941311808,-0.092615425
,-0.2906773552\H,-0.7217061455,-0.2507271197,-1.3479124794\C,-0.866976
4594,-1.3263828904,0.5203292612\H,-0.3673989572,-2.2205334568,0.137516
4497\H,-1.9514106307,-1.4846368089,0.4631818189\H,-0.5925843198,-1.198
7432426,1.5725091395\Cl,1.3354654321,0.1194553241,-0.2608767172\\Versi
on=IA32L-G03RevC.02\State=1-A\HF=-578.7436049\RMSD=2.968e-09\RMSF=2.25
7e-05\Dipole=-0.9277363,-0.101048,0.0367694\PG=C01 [X(C3H7Cl1)]\\@

n.Cl-C_CH3_3
1\1\GINC-LC12\FOpt\RB3LYP\Gen\C4H9Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C_CH3_
3.freq\\0,1\C,-0.1393369681,-0.3725335291,1.6269961136\C,0.150882319,0
.2261260029,0.250501732\C,-0.5100356463,1.5935729069,0.0756272159\H,0.
2945880498,0.272844982,2.4015623803\H,0.2998349163,-1.3696016984,1.723
7375041\H,-1.2158943633,-0.4480553583,1.8049961589\C,1.6509191076,0.27
95903615,-0.0401015839\H,2.1372001972,0.9437238848,0.6860002888\H,1.84
4284095,0.6670172342,-1.0445346986\H,2.1041639989,-0.7123839964,0.0431
22744\H,-0.0868364888,2.2963836027,0.8048052241\H,-1.5895323551,1.5337
255585,0.2414018451\H,-0.3339282248,1.9910083,-0.928061259\Cl,-0.60990
89823,-0.9138351154,-1.0124218266\\Version=IA32L-G03RevC.02\State=1-A\
HF=-618.0595984\RMSD=3.297e-09\RMSF=1.299e-04\Dipole=0.3919406,0.58723
83,0.6506037\PG=C01 [X(C4H9Cl1)]\\@

n.Cl-CCH
1\1\GINC-LC26\FOpt\RB3LYP\Gen\C2H1Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CCH.fr
eq\\0,1\C,-0.2222348776,-0.1109451205,-0.5668621324\C,-0.6550822704,-0
.3270331921,-1.6709408388\H,-1.0378481863,-0.5181193578,-2.6472750026\
Cl,0.3706912396,0.1850581902,0.9455348724\\Version=IA32L-G03RevC.02\St
ate=1-SG\HF=-536.9132555\RMSD=2.599e-09\RMSF=1.608e-05\Dipole=-0.07754
14,-0.0387106,-0.1977874\PG=C*V [C*(H1C1C1Cl1)]\\@

n.Cl-CH=C_CH3_2
1\1\GINC-LC12\FOpt\RB3LYP\Gen\C4H7Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH=C_C
H3_2.freq\\0,1\C,-0.7515214401,-0.0475403104,0.2107819115\C,0.07459853
6,-0.1920884817,-0.8290535898\H,-1.8215903728,-0.2043847248,0.14492558
88\C,1.5631995091,0.015669998,-0.7801987461\C,-0.501136565,-0.59355199
53,-2.166361914\H,-0.0546355577,-1.5344007519,-2.5154238488\H,-0.27821
10012,0.1645862139,-2.929207509\H,-1.5865132806,-0.7268174322,-2.12709
31767\H,1.8641311344,0.7956599629,-1.4923977318\H,2.087493197,-0.90919
61506,-1.0788268008\H,1.9107151646,0.3034861184,0.2135761142\Cl,-0.260
7193838,0.4122900883,1.8337318468\\Version=IA32L-G03RevC.02\State=1-A\
HF=-616.8247988\RMSD=7.449e-09\RMSF=6.759e-05\Dipole=0.0281275,-0.1940
422,-0.8119038\PG=C01 [X(C4H7Cl1)]\\@

n.Cl-CH=CH2
1\1\GINC-LC59\FOpt\RB3LYP\Gen\C2H3Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH=CH2
.freq\\0,1\C,-0.4909310906,-0.1397785193,-0.5704890688\C,0.3174950737,
-0.2852865718,-1.6130580654\H,-1.5709568244,-0.2191188719,-0.621170021
1\H,1.3960138071,-0.2003951652,-1.532202611\H,-0.1057640812,-0.4979400
728,-2.590419835\Cl,0.0777248941,0.2039908622,1.0497103101\\Version=IA
32L-G03RevC.02\State=1-A\HF=-538.1853915\RMSD=1.882e-09\RMSF=4.316e-05
\Dipole=-0.1687083,-0.1243877,-0.5985567\PG=C01 [X(C2H3Cl1)]\\@

n.Cl-CH=CHCH3
1\1\GINC-LC26\FOpt\RB3LYP\Gen\C3H5Cl1\CYL509\18-Jun-2008\0\\#B3LYP/GEN

6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CH=CHC
H3.freq\\0,1\C,-0.4335844219,0.1205055098,0.0473182646\C,0.3313041403,
-0.2994659646,-0.9568148905\H,-1.4857988915,0.3647955529,-0.0507298972
\H,1.3798672791,-0.5227117678,-0.7692600805\C,-0.1769098839,-0.4865938
888,-2.3578915818\H,0.3783895985,0.1445983317,-3.0638823025\H,-1.23938
60608,-0.2364549886,-2.4417373918\H,-0.0444749508,-1.5253549814,-2.687
4750616\Cl,0.1580320011,0.3393208185,1.6833772929\\Version=IA32L-G03Re
vC.02\State=1-A\HF=-577.5052656\RMSD=4.864e-09\RMSF=5.665e-05\Dipole=-
0.1439205,-0.1422914,-0.7930114\PG=C01 [X(C3H5Cl1)]\\@

n.Cl-CHO
1\1\GINC-LC16\FOpt\RB3LYP\Gen\C1H1Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CHO.
freq\\0,1\C,-0.4166909112,-0.1706024567,-0.6706120316\O,0.3544902458,-
0.3399215975,-1.5549419293\H,-1.511388475,-0.2302116748,-0.7296876664\
Cl,0.0691536456,0.2337175997,1.0113467818\\Version=IA32L-G03RevC.02\St
ate=1-A\HF=-574.116999\RMSD=4.216e-09\RMSF=3.397e-05\Dipole=-0.7342139
,-0.023489,0.0326442\PG=C01 [X(C1H1Cl1O1)]\\@

n.Cl-CN
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C1Cl1N1\CYL509\18-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CN.fr
eq\\0,1\C,-0.2237508022,-0.1127673588,-0.6115493363\N,-0.6175298962,-0
.3112266623,-1.6878151696\Cl,0.3332478874,0.1679523993,0.9108236591\\V
ersion=IA32L-G03RevC.02\State=1-SG\HF=-553.0082927\RMSD=2.718e-09\RMSF
=1.668e-04\Dipole=0.3563427,0.1795919,0.9739458\PG=C*V [C*(N1C1Cl1)]\\
@

n.Cl-COCH3
1\1\GINC-LC26\FOpt\RB3LYP\Gen\C2H3Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COCH
3.freq\\0,1\C,-0.1691825557,-0.0189636102,0.5158904758\C,1.1649369782,
0.2326297337,1.1622405582\O,-1.2178906331,-0.1944191689,1.0439962589\H
,1.5642297326,1.1933127833,0.8229448246\H,1.0415128271,0.2340401615,2.
2473200786\H,1.8738003325,-0.5444676787,0.8604134524\Cl,-0.0418202566,
-0.0358546268,-1.3147902724\\Version=IA32L-G03RevC.02\State=1-A\HF=-61
3.4459163\RMSD=3.068e-09\RMSF=5.918e-05\Dipole=0.9860131,0.1871632,0.5
320186\PG=C01 [X(C2H3Cl1O1)]\\@

n.Cl-CON_CH2CH3_2
1\1\GINC-LC96\FOpt\RB3LYP\Gen\C5H10Cl1N1O1\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C
ON_CH2CH3_2.freq\\0,1\C,-0.0025533137,0.3235592554,-0.9351006301\O,0.6
133962266,0.2204495705,-1.9633072132\N,0.2687040365,-0.2832638933,0.24
1230604\C,-0.466999757,-0.1150364636,1.5022324004\C,1.4372008277,-1.18
66521412,0.2460213786\H,0.2727086064,-0.1944257417,2.3066289777\C,-1.5
77788178,-1.1497225362,1.6937130715\H,-0.8731010339,0.8958493147,1.543
2475019\H,1.477424616,-1.6883896442,-0.7229996408\H,1.2477483761,-1.94
84899971,1.009065474\C,2.7512965166,-0.4544908398,0.5203344278\H,-2.34
18574494,-1.0434811988,0.917964979\H,-2.0560462194,-1.0107218508,2.669
8480712\H,-1.1838038105,-2.1713636321,1.6523246246\H,2.9476360554,0.27
98502773,-0.2661697799\H,3.5826485073,-1.1682284133,0.5395781297\H,2.7
27597815,0.0648182655,1.4850562375\Cl,-1.496234712,1.3939935095,-0.898
8179403\\Version=IA32L-G03RevC.02\State=1-A\HF=-786.7479858\RMSD=6.629
e-09\RMSF=9.532e-06\Dipole=0.3342876,-0.7578482,1.5474056\PG=C01 [X(C5
H10Cl1N1O1)]\\@

n.Cl-CON_CH3_2
1\1\GINC-LC151\FOpt\RB3LYP\Gen\C3H6Cl1N1O1\CYL509\18-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-C
ON_CH3_2.freq\\0,1\H,-1.600952582,1.6629844445,-1.7200217722\C,-1.7679
738813,1.0408598563,-0.8324007262\N,-0.4854460687,0.703241961,-0.21245
85158\H,-2.2793588375,0.1245809325,-1.1199688943\H,-2.38889778,1.60163
38693,-0.1233233767\C,-0.1727331655,-0.611219179,-0.1087387319\O,-0.83
59968914,-1.5457026463,-0.4720739273\C,0.3084225314,1.8444085936,0.223
2016346\H,0.5303287422,2.4904669289,-0.6353231133\H,1.2425759321,1.518
1205035,0.6716645775\H,-0.2567921337,2.4291295829,0.9596329734\Cl,1.44
89941978,-0.9428402582,0.6787510338\\Version=IA32L-G03RevC.02\State=1-
A\HF=-708.1148131\RMSD=3.151e-09\RMSF=1.954e-05\Dipole=-0.342933,1.680
6408,-0.1045155\PG=C01 [X(C3H6Cl1N1O1)]\\@

n.Cl-CONH2
1\1\GINC-LC16\FOpt\RB3LYP\Gen\C1H2Cl1N1O1\CYL509\18-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-CO
NH2.freq\\0,1\C,-0.113881255,-0.0193420525,0.5356098757\N,1.1117075823
,0.2670352534,1.0216465461\O,-1.1173630994,-0.2408785531,1.1471000623\
H,1.2273689655,0.3050207605,2.0248416205\H,1.8990082491,0.4373073027,0

.4162194138\Cl,-0.0756551745,-0.0334408292,-1.2931203887\\Version=IA32
L-G03RevC.02\State=1-A\HF=-629.4969904\RMSD=1.580e-09\RMSF=6.569e-05\D
ipole=1.4379074,0.3331563,0.5371838\PG=C01 [X(C1H2Cl1N1O1)]\\@

n.Cl-CONHCH3
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C2H4Cl1N1O1\CYL509\20-Aug-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\Cl-CO
NHCH3.freq\\0,1\C,-0.0926108307,-0.0045391925,0.3547675264\O,-0.087462
6505,0.0045163223,1.5530829726\N,0.9597418275,-0.0195633807,-0.4870157
194\H,0.7795286567,0.0343663089,-1.4784013523\C,2.3284321918,0.0537606
904,0.0083511827\H,2.3626120223,-0.3868883215,1.0057079744\H,2.6841337
003,1.0893520981,0.0670441996\H,2.9825627555,-0.5137092445,-0.65880901
54\Cl,-1.6613092288,-0.0245668672,-0.5958710474\\Version=IA64L-G03RevC
.02\State=1-A\HF=-668.8089245\RMSD=5.482e-09\RMSF=8.913e-05\Dipole=1.3
514197,0.049405,-0.9739459\PG=C01 [X(C2H4Cl1N1O1)]\\@

n.Cl-COOC_CH3_3
1\1\GINC-LC48\FOpt\RB3LYP\Gen\C5H9Cl1O2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COOC
_CH3_3.freq\\0,1\C,-0.7369414816,0.4595387908,-0.6455103826\O,-0.15638
33144,0.82950876,-1.6239265542\O,-0.2928346619,-0.1571587041,0.4335398
65\C,1.1603380268,-0.5015117049,0.5646422241\C,1.5543646657,-1.4691724
965,-0.5519654174\C,1.1972890857,-1.1824529932,1.9321104068\C,1.988245
1485,0.7841708976,0.5583967299\H,2.2216191377,-1.4930693993,2.16221842
56\H,0.5547362626,-2.0681471735,1.942019282\H,0.8569793807,-0.49841960
63,2.7155091112\H,2.5820338528,-1.8102754112,-0.3858597759\H,1.5032505
228,-0.9922703306,-1.5325518405\H,0.9001075066,-2.3472021938,-0.547584
8196\H,3.0343669202,0.5389817984,0.7718423037\H,1.635380151,1.47168806
88,1.3341638821\H,1.9420519684,1.2862555082,-0.4097807654\Cl,-2.506856
1508,0.7053072546,-0.4513484502\\Version=IA32L-G03RevC.02\State=1-A\HF
=-806.6170804\RMSD=6.853e-09\RMSF=1.980e-05\Dipole=1.0824226,-0.570186
5,0.7346042\PG=C01 [X(C5H9Cl1O2)]\\@

n.Cl-COOCH2CH3
1\1\GINC-LC72\FOpt\RB3LYP\Gen\C3H5Cl1O2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COOC
H2CH3.freq\\0,1\C,-0.206297747,0.2992492977,-0.6553595816\O,0.44116800
29,0.3899942148,-1.6561786134\O,0.1483823537,-0.2279523355,0.509176143
2\C,1.5084679944,-0.7607946195,0.5548076566\H,2.2010652931,0.050897426
9,0.314392078\H,1.5997687738,-1.5295013757,-0.2179077708\C,1.723049260
5,-1.3120658497,1.9491351493\H,2.7353080332,-1.7231806817,2.0262638207
\H,1.0080238969,-2.1105612483,2.1690839659\H,1.6106708749,-0.526617796
8,2.7025779478\Cl,-1.8836798101,0.893193863,-0.5241111545\\Version=IA3
2L-G03RevC.02\State=1-A\HF=-727.9837096\RMSD=6.058e-09\RMSF=3.499e-05\
Dipole=0.787122,-0.5752137,0.8186855\PG=C01 [X(C3H5Cl1O2)]\\@

n.Cl-COOCH3
1\1\GINC-LC71\FOpt\RB3LYP\Gen\C2H3Cl1O2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COOC
H3.freq\\0,1\C,0.3001703648,0.1069483167,-0.0338514548\O,1.4825890723,
0.1178001236,-0.2075194864\O,-0.5155282623,-0.9424558334,-0.0163886407
\C,0.1408670134,-2.213993766,-0.2383059373\H,0.6246048558,-2.221676465
8,-1.2175370304\H,-0.6574597548,-2.9534834274,-0.1932156909\H,0.884154
6721,-2.3946473818,0.5413397001\Cl,-0.6608241484,1.5770191559,0.252566
023\\Version=IA32L-G03RevC.02\State=1-A\HF=-688.6639086\RMSD=3.354e-09
\RMSF=2.417e-05\Dipole=-0.2224462,-1.0996375,-0.0751567\PG=C01 [X(C2H3
Cl1O2)]\\@

n.Cl-COOH
1\1\GINC-LC26\FOpt\RB3LYP\Gen\C1H1Cl1O2\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COOH
.freq\\0,1\C,0.0769479602,0.0313141944,0.4970907536\O,1.0386553718,0.2
293290436,1.1759893418\O,-1.176874639,-0.1810606553,0.9157814778\H,-1.
1486752523,-0.1417415449,1.8914837261\Cl,0.1054553899,-0.0254288663,-1
.2710702826\\Version=IA32L-G03RevC.02\State=1-A\HF=-649.354907\RMSD=8.
790e-09\RMSF=8.237e-05\Dipole=-0.6017903,-0.0894648,0.5578257\PG=C01 [
X(C1H1Cl1O2)]\\@

n.Cl-COPh
1\1\GINC-LC76\FOpt\RB3LYP\Gen\C7H5Cl1O1\CYL509\18-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\Cl-COPh
.freq\\0,1\C,-2.6118754656,-0.0079550708,-0.1030748385\C,-2.5843369816
,-0.0049550776,1.2946142584\C,-1.363035269,-0.0000292409,1.9718032657\
C,-0.1657412633,0.0019229863,1.2594131153\C,-0.1889687491,-0.001075650
8,-0.1423159398\C,-1.4211053212,-0.0060353557,-0.8211674663\C,1.024660
313,0.0006247697,-0.9933408259\O,1.0487814037,-0.0013488177,-2.1870045
108\H,-1.4226817118,-0.0083079313,-1.9057743269\H,0.7819698499,0.00574

S45

72607,1.7842945674\H,-1.341655229,0.0023021323,3.0576280296\H,-3.56112
03867,-0.0117850588,-0.6308627151\H,-3.5149471053,-0.0064579022,1.8555
698232\Cl,2.6194470456,0.0079004635,-0.0859063944\\Version=IA32L-G03Re
vC.02\State=1-A\HF=-805.1849693\RMSD=4.211e-09\RMSF=4.731e-05\Dipole=-
1.3720612,-0.00252,0.9079965\PG=C01 [X(C7H5Cl1O1)]\\@

n.CH3-H
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C1H4\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-H.freq\\
0,1\C,0.,0.,0.\H,-0.0000003042,0.0000001907,1.0933912546\H,1.030859262
2,0.0000000327,-0.3644634647\H,-0.5154293956,-0.8927503326,-0.36446373
92\H,-0.5154295624,0.8927501093,-0.3644640506\\Version=IA64L-G03RevC.0
2\State=1-A1\HF=-40.5183833\RMSD=6.431e-10\RMSF=4.407e-05\Dipole=0.,0.
,0.\PG=TD [O(C1),4C3(H1)]\\@

n.CH3-BH2
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C1H5B1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-BH2.fr
eq\\0,1\C,0.2216494897,0.1824344811,0.621922372\H,1.2946348031,0.38960
91838,0.6972815937\H,0.0463360637,-0.7259478453,1.2298603591\H,-0.3471
256936,0.9819929249,1.1088775997\B,-0.2737110652,-0.1973697855,-0.8080
761046\H,0.4624531936,-0.7164042343,-1.5989565713\H,-1.4176399787,-0.0
370079881,-1.12821669\\Version=IA64L-G03RevC.02\State=1-A\HF=-65.94666
1\RMSD=4.422e-09\RMSF=5.097e-06\Dipole=0.0739019,0.0207136,0.2648932\P
G=C01 [X(C1H5B1)]\\@

n.CH3-CH3
1\1\GINC-AC1\FOpt\RB3LYP\Gen\C2H6\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH3.freq\
\0,1\H,0.2822963016,-0.3511507746,-1.4814500269\C,0.2797944825,-0.5824
814779,-0.4099747294\H,1.311017458,-0.8151698924,-0.1201196126\H,-0.31
59496779,-1.491801474,-0.2697339625\C,-0.2798281692,0.5824184887,0.409
9788231\H,0.3149789029,1.4921958911,0.2681215418\H,-0.2805032566,0.352
1208579,1.4816777655\H,-1.3116376078,0.8141833273,0.1214797321\\Versio
n=IA64L-G03RevC.02\State=1-A\HF=-79.8304206\RMSD=1.101e-09\RMSF=2.040e
-05\Dipole=0.0000228,0.0000088,-0.0000143\PG=C01 [X(C2H6)]\\@

n.CH3-NH2
1\1\GINC-AC2\FOpt\RB3LYP\Gen\C1H5N1\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NH2.fre
q\\0,1\C,0.2327427385,0.1332439419,0.652987302\H,1.3259746814,0.199384
4458,0.6792172298\H,-0.0601148363,-0.6608088695,1.3486312443\H,-0.1703
838983,1.0853016964,1.0416746944\N,-0.1928277048,-0.2339549171,-0.6999
215149\H,-1.20935982,-0.2894533505,-0.735554401\H,0.0672213754,0.50379
68456,-1.3524419757\\Version=IA64L-G03RevC.02\State=1-A\HF=-95.8532062
\RMSD=4.976e-09\RMSF=1.851e-05\Dipole=-0.2680732,0.5041698,0.0936696\P
G=C01 [X(C1H5N1)]\\@

n.CH3-OH
1\1\GINC-AC11\FOpt\RB3LYP\Gen\C1H4O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OH.fre
q\\0,1\C,-0.0225076774,-0.0364037632,-0.6613583405\O,-0.023466076,-0.0
460553763,0.7574749515\H,0.9936984255,-0.0434745329,-1.0856441251\H,-0
.5683918944,0.8232159964,-1.0807293706\H,-0.5303712189,-0.9500274685,-
0.9821664995\H,0.4278393605,0.7571515946,1.0568904264\\Version=IA64L-G
03RevC.02\State=1-A\HF=-115.7144057\RMSD=3.257e-09\RMSF=4.726e-05\Dipo
le=0.2772331,0.495668,-0.3494451\PG=C01 [X(C1H4O1)]\\@

n.CH3-F
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C1H3F1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-F.freq
\\0,1\H,0.2250107228,-0.2237715069,-1.4008132976\C,0.2259127657,-0.483
0442984,-0.3354805411\H,1.2510905262,-0.705324199,-0.0164832482\H,-0.4
028637777,-1.3674923382,-0.177088697\F,-0.2698571186,0.5772059817,0.40
08076097\\Version=IA64L-G03RevC.02\State=1-A\HF=-139.7339157\RMSD=1.03
4e-09\RMSF=1.195e-04\Dipole=0.2415928,-0.516621,-0.3587828\PG=C01 [X(C
1H3F1)]\\@

n.CH3-SiH3
1\1\GINC-AC19\FOpt\RB3LYP\Gen\C1H6Si1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-SiH3.
freq\\0,1\H,0.6042320567,-1.0464936201,-1.5120490232\C,0.5896452789,-1
.0212947333,-0.4169416595\H,1.6269655135,-1.0465260769,-0.0656042063\H
,0.0927986196,-1.9322564375,-0.0656582033\Si,-0.3006882558,0.520806903
7,0.2126184417\H,-1.7106289079,0.5521099501,-0.2666723592\H,-0.3187478
216,0.5521345956,1.7016868159\H,0.3771444471,1.757503337,-0.2667112507
\\Version=IA64L-G03RevC.02\State=1-A\HF=-331.2108723\RMSD=7.186e-09\RM

SF=1.199e-05\Dipole=0.1516897,-0.262734,-0.1072606\PG=C03 [C3(C1Si1),X (H6)]\\@

n.CH3-PH2
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C1H5P1\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-PH2.fr eq\\0,1\C,-0.5683148254,0.9898873182,0.3666473545\H,0.1510309782,1.751 7945247,0.6826951466\H,-1.2124220714,0.7687267922,1.2234209889\H,-1.18 18181644,1.3963397834,-0.4413641386\P,0.3663047437,-0.5664715006,-0.10 62285714\H,-0.720976263,-1.2565397534,-0.7182402006\H,0.8795033181,-0. 1025727479,-1.3529673516\\Version=IA64L-G03RevC.02\State=1-A'\HF=-382. 4577748\RMSD=5.469e-09\RMSF=1.610e-05\Dipole=-0.3293845,0.3709887,-0.1 560742\PG=CS [SG(C1H1P1),X(H4)]\\@

n.CH3-SH
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C1H4S1\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-SH.fre q\\0,1\C,0.329828014,0.2947706031,1.0779089523\H,1.4148829366,0.412429 2451,1.123814636\H,0.0021478487,-0.461294262,1.7950251174\H,-0.1369681 059,1.2481048785,1.3363958321\S,-0.2309060771,-0.1058464119,-0.6236566 073\H,0.4354664694,-1.2743208899,-0.7441835819\\Version=IA64L-G03RevC. 02\State=1-A\HF=-438.6983423\RMSD=7.606e-09\RMSF=8.115e-06\Dipole=0.36 72239,-0.1708446,0.5499149\PG=C01 [X(C1H4S1)]\\@

n.CH3-Cl
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C1H3Cl1\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-Cl.fr eq\\0,1\H,0.4032782554,-0.5921458858,-1.6616300541\C,0.4111697868,-0.8 712830258,-0.6078476021\H,1.4298376382,-1.07392363,-0.2766529778\H,-0. 22376772,-1.7412944652,-0.4398672834\Cl,-0.239786288,0.5079448316,0.35 44256427\\Version=IA64L-G03RevC.02\State=1-A\HF=-500.1085334\RMSD=2.24 1e-09\RMSF=5.286e-05\Dipole=0.2959815,-0.6266538,-0.4373722\PG=C01 [X(C1H3Cl1)]\\@

n.CH3-Br
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C1H3Br1\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-Br.fr eq\\0,1\H,0.5450881132,-0.8872049211,-1.8725336704\C,0.5582973233,-1.1 785786011,-0.8237959709\H,1.5744460099,-1.3702961291,-0.4837811193\H,- 0.0827015589,-2.0407058746,-0.6485803435\Br,-0.1539033286,0.324847958, 0.2270763132\\Version=IA64L-G03RevC.02\State=1-A\HF=-2613.7955729\RMSD =8.329e-09\RMSF=4.669e-05\Dipole=0.2950393,-0.6225217,-0.4352365\PG=C0 1 [X(C1H3Br1)]\\@

n.CH3-N_CH3_2
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C3H9N1\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-N_CH3_ 2.freq\\0,1\C,0.6309694629,-0.0479964995,1.2378699908\H,1.7248755103,0 .015283008,1.2357973162\H,0.3390381549,-0.8647513744,1.9074421443\H,0. 2350403944,0.8980866197,1.6605513577\N,0.1522058273,-0.321528837,-0.10 83733824\C,-1.2919848181,-0.4947347766,-0.1367614288\C,0.58603581,0.70 11509797,-1.0477141649\H,-1.5798606603,-1.3116636521,0.534349429\H,-1. 6131322084,-0.7586486099,-1.1505887823\H,-1.8490216656,0.4134006807,0. 172322105\H,1.6799597954,0.7640575605,-1.0469562961\H,0.1858883136,1.7 091671296,-0.8146768634\H,0.2616488454,0.4352522752,-2.0599931153\\Ver sion=IA64L-G03RevC.02\State=1-A\HF=-174.4744033\RMSD=1.388e-09\RMSF=1. 068e-05\Dipole=-0.0926285,0.1954838,0.0658847\PG=C01 [X(C3H9N1)]\\@

n.CH3-NHCH3
1\1\GINC-AC2\FOpt\RB3LYP\Gen\C2H7N1\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6 D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NHCH3.f req\\0,1\C,0.8373621362,0.2405194459,0.8735800623\H,1.9278042334,0.340 1230919,0.850710369\H,0.5907306021,-0.5543118724,1.5882632911\H,0.4109 866805,1.1835296623,1.2677945497\N,0.3518696027,-0.1341564229,-0.44817 41069\C,-1.1017347834,-0.2107035977,-0.513764155\H,-1.4502181784,-1.02 9131709,0.1281755775\H,-1.412599271,-0.43733262,-1.5391929074\H,-1.624 0643687,0.7100291033,-0.1883205148\N,0.6805089665,0.5472942152,-1.1291 070604\\Version=IA64L-G03RevC.02\State=1-A\HF=-135.1628563\RMSD=2.072e -09\RMSF=1.380e-05\Dipole=-0.100408,0.391435,0.0130459\PG=C01 [X(C2H7N 1)]\\@

n.CH3-NHCHO
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H5N1O1\CYL509\07-Apr-2008\0\\#B3LYP/GE N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NHCH O.freq\\0,1\C,-0.0913365543,-0.4110003383,1.4548678243\H,0.9538962324, -0.1270843243,1.3250566119\H,-0.1410506705,-1.4569335617,1.7795984681\ H,-0.5413200921,0.2219888319,2.2286559929\N,-0.7502092551,-0.225393887

4,0.1734899204\H,-1.7345023037,-0.437983103,0.0907050695\C,-0.10036939
36,0.2263407607,-0.9355531248\O,1.0805208288,0.5234890044,-0.993237000
6\H,-0.7794893241,0.2978147993,-1.8084377774\\Version=IA64L-G03RevC.02
\State=1-A\HF=-209.2004279\RMSD=4.548e-09\RMSF=3.145e-06\Dipole=-1.284
2945,-0.4713998,0.6169694\PG=C01 [X(C2H5N1O1)]\\@

n.CH3-NHCOCH3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C3H7N1O1\CYL509\07-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NHCO
CH3.freq\\0,1\C,0.3274798799,-0.9948528606,1.6781220184\H,1.305319446,
-0.5165222938,1.6056818645\H,0.459318403,-2.0836870188,1.6789005843\H,
-0.1495055756,-0.696569268,2.6196449692\N,-0.4476575007,-0.5577828448,
0.5319530962\H,-1.3908867688,-0.9002740936,0.426395989\C,0.0505105704,
0.3009214844,-0.4107949169\O,1.1830425296,0.764152592,-0.3602615661\C,
-0.9070332428,0.6485046922,-1.5427347508\H,-0.4460438468,0.3631565888,
-2.4932977714\H,-1.0487533994,1.7334151116,-1.5627085455\H,-1.88592923
58,0.1643002554,-1.4637503391\\Version=IA64L-G03RevC.02\State=1-A\HF=-
248.5235631\RMSD=2.275e-09\RMSF=2.080e-06\Dipole=-1.2245759,-0.7017669
,0.2417766\PG=C01 [X(C3H7N1O1)]\\@

n.CH3-NO2
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C1H3N1O2\CYL509\05-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NO2.
freq\\0,1\H,0.5379650314,-0.6195690809,-1.7586975281\C,0.5516536625,-0
.9643410662,-0.7220822824\H,1.5763342561,-1.1027280531,-0.3817277338\H
,-0.0539260152,-1.8622821246,-0.6128230525\N,-0.0707606588,0.120063238
6,0.1045618431\O,0.677720125,0.9908489403,0.5363724926\O,-1.2870914549
,0.0754239327,0.2578536457\\Version=IA64L-G03RevC.02\State=1-A\HF=-245
.0093321\RMSD=2.841e-09\RMSF=6.698e-05\Dipole=0.5669415,-0.9855271,-0.
7602955\PG=C01 [X(C1H3N1O2)]\\@

n.CH3-OCF3
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C2H3F3O1\CYL509\07-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OCF3
.freq\\0,1\C,-1.0892492068,-0.0814840395,-1.6200890318\O,-0.797674315,
0.5819587208,-0.3784100316\C,0.2034289736,0.048342946,0.3442854116\F,1
.3813982203,0.0474790468,-0.3221746906\F,-0.0381808949,-1.235875685,0.
6966894836\F,0.3483274803,0.7700017417,1.4551596899\H,-0.2200250546,-0
.0545797676,-2.2834246226\H,-1.3949211636,-1.1161498323,-1.4403162162\
H,-1.9126411137,0.479460464,-2.0612275333\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-452.7654984\RMSD=2.148e-09\RMSF=8.623e-05\Dipole=-0.393321
5,-0.2009527,-0.801015\PG=C01 [X(C2H3F3O1)]\\@

n.CH3-OCH2CH3
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C3H8O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OCH2CH
3.freq\\0,1\C,-1.7265935923,0.4365942314,0.3377971338\H,-2.0504344629,
0.7704084454,-0.6620716979\H,-1.5899063884,1.3300549413,0.9695632281\H
,-2.5116052282,-0.1874255326,0.7735714981\O,-0.5556533466,-0.346197154
4,0.2757549969\C,0.5439331033,0.356030615,-0.2760344386\C,1.7470901796
,-0.5724107409,-0.2967811265\H,0.7596250111,1.257427513,0.3244233897\H
,0.3017463505,0.7003467494,-1.2970062257\H,2.6193413419,-0.0611599758,
-0.7187928529\H,1.5360738301,-1.4591518827,-0.9032151891\H,1.993808174
8,-0.9022076558,0.7175984626\\Version=IA64L-G03RevC.02\State=1-A\HF=-1
94.3442992\RMSD=4.755e-09\RMSF=3.859e-05\Dipole=-0.0065044,0.4269246,-
0.1447386\PG=C01 [X(C3H8O1)]\\@

n.CH3-OCH3
1\1\GINC-AC11\FOpt\RB3LYP\Gen\C2H6O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OCH3.f
req\\0,1\C,-0.4899387354,0.0034990738,-1.0812806275\O,-0.4905709788,0.
0026778129,0.3291236237\C,0.8146986091,-0.0052749263,0.8633984397\H,0.
0057810252,-0.8921477998,-1.4913405983\H,-1.5338450974,0.0102183377,-1
.4063910968\H,0.0169426886,0.8933601465,-1.4902856364\H,1.3784805323,-
0.9012430478,0.5544306152\H,0.7196468783,-0.0052228302,1.9526402693\H,
1.3890025618,0.8842678048,0.555250584\\Version=IA64L-G03RevC.02\State=
1-A\HF=-155.0250508\RMSD=8.051e-09\RMSF=1.247e-04\Dipole=0.4173848,-0.
0022503,-0.2800236\PG=C01 [X(C2H6O1)]\\@

n.CH3-OCHO
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H4O2\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OCHO.f
req\\0,1\C,-1.3685435718,-0.3990834186,-0.0052996195\O,-0.4774432927,0
.7328594798,0.0032456334\C,0.8304841127,0.4320943216,0.0044203863\O,1.
3029277834,-0.678117019,-0.001187994\H,-1.2080916184,-1.0177459476,0.8
814136485\H,-1.204943786,-1.0063521312,-0.8993099362\H,-2.3740882143,0
.0212881877,-0.0042778274\H,1.4116044481,1.3668047864,0.0109883989\\Ve

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rsion=IA64L-G03RevC.02\State=1-A\HF=-229.0630092\RMSD=7.982e-09\RMSF=6
.826e-05\Dipole=-0.6595265,0.3001289,0.0004366\PG=C01 [X(C2H4O2)]\\@

n.CH3-OCOCH3
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C3H6O2\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-OCOCH3
.freq\\0,1\C,-0.8804257779,0.0598136811,-1.6590154362\O,-0.8757360389,
0.0968789209,-0.2229866054\C,0.3426526247,-0.0303463886,0.3541209644\C
,0.2307348566,0.0203668591,1.8601684801\O,1.3685768249,-0.1662848251,-
0.2748628539\H,-0.2754618584,0.8738528514,-2.0675180958\H,-0.482266531
4,-0.8919040107,-2.0212820545\H,-1.9246950009,0.1744455643,-1.95153945
13\H,1.2236854855,-0.0737014734,2.3008031958\H,-0.4131363964,-0.790104
0633,2.2174504168\H,-0.2286222068,0.9636534554,2.1732376134\\Version=I
A64L-G03RevC.02\State=1-A\HF=-268.388484\RMSD=6.367e-09\RMSF=3.136e-05
\Dipole=-0.6821362,0.0816115,0.1352391\PG=C01 [X(C3H6O2)]\\@

n.CH3-Si_CH3_3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H12Si1\CYL509\05-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-Si_C
H3_3.freq\\0,1\H,0.9123922966,-1.5813407482,-1.7282637361\C,0.8934991l
,-1.5476843555,-0.6319087206\H,1.9337240459,-1.5808878418,-0.285052951
7\H,0.4026938003,-2.465152341,-0.2842811424\Si,-0.0000139699,0.0000252
714,0.0000161\C,-1.7871729994,0.0000405237,-0.6317975903\C,0.000038867
8,-0.0000546186,1.8955732663\C,0.893642085,1.5476752889,-0.6318875812\
H,-1.8257813505,0.0004613189,-1.7281484588\H,-2.3362833972,0.883857057
7,-0.2841919891\H,-2.3360500585,-0.884194417,-0.2848915348\H,1.9334435
52,1.5815185025,-0.2838240163\H,0.402075982,2.4651974619,-0.2854903476
\H,0.9138204216,1.5805630668,-1.7282404022\H,1.0208259185,-0.000098205
2,2.2974160325\H,-0.5103842448,-0.8840877459,2.2973623876\H,-0.5103237
666,0.8839490607,2.2975045134\\Version=IA64L-G03RevC.02\State=1-A\HF=-
449.1916976\RMSD=4.752e-09\RMSF=1.721e-04\Dipole=0.0000112,0.0000303,0
.0000336\PG=C01 [X(C4H12Si1)]\\@

n.CH3-P_CH3_2
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C3H9P1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-P_CH3_
2.freq\\0,1\C,-0.6172245734,1.3106163547,0.8256316504\H,0.0732110323,2
.1046517271,1.1300297944\H,-1.2939826874,1.1206613013,1.6655694387\H,-
1.2083381592,1.6677666107,-0.027371338\P,0.3462371766,-0.2407440985,0.
4349428439\C,-1.0311738668,-1.2803547567,-0.278741117\C,1.1670130972,0
.3044664264,-1.1514016051\H,-0.6140193398,-2.1981244297,-0.7073568574\
H,-1.5979293585,-0.7553074805,-1.0580047728\H,-1.7218155533,-1.5726939
561,0.5197464935\H,1.9270526469,1.0616504027,-0.9299367481\H,0.4552822
198,0.7228347966,-1.874269392\H,1.6752936075,-0.5486456416,-1.61386284
6\\Version=IA64L-G03RevC.02\State=1-A\HF=-461.0984129\RMSD=5.701e-09\R
MSF=5.926e-06\Dipole=-0.3031785,0.2107677,-0.3809246\PG=C01 [X(C3H9P1)
]\\@

n.CH3-SC_CH3_2CN
1\1\GINC-SC24\FOpt\RB3LYP\6-31G(d)\C5H9N1S1\MLC501\23-Sep-2002\0\\#N B
3LYP/6-31G(D) OPT=(MAXCYC=100) FREQ MAXDISK=52428800 GEOM=CHECK\\ch3sc
me2cn-c1b2-6dub3\\0,1\C,2.0004608618,0.9668672623,0.3091125322\H,1.999
9993174,0.9636095319,1.402206942\H,3.0568058107,0.9668243234,-0.041280
1942\S,1.2416814904,-0.5438703598,-0.3838305371\C,-0.5503501855,-0.3539
747574,0.1076597413\C,-0.7388086095,-0.429265126,1.635054428\C,-1.3023
225301,-1.501267512,-0.5974700784\C,-1.035494258,0.9424549998,-0.38849
77241\H,-0.3703085291,-1.3927528237,1.9987089375\H,-0.1981988796,0.370
0798125,2.1489303456\H,-1.8009991951,-0.3359079691,1.8893357496\H,-1.1
916771354,-1.4397566369,-1.6831554124\H,-2.3679363761,-1.4558307861,-0
.3504707881\H,-0.906511597,-2.4628171846,-0.2554545166\N,-1.4011523275
,1.9824019672,-0.7563977594\H,1.4998250629,1.8627745195,-0.0679015481\
\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-648.8781177\RMSD=8.129e-09\RMS
F=4.157e-06\Dipole=0.2984912,-0.8362157,0.8124852\PG=C01 [X(C5H9N1S1)]
\\@

n.CH3-SCH2COOCH3
1\1\GINC-SC28\FOpt\RB3LYP\6-31G(d)\C4H8O2S1\MLC501\20-Sep-2002\1\\#N B
3LYP/6-31G(D) OPT=(Z-MATRIX,MAXCYC=100) FREQ MAXDISK=52428800 GEOM=CHE
CK\\ch3sch2co2ch3-c1p-6dub3\\0,1\S\C,1,B1\H,2,B2,1,A1\H,2,B3,1,A2,3,D1
,0\C,1,B4,2,A3,3,D2,0\C,5,B5,1,A4,2,D3,0\O,6,B6,5,A5,1,D4,0\O,6,B7,5,A
6,7,D5,0\C,8,B8,6,A7,5,D6,0\H,5,B9,1,A8,6,D7,0\H,5,B10,1,A9,6,D8,0\H,9
,B11,8,A10,6,D9,0\H,9,B12,8,A11,12,D10,0\H,9,B13,8,A12,12,D11,0\H,2,B1
4,1,A13,4,D12,0\\B14=1.09407907\A13=110.98917864\D12=-122.32599148\B1=
1.82941218\B2=1.09320983\B3=1.09179061\B4=1.84120939\B5=1.51326922\B6=
1.21430186\B7=1.34788275\B8=1.43778776\B9=1.09325654\B10=1.09174033\B1
1=1.09310389\B12=1.09323525\B13=1.09017352\A1=106.45059106\A2=110.8007
717\A3=100.17137515\A4=111.04905442\A5=124.57420924\A6=111.47577278\A7

=115.34918093\A8=109.61040514\A9=106.06955231\A10=110.56850432\A11=110
.39708436\A12=105.51426102\D1=-119.0645737\D2=175.11314455\D3=-70.7090
079\D4=81.86780755\D5=-178.35716699\D6=176.4774588\D7=120.89987776\D8=
-120.6551676\D9=59.44174906\D10=-120.72743755\D11=119.73808134\\Versio
n=DEC-AXP-OSF/1-G98RevA.11.3\HF=-705.8848169\RMSD=7.903e-09\RMSF=2.103
e-05\Dipole=-0.2739871,-0.1599817,-0.1633175\PG=C01 [X(C4H8O2S1)]\\@

n.CH3-SCH2Ph
1\1\GINC-SC29\FOpt\RB3LYP\6-31G(d)\C8H10S1\MLC501\29-Jan-2003\0\\#N B3
LYP/6-31G(D) OPT(MAXCYC=100) FREQ MAXDISK=39321600 GEOM=CHECK GUESS=RE
AD\\CH3SB2 (based on c1cy)//B3\\0,1\C,2.2716097518,1.1121065137,-0.997
3390939\S,2.4284127182,-0.4787724374,-0.1153723018\C,1.0853222086,-0.2
985429716,1.1422050296\H,1.2732481361,1.2266499171,-1.4278935723\H,3.0
083318311,1.0980264415,-1.804834343\C,-0.3064073801,-0.1601063939,0.57
40714721\H,1.3243469567,0.5507382422,1.7912300283\H,1.1749078686,-1.20
73821913,1.7469281007\C,-0.9937221494,1.0564749042,0.6650093261\C,-0.9
397240463,-1.2425042601,-0.0546658397\C,-2.2834744781,1.1918881437,0.1
448090955\C,-2.2266742838,-1.1118376907,-0.5716986532\C,-2.9038127115,
0.1075313971,-0.4741765207\H,-3.9076158778,0.2087023447,-0.8780254106\
H,-2.7042121176,-1.962380853,-1.0511911286\H,-2.8009101292,2.144302445
6,0.2259204072\H,-0.4126995505,-2.1894404946,-0.1430459346\H,-0.517664
1431,1.9038244544,1.1539361163\H,2.488962066,1.9572608373,-0.336356329
5\\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-709.0645592\RMSD=4.540e-09\R
MSF=5.598e-06\Dipole=-0.4507539,0.4538128,0.0558314\PG=C01 [X(C8H10S1)
]\\@

n.CH3-SCH3
1\1\GINC-SC32\FOpt\RB3LYP\6-31G(d)\C2H6S1\MLC501\16-Mar-2004\0\\# B3LY
P/6-31G* OPT FREQ MAXDISK=65536000\\CH3SCH3-geom-6dub3\\0,1\S,-0.36978
21769,-0.5514550776,0.\C,1.4449112088,-0.3482505121,0.\C,-0.8707345203
,1.2045205438,0.\H,1.8814896329,-1.3505755523,0.\H,-1.9637607463,1.227
8848837,0.\H,1.785254922,0.1830801241,0.8945611212\H,-0.5083920151,1.7
21101736,0.8945611186\H,1.785254922,0.1830801241,-0.8945611212\H,-0.50
83920151,1.721101736,-0.8945611186\\Version=DEC-AXP-OSF/1-G03RevB.03\S
tate=1-A'\HF=-478.0138083\RMSD=4.490e-09\RMSF=3.553e-05\Dipole=0.37734
84,0.5627385,0.\PG=CS [SG(C2H2S1),X(H4)]\\@

n.CH3-SO2CH3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H6O2S1\CYL509\05-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-SO2C
H3.freq\\0,1\C,-0.5693464435,-1.4882201784,-0.5811886756\S,-0.06930397
9,0.0848752568,0.1612097726\C,1.227989534,0.6817367339,-0.9507725321\O
,-1.2071536857,1.0105358861,0.062518508\O,0.5522585167,-0.2086078218,1
.4607548021\H,2.0565938955,-0.0294479748,-0.9636026922\H,1.5616507837,
1.6367294395,-0.5379488086\H,0.8147584878,0.8310526665,-1.9505116709\H
,0.2810444895,-2.1731259033,-0.5985765865\H,-0.9607486664,-1.312654425
,-1.5854515336\H,-1.3571325171,-1.8870817594,0.0623156952\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-628.4008216\RMSD=8.678e-09\RMSF=1.791e-05\
Dipole=0.6444631,-0.7891339,-1.4989924\PG=C01 [X(C2H6O2S1)]\\@

n.CH3-SOCH3
1\1\GINC-AC7\FOpt\RB3LYP\Gen\C2H6O1S1\CYL509\11-Apr-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-SOCH3
.b1.freq\\0,1\H,0.5011333965,1.1134772663,-1.6152834588\C,0.703141249,
1.3258550683,-0.5611813272\H,1.7799391642,1.4339084427,-0.4104052859\H
,0.1905120969,2.2380020504,-0.2403112153\S,0.1570310499,-0.0958184515,
0.467155375\O,0.7771757481,-1.3442953328,-0.1168188472\C,-1.6000412927
,-0.0484626761,-0.0688693757\H,-2.1056201907,-0.8846195384,0.420144301
1\H,-1.6544944198,-0.1727940147,-1.154511758\H,-2.0599725682,0.8951293
284,0.2407364122\\Version=IA64L-G03RevC.02\State=1-A'\HF=-553.1869341\
RMSD=5.114e-09\RMSF=1.127e-05\Dipole=-0.7995656,1.3212387,-0.0522912\P
G=CS [SG(O1S1),X(C2H6)]\\@

n.CH3-Ph
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C7H8\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-Ph.freq\
\0,1\C,0.8370875263,0.4312198302,2.2352514059\H,1.922021,0.6018739263,
2.2178876395\H,0.6531340685,-0.4134973976,2.9078264328\H,0.3765159687,
1.3215844198,2.6766899025\C,0.3018642167,0.1610210578,0.8474806067\C,-
0.6431077018,-0.3371566985,-1.7612937383\C,-0.1294726256,1.2108443571,
0.0256885811\C,0.2458969242,-1.1436564459,0.3393401996\C,-0.2201696899
,-1.3930929008,-0.9522027675\C,-0.596481269,0.9673169011,-1.2666414937
\H,-0.1004950958,2.2306000596,0.4040615462\H,0.569753954,-1.9735289326
,0.9641087752\H,-0.2569032036,-2.4138084874,-1.3245636571\H,-0.9282545
513,1.797234492,-1.8855320033\H,-1.0094764249,-0.529434739,-2.76621539
91\\Version=IA64L-G03RevC.02\State=1-A\HF=-271.5666377\RMSD=7.836e-09\
RMSF=2.415e-05\Dipole=0.0559009,0.0235781,0.1100932\PG=C01 [X(C7H8)]\\

@

n.CH3-C6H4CN
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C8H7N1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-C6H4CN
.freq\\0,1\C,1.1540637282,0.5741186195,2.9352620447\H,2.2519353185,0.5
912248458,2.9158835196\H,0.8536777139,-0.1996203433,3.6491940984\H,0.8
207707334,1.5428706005,3.3213323433\C,0.5940997475,0.3046799724,1.5594
729852\C,-0.3981390926,-0.2011319518,-1.0291522532\C,0.316866808,1.358
4820383,0.6765886322\C,0.3596393375,-1.0071307044,1.1224335261\C,-0.12
86785717,-1.2661377843,-0.1539345037\C,-0.1717836213,1.1180541811,-0.6
032751198\H,0.4851364921,2.3833456904,0.9978274811\H,0.5614692816,-1.8
382877032,1.7934734734\H,-0.3074414831,-2.2861266671,-0.4790271438\H,-
0.3839006735,1.9429090631,-1.2760610148\C,-0.9048484622,-0.4583687425,
-2.3452216143\N,-1.3155666605,-0.6673870366,-3.4136664201\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-363.811129\RMSD=4.310e-09\RMSF=2.055e-06\D
ipole=0.7295346,0.3610479,1.8446661\PG=C01 [X(C8H7N1)]\\@

n.CH3-C6H4NO2
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C7H7N1O2\CYL509\07-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-C6H4
NO2.freq\\0,1\C,1.2257979093,0.634562304,3.2964905395\H,2.3105244171,0
.8040258582,3.2704357455\H,1.0450434315,-0.2109312357,3.9678535732\H,0
.7680811976,1.5263070931,3.7364297259\C,0.6910299555,0.3647873724,1.91
13572401\C,-0.2456731711,-0.1281947049,-0.6683087123\C,0.2589526341,1.
4178902698,1.0904204314\C,0.6353259713,-0.9429063361,1.404910888\C,0.1
710690208,-1.2001109514,0.1188657536\C,-0.2089327707,1.1834451978,-0.1
986565691\H,0.2879876237,2.4368935671,1.467559427\H,0.9590579739,-1.77
23861494,2.0282931167\H,0.1228303337,-2.2059079522,-0.2799159995\H,-0.
5460148108,1.9894140771,-0.8387904225\N,-0.740650033,-0.3880115817,-2.
0263112192\O,-1.1032011661,0.5781761666,-2.6983324546\O,-0.7628459878,
-1.5566978036,-2.4139380528\\Version=IA64L-G03RevC.02\State=1-A\HF=-47
6.0696457\RMSD=8.613e-09\RMSF=8.752e-05\Dipole=0.7075901,0.3640844,1.8
862635\PG=C01 [X(C7H7N1O2)]\\@

n.CH3-C6H4OCH3
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H10O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-C6H4O
CH3.freq\\0,1\C,-0.9744537048,-0.0476318403,-0.9819541032\C,-0.9155034
449,-0.0098185008,0.4195567308\C,0.3295587119,0.0349823694,1.051978067
7\C,1.4963975772,0.0414065023,0.2786937443\C,1.4589980319,0.0042711032
,-1.1156962348\C,0.1951762476,-0.0404531881,-1.7292410555\C,2.72373376
51,0.0115385436,-1.9430707741\O,-2.1215407814,-0.0204143068,1.06514925
32\C,-2.1191187748,0.0157234004,2.4818296613\H,2.8014621641,-0.8852755
695,-2.5709994032\H,3.6147175654,0.0480782831,-1.3078567087\H,2.761596
1876,0.8774036359,-2.6164653395\H,0.1283555699,-0.0702349486,-2.814969
0431\H,2.4581466789,0.0764990443,0.7860263142\H,0.4084392774,0.0649351
914,2.1329182506\H,-1.9491972466,-0.0822443621,-1.4590389604\H,-1.6054
859504,-0.856463496,2.9085857745\H,-3.1678422911,-0.0006589297,2.78495
54749\H,-1.6465961593,0.9311652665,2.863073396\\Version=IA64L-G03RevC.
02\State=1-A\HF=-386.0887974\RMSD=6.789e-09\RMSF=1.794e-05\Dipole=0.16
94823,0.0144961,0.4220463\PG=C01 [X(C8H10O1)]\\@

n.CH3-C6H4OH
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C7H8O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-C6H4OH
.freq\\0,1\C,-1.2476636726,-0.0702393146,-0.6763194152\C,-1.2487487545
,-0.0043113748,0.7217382411\C,-0.0359789763,0.0658881736,1.4097170004\
C,1.1669497763,0.0696556224,0.6996266378\C,1.1922721651,0.0042653113,-
0.6963002282\C,-0.0399801846,-0.0653638618,-1.3658553815\C,2.494480472
6,0.0062156904,-1.4639031819\O,-2.4643304638,-0.0120096721,1.353901703
9\H,3.3535335979,0.0854515155,-0.7898038762\H,2.5477505078,0.846171527
1,-2.1681313473\H,2.619207491,-0.9123962638,-2.0514958541\H,-0.0541886
181,-0.1167899141,-2.452688234\H,2.1032565564,0.1250341176,1.250428140
8\H,-0.0274577399,0.1179484311,2.4974326954\H,-2.1968954097,-0.1240196
647,-1.2004361761\H,-2.3185476304,0.0380161489,2.3112589846\\Version=I
A64L-G03RevC.02\State=1-A\HF=-346.7822401\RMSD=8.952e-09\RMSF=1.008e-0
5\Dipole=0.3380928,0.0284806,0.3930471\PG=C01 [X(C7H8O1)]\\@

n.CH3-CF2CF3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C3H3F5\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CF2CF3
.freq\\0,1\F,-0.7433845018,0.0994767838,-1.5840848079\C,-0.730369159,0
.0086712347,-0.2210437773\C,0.7498207213,0.0176611661,0.2118993003\C,-
1.507711401,-1.2028987418,0.2334559497\F,-1.2940061948,1.1496085077,0.
2753178389\F,1.3831231775,-1.0611967378,-0.2843751351\F,0.8394943351,-
0.0227653524,1.5543965789\F,1.3743057994,1.117280856,-0.2242547237\H,-

S51

2.5357778998,-1.1088352039,-0.1249989261\H,-1.5079930556,-1.261792782,
1.3243109478\H,-1.0624635518,-2.1116104837,-0.1781786183\\Version=IA64
L-G03RevC.02\State=1-A\HF=-615.3356283\RMSD=3.089e-09\RMSF=8.908e-05\D
ipole=-0.4521327,-0.6190448,0.215737\PG=C01 [X(C3H3F5)]\\@

n.CH3-CF2H
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H4F2\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CF2H.f
req\\0,1\C,0.3168212601,0.0145880806,-0.1794375532\C,0.349943197,0.046
5566125,1.327784024\H,0.8167293845,0.9721733211,1.6765718164\H,-0.6736
607659,-0.0041707023,1.7105835958\H,1.3077378787,0.0615052985,-0.64602
77915\F,-0.4166975612,1.0711553111,-0.6524812193\F,-0.2909667623,-1.13
67475986,-0.6078469306\H,0.9175856719,-0.8060454885,1.711746904\\Versi
on=IA64L-G03RevC.02\State=1-A\HF=-278.3016091\RMSD=7.754e-09\RMSF=5.02
5e-05\Dipole=0.5583501,0.0425574,0.5261017\PG=C01 [X(C2H4F2)]\\@

n.CH3-CF3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H3F3\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CF3.fr
eq\\0,1\F,0.029126865,0.078856162,-1.3603925821\C,0.0143922493,0.02365
93746,-0.009710629\F,1.3004567558,0.0278002594,0.4068650874\C,-0.72436
20108,-1.1911891567,0.4868208096\F,-0.555087546,1.1670885098,0.4329781
101\H,-1.7572072871,-1.1612779732,0.1327454\H,-0.715307047,-1.20315946
37,1.5791611519\H,-0.2381317705,-2.0940882517,0.1103768268\\Version=IA
64L-G03RevC.02\State=1-A\HF=-377.5549316\RMSD=2.542e-09\RMSF=3.766e-05
\Dipole=-0.3934698,-0.647387,0.2644714\PG=C01 [X(C2H3F3)]\\@

n.CH3-CCl2H
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H4Cl2\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CCl2H
.freq\\0,1\C,0.5317915244,-0.0377280063,0.1236991044\C,0.6107708223,-0
.0395155509,1.6375076469\H,1.5101629807,-0.1105488926,-0.3474423091\Cl
,-0.1944835848,1.503122148,-0.4821759479\Cl,-0.4097412616,-1.462214573
4,-0.4736523758\H,1.2115317109,0.8110742497,1.9741120338\H,-0.38735935
54,0.0340498933,2.0765340653\H,1.0821129729,-0.9665426742,1.9786372041
\\Version=IA64L-G03RevC.02\State=1-A\HF=-999.0165063\RMSD=6.693e-09\RM
SF=6.816e-05\Dipole=0.6538226,-0.0441606,0.6070099\PG=C01 [X(C2H4Cl2)]
\\@

n.CH3-CCl3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H3Cl3\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CCl3.
freq\\0,1\C,0.0109801763,0.003029888,0.2529598023\C,0.0732843871,0.019
7009895,1.772199865\Cl,1.6718716277,-0.1726983197,-0.4315163779\Cl,-0.
7133263944,1.5426734429,-0.3523841561\Cl,-1.0038325632,-1.3821151978,-
0.3078924416\H,0.6879726062,0.8604897175,2.1025846922\H,0.5123827621,-
0.9150058782,2.1295219885\H,-0.9360581401,0.1245121649,2.1774158991\\V
ersion=IA64L-G03RevC.02\State=1-A\HF=-1458.5990036\RMSD=3.468e-09\RMSF
=1.238e-04\Dipole=0.0343023,0.0090281,0.7831731\PG=C01 [X(C2H3Cl3)]\\@

n.CH3-CH2Cl
1\1\GINC-AC19\FOpt\RB3LYP\Gen\C2H5Cl1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH2Cl
.freq\\0,1\H,0.152939702,-1.6766343048,-1.1951110927\C,0.1435919935,-1
.6482902457,-0.1015344938\H,1.1777416708,-1.6766340082,0.2541783383\H,
-0.3718289714,-2.5458447524,0.2629232015\C,-0.5788235967,-0.4141291988
,0.4092900091\Cl,0.2261145327,1.1178256213,-0.1598872833\H,-0.58297858
1,-0.3647027667,1.4998849735\H,-1.6084312567,-0.3647030635,0.049675303
8\\Version=IA64L-G03RevC.02\State=1-A'\HF=-539.4262592\RMSD=4.179e-09\
RMSF=4.191e-05\Dipole=-0.3397106,-0.7898793,0.2402117\PG=CS [SG(C2H1Cl
1),X(H4)]\\@

n.CH3-CH2F
1\1\GINC-AC19\FOpt\RB3LYP\Gen\C2H5F1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH2F.f
req\\0,1\C,-0.5965306137,-0.3851921941,0.9846348645\C,-0.347681331,0.1
596739261,-0.4081612519\F,1.0227537398,0.2506683277,-0.6407626222\H,-0
.7793152501,1.1617767341,-0.5278531378\H,-0.7793152046,-0.4951980711,-
1.1760667756\H,-0.1541556111,0.2726100659,1.7398324051\H,-0.1541555396
,-1.3808242827,1.0930037928\H,-1.6725703847,-0.461269784,1.179105642\\
Version=IA64L-G03RevC.02\State=1-A\HF=-179.0564227\RMSD=3.869e-09\RMSF
=9.244e-05\Dipole=-0.6467537,-0.0706048,0.1804812\PG=C01 [X(C2H5F1)]\\
@

n.CH3-CH2OH
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C2H6O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH2OH.

freq\\0,1\C,-0.4129563554,0.0000000097,-1.1721226719\C,-0.4336937028,-
0.0000000474,0.3474741898\O,0.9172385285,0.0000000442,0.8013387676\H,0
.109161998,0.8868592504,-1.5460133939\H,0.1091621401,-0.8868591199,-1.
5460134587\H,-1.4328551688,-0.0000000573,-1.5725072617\H,-0.9744341204
,-0.8875625033,0.7156739292\H,-0.9744342627,0.8875622949,0.7156739941\
H,0.9053915348,0.0000000078,1.770366943\\Version=IA64L-G03RevC.02\Stat
e=1-A'\HF=-155.0337992\RMSD=1.846e-09\RMSF=3.755e-05\Dipole=-0.475568,
0.,0.3898336\PG=CS [SG(C2H2O1),X(H4)]\\@

n.CH3-CH2Ph
1\1\GINC-SC122\FOpt\RB3LYP\6-31G(d)\C8H10\MLC501\11-Sep-2002\0\\#P B3L
YP/6-31G(D) FOPT=(MAXCYC=100) FREQ MAXDISK=52428800 SCF=(TIGHT,MAXCYC=
100) GEOM=CHECK\\etbz-cs-6drb3\\0,1\C,-2.2284396309,1.7737516665,0.\C,
-0.6937105063,1.8926699354,0.\C,0.,0.546181554,0.\C,0.3118254669,-0.10
23160492,1.2026834225\C,0.3118254669,-0.1023160492,-1.2026834225\C,0.9
132220777,-1.3616103083,1.2059190433\C,0.9132220777,-1.3616103083,-1.2
059190433\C,1.2153222385,-1.9966792384,0.\H,1.6863498799,-2.976105526,
0.\H,1.150067146,-1.8447129978,2.1505767223\H,1.150067146,-1.844712997
8,-2.1505767223\H,0.0837929653,0.387950677,2.1471919348\H,0.0837929653
,0.387950677,-2.1471919348\H,-0.3779096411,2.4687487917,-0.8791267801\
H,-0.3779096411,2.4687487917,0.8791267801\H,-2.5794995785,1.2298765659
,0.8842051352\H,-2.5794995785,1.2298765659,-0.8842051352\H,-2.69885480
66,2.7639522374,0.\\Version=DEC-AXP-OSF/1-G98RevA.11.3\State=1-A'\HF=-
310.8802404\RMSD=5.588e-09\RMSF=2.772e-06\Dipole=-0.0632775,0.0900445,
0.\PG=CS [SG(C4H2),X(C4H8)]\\@

n.CH3-CH_CH2_2
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H8\CYL509\14-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH_CH2_2
.freq\\0,1\C,-0.9069040941,-0.355602893,-0.7482824075\C,-0.8972401886,
-0.3470834824,0.7633143755\C,0.4046838034,-0.3445871529,-0.0009189447\
C,1.2845391857,0.8875220518,-0.0127549402\H,1.9351920314,0.9231729204,
0.8701345955\H,0.6784090887,1.8017382783,-0.013879115\H,1.9254396361,0
.9136462762,-0.9028982028\H,0.9512181151,-1.2869214215,0.0008418546\H,
-1.1908547276,0.5702536364,1.2684892494\H,-1.1933206441,-1.2525206468,
1.2865583382\H,-1.2068330634,0.5560140287,-1.2600559969\H,-1.209722674
9,-1.2668742122,-1.2573392218\\Version=IA64L-G03RevC.02\State=1-A\HF=-
157.2120142\RMSD=3.216e-09\RMSF=5.218e-05\Dipole=0.0408506,-0.0105918,
-0.0001185\PG=C01 [X(C4H8)]\\@

n.CH3-CH2CH=CH2
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C4H8\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH2CH=CH
2.freq\\0,1\H,0.2104087115,-1.5083209749,-1.441292261\C,0.3119965082,-
1.7049522569,-0.3682921263\H,1.3821949935,-1.7971787767,-0.1468568848\
H,-0.1581677346,-2.6709489982,-0.1519805649\C,-0.3314799566,-0.5796468
885,0.4599017926\C,0.3158179096,0.7584943927,0.2252240637\H,-0.2532648
32,-0.8383442948,1.526658146\H,-1.4030697738,-0.5148252156,0.232286344
7\H,1.3814476627,0.8148946385,0.4576315215\C,-0.3004810895,1.842669242
2,-0.2468437574\H,0.2255531064,2.7812206181,-0.4009085113\H,-1.3602223
639,1.834116066,-0.4954776251\\Version=IA64L-G03RevC.02\State=1-A\HF=-
157.2210723\RMSD=3.477e-09\RMSF=7.498e-06\Dipole=0.0201067,-0.1254964,
0.0373354\PG=C01 [X(C4H8)]\\@

n.CH3-CH2CH3
1\1\GINC-AC18\FOpt\RB3LYP\Gen\C3H8\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH2CH3.f
req\\0,1\H,0.3433093172,-0.3757188915,-2.1473334273\C,0.3586489515,-0.
6325608865,-1.0817319361\H,1.3957339377,-0.8657222481,-0.8098130521\H,
-0.2301997608,-1.5489412973,-0.9507199756\C,-0.1946819459,0.5071097342
,-0.2203283523\H,0.3923630535,1.4180693686,-0.3997896001\C,-0.18613778
63,0.1830190752,1.2770282005\H,-1.2205001888,0.7392505519,-0.537344938
1\H,0.8321376706,-0.0200527907,1.6315662818\H,-0.7931697188,-0.7051248
961,1.4927533205\H,-0.5866496266,1.0128326658,1.8708739179\\Version=IA
64L-G03RevC.02\State=1-A\HF=-119.1442428\RMSD=4.751e-09\RMSF=2.528e-05
\Dipole=-0.00723,0.0188855,-0.0082204\PG=C01 [X(C3H8)]\\@

n.CH3-CH_CH3_2
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH_CH3_
2.freq\\0,1\C,-0.8154522391,1.2088090314,0.141554704\H,-0.5537675912,1
.4205163378,1.1867798271\H,-1.9052971282,1.0989818085,0.0877526865\H,-
0.5364641997,2.0858347908,-0.4548637092\C,-0.100461725,-0.0558427644,-
0.3548862041\C,1.4240519283,0.1219811794,-0.3216646\H,-0.3969292358,-0
.220520761,-1.40179813\C,-0.5311159233,-1.2877423315,0.4537541585\H,-0
.0486911679,-2.1992763073,0.0808136495\H,-1.6163484951,-1.4382240336,0
.405292065\H,-0.2578235347,-1.1756708207,1.5113624215\H,1.938531212,-0

.7665017775,-0.7071864067\H,1.7752251033,0.2903716972,0.7050219206\H,1
.7394327916,0.9812583762,-0.9257226751\\Version=IA64L-G03RevC.02\State
=1-A\HF=-158.4588096\RMSD=1.754e-09\RMSF=1.705e-05\Dipole=-0.0090381,-
0.0050283,-0.0319434\PG=C01 [X(C4H10)]\\@

n.CH3-C_CH3_3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C5H12\CYL509\05-Apr-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-C_CH3_3
.freq\\0,1\C,-0.2605458925,-0.5530850164,1.4138431575\C,0.0000101688,0
.0000013458,0.0000093653\C,-0.628822628,1.400374715,-0.1274461111\C,-0
.6288254906,-0.9421644505,-1.0438605495\H,0.1767545644,0.0982977292,2.
1807467753\H,0.1765678042,-1.5520408016,1.5350661155\H,-1.3359455426,-
0.6321275361,1.6161825135\C,1.5181947246,0.0948794909,-0.2425431865\H,
-0.1997405863,-1.9497087146,-0.9773913938\H,-0.4593225663,-0.573401587
8,-2.0631518804\H,-1.7124155395,-1.0300706297,-0.8962253071\H,1.994953
2099,0.7608965147,0.4873892977\H,1.7355089002,0.4865177741,-1.24407525
08\H,1.9950346124,-0.8895779284,-0.157984684\H,-0.1997954786,2.0952547
737,0.6051832325\H,-1.7124115163,1.3646650729,0.0405791793\H,-0.459253
1559,1.8212588254,-1.1263346518\\Version=IA64L-G03RevC.02\State=1-A\HF
=-197.7729779\RMSD=3.533e-09\RMSF=1.210e-05\Dipole=-0.0000044,-0.00000
37,0.0000067\PG=C01 [X(C5H12)]\\@

n.CH3-CCH
1\1\GINC-AC2\FOpt\RB3LYP\Gen\C3H4\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CCH.freq\
\0,1\C,0.4457552152,0.2225294111,1.1369810945\H,1.5288718374,0.3918758
605,1.1119682126\H,0.2562425832,-0.622343289,1.8098143395\H,-0.0201646
545,1.1114055542,1.5788489484\C,-0.0788363392,-0.0392700264,-0.2004234
436\C,-0.5119842433,-0.2556345702,-1.3062159844\H,-0.8945575624,-0.446
6870126,-2.282681499\\Version=IA64L-G03RevC.02\State=1-A\HF=-116.65326
93\RMSD=2.169e-09\RMSF=1.499e-05\Dipole=0.0971577,0.0484488,0.2473448\
PG=C01 [X(C3H4)]\\@

n.CH3-CH=C_CH3_2
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H10\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH=C_CH
3_2.freq\\0,1\C,-0.4149566233,0.4394676962,2.0285066869\H,0.6553930442
,0.6136195718,2.1676045371\H,-0.7200766483,-0.3398884641,2.7405527152\
H,-0.9422717814,1.3561076889,2.327161991\C,-0.7752677503,0.049504578,0
.6222756597\C,0.0323179519,-0.1025493371,-0.4383453808\H,-1.840320066,
-0.1290862454,0.4640912058\C,1.5280935621,0.0984304422,-0.4213755554\C
,-0.5275061873,-0.5036856416,-1.7831507047\H,-0.0789961363,-1.44350132
,-2.1357091316\H,-0.3021929344,0.2525643843,-2.548682263\H,-1.61335307
97,-0.6385583501,-1.7502999777\H,1.8233886782,0.8744388098,-1.14159846
35\H,2.0464863825,-0.8208107435,-0.7285322611\H,1.9158568229,0.3881082
421,0.5579474133\\Version=IA64L-G03RevC.02\State=1-A\HF=-196.5435771\R
MSD=5.092e-09\RMSF=7.881e-06\Dipole=0.0676068,0.0051303,-0.0157486\PG=
C01 [X(C5H10)]\\@

n.CH3-CH=CH2
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H6\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH=CH2.f
req\\0,1\C,0.041981285,0.2345551139,1.2227682436\H,1.1336755235,0.3128
042826,1.2625753495\H,-0.2693715704,-0.5507246578,1.9250050389\H,-0.38
14858116,1.1759665191,1.5982544835\C,-0.4392576508,-0.0604143514,-0.16
90868163\C,0.3432749945,-0.2125278429,-1.2377783683\H,-1.5198236356,-0
.1528463678,-0.2899559369\H,1.4264612508,-0.1294512662,-1.1692799408\H
,-0.0654475296,-0.4254260272,-2.2220173487\\Version=IA64L-G03RevC.02\S
tate=1-A\HF=-117.9075585\RMSD=7.366e-09\RMSF=3.818e-05\Dipole=-0.04674
48,0.0216798,0.1299055\PG=C01 [X(C3H6)]\\@

n.CH3-CH=CHCH3
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H8\CYL509\07-Apr-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH=CHCH3
.freq\\0,1\C,0.1270540134,0.4006759751,1.9196455786\H,1.1902174935,0.1
513307189,2.007054982\H,-0.4274730333,-0.2285090106,2.6294287839\H,-0.
0053934852,1.4391162808,2.2531929576\C,-0.3700147986,0.2095373485,0.51
48570174\C,0.3698982794,-0.2098618659,-0.5147682465\H,-1.4241222579,0.
4379319115,0.3432992776\H,1.4240829189,-0.4378945612,-0.3432497565\C,-
0.1269876328,-0.4005254188,-1.9196877366\H,0.4277172345,0.2288627194,-
2.6291401884\H,-1.190086875,-0.1509392593,-2.0072781579\H,0.0053588353
,-1.4388550329,-2.2535875754\\Version=IA64L-G03RevC.02\State=1-A\HF=-1
57.2269102\RMSD=2.250e-09\RMSF=7.872e-06\Dipole=0.0000461,0.0001996,-0
.0000533\PG=C01 [X(C4H8)]\\@

n.CH3-CHO
1\1\GINC-AC18\FOpt\RB3LYP\Gen\C2H4O1\CYL509\05-Apr-2008\0\\#B3LYP/GEN

S54

6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CHO.fr
eq\\0,1\C,0.0526477067,0.2645017475,1.1492676754\H,1.1415237494,0.3252
469362,1.2110074148\H,-0.3209206199,-0.4967545375,1.8468769331\H,-0.39
45072797,1.2194465372,1.4556458105\C,-0.378866289,-0.0743253817,-0.255
7156299\O,0.3765116046,-0.2544258868,-1.1844050461\H,-1.4808771926,-0.
1535900364,-0.3996020622\\Version=IA64L-G03RevC.02\State=1-A\HF=-153.8
301199\RMSD=4.014e-09\RMSF=1.754e-05\Dipole=-0.4918775,0.1838219,0.896
6509\PG=C01 [X(C2H4O1)]\\@

n.CH3-CN
1\1\GINC-AC18\FOpt\RB3LYP\Gen\C2H3N1\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CN.fre
q\\0,1\C,0.3997362777,0.2014618411,1.0925484639\H,1.4930422859,0.25515
96826,1.0937030381\H,0.0891175623,-0.6038364438,1.7657598013\H,0.00339
49205,1.1477755687,1.4741328926\C,-0.0949412412,-0.0478491403,-0.25949
08519\N,-0.4877607125,-0.2458250017,-1.3331344862\\Version=IA64L-G03Re
vC.02\State=1-A1\HF=-132.7549292\RMSD=7.634e-09\RMSF=7.263e-05\Dipole=
0.5079392,0.2559947,1.3882858\PG=C03V [C3(C1C1N1),3SGV(H1)]\\@

n.CH3-COCH3
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C3H6O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COCH3.
freq\\0,1\C,-0.1148826767,-0.051284736,-1.4262472258\C,-0.1578277899,-
0.0260899841,0.0935274626\C,1.1621393328,0.2244214847,0.8056533694\O,-
1.1932497837,-0.1972727831,0.7071077152\H,-1.1150494767,-0.2379135844,
-1.8221363055\H,0.5714031133,-0.8317436189,-1.7786034804\H,0.262645811
1,0.902521121,-1.8160973232\H,1.5873261758,1.1886057613,0.4993478654\H
,1.0068092941,0.2200565354,1.8862761447\H,1.8962901554,-0.545624537,0.
5367497397\\Version=IA64L-G03RevC.02\State=1-A\HF=-193.1556928\RMSD=4.
732e-09\RMSF=1.816e-06\Dipole=0.9434492,0.1559708,-0.5590769\PG=C01 [X
(C3H6O1)]\\@

n.CH3-CON_CH2CH3_2
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C6H13N1O1\CYL509\07-Apr-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CON
_CH2CH3_2.freq\\0,1\C,-1.434751685,1.5048996524,-1.0552379586\H,-1.601
1983621,1.8082363541,-2.0895225519\H,-1.2297671723,2.4024145018,-0.459
0413928\H,-2.3477579782,1.0445913859,-0.6631414873\C,-0.2423285737,0.5
536524069,-1.0500258576\O,0.4332614086,0.3884567909,-2.0626829602\N,0.
05004452,-0.1009087866,0.1226837777\C,-0.6836991332,0.0700804237,1.375
5131245\C,1.1976480271,-1.0153601091,0.1266079735\H,0.0465777637,0.065
0388117,2.194442999\C,-1.7446196049,-1.0098831986,1.6210996892\H,-1.14
69872691,1.0595767081,1.3907516337\H,1.247368384,-1.48771385,-0.856653
0045\H,0.999543169,-1.7979971486,0.8679220209\C,2.5220709141,-0.309700
6992,0.4305965222\H,-2.5131451457,-0.9908143148,0.8408120777\H,-2.2340
968336,-0.8529646087,2.5894538355\H,-1.2981262523,-2.0101726126,1.6267
88343\H,2.7342074793,0.434172246,-0.3426129627\H,3.3455809071,-1.03325
07661,0.4485971277\H,2.4954787347,0.195459615,1.4035596399\\Version=IA
64L-G03RevC.02\State=1-A\HF=-366.4618066\RMSD=3.612e-09\RMSF=4.242e-06
\Dipole=-0.536923,-0.0516932,1.3464833\PG=C01 [X(C6H13N1O1)]\\@

n.CH3-CON_CH3_2
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C4H9N1O1\CYL509\07-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CON_
CH3_2.freq\\0,1\H,-1.3506656664,1.4996474101,-1.6016687142\C,-1.502762
6077,0.8796119124,-0.7077321736\N,-0.2269643951,0.5503371077,-0.090792
7956\H,-1.9973980168,-0.0493648329,-0.9875246976\H,-2.1377139038,1.438
3649008,-0.0067828291\C,0.133284009,-0.7734330839,0.0360187592\O,-0.59
07829824,-1.682653515,-0.356338481\C,1.4779439039,-1.0815307811,0.6877
140023\H,1.5860387385,-2.1664101357,0.6992900737\H,1.5320723694,-0.709
7611048,1.7172491814\H,2.3156963713,-0.6486291028,0.1292758544\C,0.566
001743,1.684927611,0.3441663703\H,0.8007224123,2.3423985542,-0.5050635
305\H,1.5038469786,1.3639514929,0.7946517379\H,0.0156130523,2.28121723
36,1.0858285916\\Version=IA64L-G03RevC.02\State=1-A\HF=-287.830206\RMS
D=2.908e-09\RMSF=4.528e-05\Dipole=0.5948392,1.2651447,0.3422538\PG=C01
 [X(C4H9N1O1)]\\@

n.CH3-CONH2
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C2H5N1O1\CYL509\08-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CONH
2.freq\\0,1\C,-0.1520840434,-0.0417695178,-1.3983386089\C,-0.109019234
9,-0.027394312,0.1241614881\N,1.1228379041,0.2119941621,0.6738998618\O
,-1.1023992949,-0.2170071156,0.8086012197\H,-0.6917611699,0.8455434296
,-1.7467178144\H,0.8366966321,-0.0587203322,-1.8674331765\H,-0.7187452
073,-0.9181983285,-1.7230589281\H,1.1783740817,0.3201686199,1.67707821
39\H,1.9213843641,0.47828738,0.1190861682\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-209.212201\RMSD=7.638e-09\RMSF=1.076e-05\Dipole=1.2982588,

0.400104,-0.5345889\PG=C01 [X(C2H5N1O1)]]\\@

n.CH3-CONHCH3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C3H7N1O1\CYL509\05-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CONH
CH3.freq\\0,1\C,0.2176547273,0.438257633,0.1497100573\O,1.3677712313,0
.4117585396,-0.270152217\C,-0.3160287937,1.6196078296,0.9488245586\H,0
.3085212794,1.7539374875,1.8373048108\H,-1.3597093097,1.5116820151,1.2
618916581\H,-0.2194646293,2.5260121248,0.3433314892\N,-0.6769370859,-0
.576853112,-0.0590302447\H,-1.6091930831,-0.4870244442,0.316410178\C,-
0.3374540549,-1.7775261456,-0.7997660068\H,0.7022382826,-1.6772188025,
-1.1147236619\H,-0.972132006,-1.8919449557,-1.6869244232\H,-0.43890205
45,-2.6735758603,-0.1754722569\\Version=IA64L-G03RevC.02\State=1-A\HF=
-248.5235631\RMSD=2.265e-09\RMSF=2.373e-06\Dipole=-1.3629116,-0.286514
1,0.332993\PG=C01 [X(C3H7N1O1)]]\\@

n.CH3-COOC_CH3_3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H12O2\CYL509\07-Apr-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COOC_
CH3_3.freq\\0,1\C,-2.5979884745,0.7722157134,-0.5521020849\H,-2.982917
4026,1.2816945487,-1.4362155178\H,-2.8051368384,1.3692237887,0.3421207
78\H,-3.1053065869,-0.1898571463,-0.4256005553\C,-1.1057657938,0.55960
032,-0.70374185\O,-0.4586196266,0.9102641421,-1.668340535\O,-0.6165819
463,-0.0707781962,0.3845417738\C,0.8143437937,-0.4081667263,0.51021722
76\C,1.2240767838,-1.3782743401,-0.603064805\C,0.875626538,-1.09367587
97,1.8776310447\C,1.6572034423,0.8716633152,0.5054641371\H,1.903099735
9,-1.4008316139,2.0997680251\H,0.2367023333,-1.9826333495,1.8936273445
\H,0.5386262183,-0.4135634303,2.666680424\H,2.2513448143,-1.7195958814
,-0.4319287316\H,1.1722260857,-0.9003044526,-1.5824694579\H,0.57032914
47,-2.2575040633,-0.6016555369\H,2.7023341083,0.6229040076,0.722008739
9\H,1.3057387831,1.5619492505,1.2803215526\H,1.6095704501,1.3724563592
,-0.4626889912\\Version=IA64L-G03RevC.02\State=1-A\HF=-386.3389759\RMS
D=6.669e-09\RMSF=2.249e-06\Dipole=-0.0684515,-0.3169678,0.6701415\PG=C
01 [X(C6H12O2)]]\\@

n.CH3-COOCH2CH3
1\1\GINC-AC22\FOpt\RB3LYP\Gen\C4H8O2\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COOCH2
CH3.freq\\0,1\C,-1.9943537601,0.9794386963,-0.6551195229\H,-2.28392359
47,1.4121680137,-1.6132382128\H,-2.0759179555,1.7340181348,0.134179473
\H,-2.6742542114,0.1613658368,-0.3952530826\C,-0.5743080426,0.46863067
01,-0.742579783\O,0.1365411801,0.5281317178,-1.721952338\O,-0.18568585
69,-0.0754797744,0.4336604659\C,1.1611474766,-0.6004301239,0.470898073
9\H,1.8612408175,0.2054043642,0.2274414124\H,1.2624372471,-1.368624433
2,-0.302669472\C,1.3951504366,-1.1580859423,1.8623620077\H,2.408735594
6,-1.5676390385,1.9333946202\H,0.6834889024,-1.9588057222,2.0880951682
\H,1.2855339522,-0.3764225036,2.6210204154\\Version=IA64L-G03RevC.02\S
tate=1-A\HF=-307.7074381\RMSD=3.499e-09\RMSF=4.611e-06\Dipole=-0.19106
24,-0.1724817,0.7278301\PG=C01 [X(C4H8O2)]]\\@

n.CH3-COOCH3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C3H6O2\CYL509\05-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COOCH3
.freq\\0,1\C,0.1371807364,0.4736397932,0.0261577628\O,1.3331103026,0.4
178588566,-0.1563999345\C,-0.6612560761,1.7333439688,0.2681254709\H,0.
0071127132,2.5947643499,0.2531176199\H,-1.1729278978,1.67565631,1.2344
603929\H,-1.4311728766,1.845662632,-0.5022820661\O,-0.6677619397,-0.61
53524795,0.0384613066\C,-0.0043814533,-1.8700665236,-0.1829610357\H,0.
4875942196,-1.8789309425,-1.159383319\H,-0.7882610642,-2.6271506958,-0
.1420939568\H,0.7455587607,-2.0515561008,0.5917571653\\Version=IA64L-G
03RevC.02\State=1-A\HF=-268.3884841\RMSD=2.436e-09\RMSF=4.276e-06\Dipo
le=-0.6635005,-0.209278,0.0777448\PG=C01 [X(C3H6O2)]]\\@

n.CH3-COOH
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C2H4O2\CYL509\07-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COOH.f
req\\0,1\C,0.1477553891,-0.0220613277,-1.3937290281\C,0.1047512295,0.0
228743191,0.1130819925\O,1.0450278752,0.2190442596,0.8491361639\O,-1.1
537188103,-0.1886646792,0.5792324961\H,1.1687503505,0.1508194609,-1.73
43002485\H,-0.5196475414,0.7393537646,-1.8105777555\H,-0.2057094253,-0
.9952746054,-1.7498981231\H,-1.0889056142,-0.1428132121,1.5516604609\\
Version=IA64L-G03RevC.02\State=1-A\HF=-229.0817862\RMSD=5.739e-09\RMSF
=6.377e-05\Dipole=-0.5173375,-0.1051791,-0.327732\PG=C01 [X(C2H4O2)]\\
@

n.CH3-COPh
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H8O1\CYL509\07-Apr-2008\0\\#B3LYP/GEN

6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-COPh.f
req\\0,1\C,-2.2694230452,-0.0069540121,-0.1014754516\C,-2.2482417085,-
0.004016837,1.296707005\C,-1.0286767692,0.0010397892,1.9759337751\C,0.
1684845258,0.003154631,1.2601502514\C,0.1570106677,0.0002451211,-0.142
7835137\C,-1.075347392,-0.004832089,-0.8153076231\C,1.4117626688,0.002
3461437,-0.9644405608\O,1.3571956036,-0.000463673,-2.1850659197\C,2.75
61707459,0.0074575057,-0.2542581648\H,3.5472731402,0.007988802,-1.0058
832877\H,2.8671119022,-0.8741495209,0.3883847376\H,2.8623649221,0.8923
917285,0.3846039877\H,-1.066530938,-0.0070203659,-1.9003602372\H,1.110
2131661,0.0070851729,1.8004137369\H,-1.0094383151,0.0033360705,3.06233
03922\H,-3.218269913,-0.0108946644,-0.6311079883\H,-3.1807269532,-0.00
56693536,1.8549917111\\Version=IA64L-G03RevC.02\State=1-A\HF=-384.8959
85\RMSD=6.742e-09\RMSF=4.050e-05\Dipole=-0.2248787,0.0017239,1.1578317
\PG=C01 [X(C8H8O1)]\\@

n.H-H
1\1\GINC-AC9\FOpt\RB3LYP\Gen\H2\CYL509\20-Jun-2008\0\\#B3LYP/GEN 6D IN
T(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.H.freq\\0,1\H
,0.,0.,-0.3715996858\H,0.,0.,0.3715996858\\Version=IA64L-G03RevC.02\St
ate=1-SGG\HF=-1.1754823\RMSD=2.224e-12\RMSF=1.693e-04\Dipole=0.,0.,0.\
PG=D*H [C*(H1.H1)]\\@

n.BH2-BH2
1\1\GINC-AC18\FOpt\RB3LYP\Gen\B2H4\CYL509\20-Aug-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.BH2.freq\\
0,1\B,-0.2640697042,-0.2132308244,-0.7467782146\H,0.4902352337,-0.4582
650407,-1.648426577\H,-1.4315992257,-0.3021519747,-1.0131623925\B,0.26
42276177,0.2132672263,0.7467119039\H,0.4577319411,1.35724163,1.0563419
292\H,0.4828424833,-0.5970066242,1.6055785939\\Version=IA64L-G03RevC.0
2\State=1-A\HF=-52.0444634\RMSD=4.189e-09\RMSF=2.581e-05\Dipole=0.0002
2,0.0000571,-0.000094\PG=C01 [X(B2H4)]\\@

n.CH3-CH3
1\1\GINC-LC111\FOpt\RB3LYP\Gen\C2H6\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH3.freq\
\0,1\C,-0.2797944899,0.582477219,0.4099745318\H,0.3149526622,1.4922966
127,0.2681758199\H,-0.2804581568,0.3521695162,1.4816835545\H,-1.311611
9612,0.8142391972,0.1214572411\C,0.2797944899,-0.582477219,-0.40997453
18\H,-0.3149526622,-1.4922966127,-0.2681758199\H,0.2804581568,-0.35216
95162,-1.4816835545\H,1.3116119612,-0.8142391972,-0.1214572411\\Versio
n=IA32L-G03RevC.02\State=1-AG\HF=-79.8304207\RMSD=1.686e-09\RMSF=4.666
e-06\Dipole=0.,0.,0.\PG=CI [X(C2H6)]\\@

n.NH2-NH2
1\1\GINC-AC9\FOpt\RB3LYP\Gen\H4N2\CYL509\25-Sep-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.NH2-NH2.fre
q\\0,1\N,0.,0.7183,-0.0775\N,0.,-0.7183,-0.0775\H,-0.2128,1.0984,0.847
\H,0.2128,-1.0984,0.847\H,0.9477,1.0101,-0.3045\H,-0.9477,-1.0101,-0.3
045\\Version=IA64L-G03RevC.02\State=1-A\HF=-111.8564475\RMSD=2.140e-09
\RMSF=4.550e-05\Dipole=0.,0.,0.8652721\PG=C02 [X(H4N2)]\\@

n.OH-OH
1\1\GINC-AC30\FOpt\RB3LYP\Gen\H2O2\CYL509\20-Aug-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.OH.freq\\0
,1\O,-0.0864926865,-0.0303245407,0.7245153407\H,0.5776459034,0.6420062
552,0.9587958739\O,-0.0191992984,0.0564723967,-0.7278497763\H,0.267889
9758,-0.8511891037,-0.9321203892\\Version=IA64L-G03RevC.02\State=1-A\H
F=-151.5332132\RMSD=1.828e-09\RMSF=1.646e-04\Dipole=0.6805144,-0.16835
71,0.0214693\PG=C02 [X(H2O2)]\\@

n.F-F
1\1\GINC-LC84\FOpt\RB3LYP\Gen\F2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D I
NT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.F.freq\\0,1\
F,-0.2515095499,0.537876976,0.3735274133\F,0.2515095499,-0.537876976,-
0.3735274133\\Version=IA32L-G03RevC.02\State=1-SGG\HF=-199.4982522\RMS
D=3.458e-10\RMSF=2.712e-06\Dipole=0.,0.,0.\PG=D*H [C*(F1.F1)]\\@

n.SiH3-SiH3
1\1\GINC-LC19\FOpt\RB3LYP\Gen\H6Si2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SiH3.freq
\\0,1\Si,-0.5537405154,0.959105483,0.3915531646\H,-1.9625449383,0.9853
473145,-0.0904345424\H,-0.568877824,0.9853724996,1.8804492628\H,0.1279
062605,2.1922875713,-0.0904741119\Si,0.5537405154,-0.959105483,-0.3915
531646\H,1.9625449383,-0.9853473145,0.0904345424\H,0.568877824,-0.9853
724996,-1.8804492628\H,-0.1279062605,-2.1922875713,0.0904741119\\Versi
on=IA32L-G03RevC.02\State=1-A1G\HF=-582.5827312\RMSD=4.260e-09\RMSF=8.
078e-05\Dipole=0.,0.,0.\PG=D03D [C3(Si1.Si1),3SGD(H2)]\\@

n.PH2-PH2
1\1\GINC-LC86\FOpt\RB3LYP\Gen\H4P2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.PH2.freq\\
0,1\P,0.5638470058,-0.9404559261,-0.2880261799\H,-0.5665342781,-1.5578
466871,-0.900768818\H,1.022505596,-0.4121128669,-1.5309506477\P,-0.563
8470058,0.9404559261,0.2880261799\H,0.5665342781,1.5578466871,0.900768
818\H,-1.022505596,0.4121128669,1.5309506477\\Version=IA32L-G03RevC.02
\State=1-AG\HF=-685.0949308\RMSD=1.561e-09\RMSF=1.269e-05\Dipole=0.,0.
,0.\PG=CI [X(H4P2)]\\@

n.SH-SH
1\1\GINC-AC28\FOpt\RB3LYP\Gen\H2S2\CYL509\22-Aug-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.SH.fail.fr
eq\\0,1\S,-0.0828112793,0.0292709984,1.0467406361\H,1.0530734042,0.731
0920402,1.2764501557\S,-0.0245688532,-0.0027055001,-1.0501283304\H,0.6
650087157,-1.1561400133,-1.2222470469\\Version=IA64L-G03RevC.02\State=
1-A\HF=-797.5717827\RMSD=2.877e-09\RMSF=1.901e-05\Dipole=0.5765659,-0.
1426405,0.0181899\PG=C02 [X(H2S2)]\\@

n.Cl-Cl
1\1\GINC-LC84\FOpt\RB3LYP\Gen\Cl2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Cl.freq\\0,
1\Cl,0.,0.,-1.0208438617\Cl,0.,0.,1.0208438617\\Version=IA32L-G03RevC.
02\State=1-SGG\HF=-920.3498788\RMSD=4.545e-09\RMSF=1.560e-05\Dipole=0.
,0.,0.\PG=D*H [C*(Cl1.Cl1)]\\@

n.Br-Br
1\1\GINC-LC104\FOpt\RB3LYP\Gen\Br2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Br.freq\\0
,1\Br,-0.4210408625,0.8888002597,0.6212577354\Br,0.4210408625,-0.88880
02597,-0.6212577354\\Version=IA32L-G03RevC.02\State=1-SGG\HF=-5147.754
7515\RMSD=1.117e-09\RMSF=8.857e-08\Dipole=0.,0.,0.\PG=D*H [C*(Br1.Br1)
]\\@

n.N_CH3_2-N_CH3_2
1\1\GINC-LC122\FOpt\RB3LYP\Gen\C4H12N2\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.N_CH3_
2.freq\\0,1\C,0.2745095964,-0.3243607972,1.7950223157\H,1.3639340675,-
0.3385478236,1.8700600706\H,-0.1028054762,-1.1287606194,2.4322385555\H
,-0.0978669624,0.6412926606,2.180036082\N,-0.163610616,-0.5908880685,0
.420844486\C,-1.6199341065,-0.764240349,0.4408305951\H,-1.858443849,-1
.5367037513,1.1769565135\H,-1.9872164119,-1.1162913389,-0.5255241872\H
,-2.1546929469,0.1636102634,0.7101068471\C,-0.2745095964,0.3243607972,
-1.7950223157\H,-1.3639340675,0.3385478236,-1.8700600706\H,0.102805476
2,1.1287606194,-2.4322385555\H,0.0978669624,-0.6412926606,-2.180036082
\N,0.163610616,0.5908880685,-0.420844486\C,1.6199341065,0.764240349,-0
.4408305951\H,1.858443849,1.5367037513,-1.1769565135\H,1.9872164119,1.
1162913389,0.5255241872\H,2.1546929469,-0.1636102634,-0.7101068471\\Ve
rsion=IA32L-G03RevC.02\State=1-AG\HF=-269.090437\RMSD=6.906e-09\RMSF=3
.936e-05\Dipole=0.,0.,0.\PG=CI [X(C4H12N2)]\\@

n.NHCH3-NHCH3
1\1\GINC-LC109\FOpt\RB3LYP\Gen\C2H8N2\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCH3.f
req\\0,1\N,-0.1726090381,-0.2588896412,-0.6688151058\C,-1.632365693,-0
.2987841936,-0.7752785845\H,-2.0191250411,-1.1118385396,-0.1482060441\
H,-1.8973666016,-0.5272620392,-1.8126590391\H,-2.1248234705,0.63677528
68,-0.466072443\H,0.1421111887,0.4885885265,-1.2920599315\N,0.17260903
81,0.2588896412,0.6688151058\C,1.632365693,0.2987841936,0.7752785845\H
,2.0191250411,1.1118385396,0.1482060441\H,1.8973666016,0.5272620392,1.
8126590391\H,2.1248234705,-0.6367752868,0.466072443\H,-0.1421111887,-0
.4885885265,1.2920599315\\Version=IA32L-G03RevC.02\State=1-AG\HF=-190.
4760079\RMSD=7.481e-09\RMSF=6.101e-05\Dipole=0.,0.,0.\PG=CI [X(C2H8N2)
]\\@

n.NHCHO-NHCHO
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C2H4N2O2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCHO.
freq\\0,1\N,-0.931188354,0.5403009491,-0.1755771394\H,-1.8168879508,0.
0592565728,-0.274425333\C,-0.200331623,0.8306296877,-1.3111166293\O,0.
9730715398,1.1299828746,-1.3141719276\H,-0.8437115815,0.8187359904,-2.
2116139823\N,-0.2694987893,0.287928426,1.0170161437\H,0.1234302935,1.1
088686744,1.4612016406\C,0.3483491678,-0.9326920773,1.2073827818\O,0.1
602307009,-1.9117506781,0.5199583904\H,0.9874560479,-0.9179500976,2.11
08760269\\Version=IA64L-G03RevC.02\State=1-A\HF=-338.5407411\RMSD=4.03
0e-09\RMSF=1.090e-04\Dipole=-0.9769546,0.6739267,0.6846318\PG=C01 [X(C

2H4N2O2)]\\@

n.NHCOCH3-NHCOCH3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4H8N2O2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCOCH
3.freq\\0,1\N,-0.5751211114,-0.745458936,-0.7098356538\H,-1.5823764353
,-0.7982557362,-0.6236097473\C,-0.0344473816,0.2622075381,-1.505719578
9\O,1.1215376292,0.6217052597,-1.3811675114\C,-0.9887449605,0.81322209
61,-2.5473991694\H,-0.4240106675,1.0693941784,-3.4460314236\H,-1.44349
55651,1.7311995532,-2.1570635029\H,-1.7890215265,0.1121143646,-2.80458
02173\N,0.0881797106,-1.0797266707,0.4655925913\H,0.9436026499,-1.5961
165095,0.303169488\C,0.0596564774,-0.1676198853,1.5184055261\O,-0.7609
577309,0.7300062921,1.562099792\C,1.0909720351,-0.43021621,2.598604237
4\H,1.9617892145,0.2103916988,2.4165447062\H,0.6668567904,-0.159680986
6,3.5676347997\H,1.4259891369,-1.4720009637,2.6228329979\\Version=IA64
L-G03RevC.02\State=1-A\HF=-417.1908706\RMSD=4.281e-09\RMSF=6.072e-06\D
ipole=-0.2635788,-0.988108,-0.1322731\PG=C01 [X(C4H8N2O2)]\\@

n.NO2-NO2
1\1\GINC-LC22\FOpt\RB3LYP\Gen\N2O4\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NO2.freq\\
0,1\N,-0.3708249212,0.648999639,0.4828806765\O,0.4295845941,1.44736082
35,0.8739055024\O,-1.5552790484,0.522593694,0.5925453708\N,0.370824921
2,-0.648999639,-0.4828806765\O,-0.4295845941,-1.4473608235,-0.87390550
24\O,1.5552790484,-0.522593694,-0.5925453708\\Version=IA32L-G03RevC.02
\State=1-AG\HF=-410.1682402\RMSD=8.427e-09\RMSF=1.421e-04\Dipole=0.,0.
,0.\PG=C02H [SGH(N2),X(O4)]\\@

n.OCF3-OCF3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C2F6O2\CYL509\21-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCF3.fre
q\\0,1\O,0.5187218102,0.8278353565,0.1119951753\C,1.1554567667,0.11266
48315,1.1228425603\F,2.2826228686,-0.4512604658,0.693408725\F,0.376945
0566,-0.8373142365,1.6390063036\F,1.4276126195,1.0289243276,2.04671149
81\O,0.2300324636,-0.1202151684,-0.9484445365\C,-1.1506118497,-0.10805
1196,-1.1282347458\F,-1.8066639281,-0.5144633714,-0.0420664781\F,-1.59
4112497,1.1021125105,-1.4620707711\F,-1.3551934186,-0.9600702442,-2.12
78839439\\Version=IA64L-G03RevC.02\State=1-A\HF=-825.6152611\RMSD=3.15
8e-09\RMSF=3.267e-05\Dipole=-0.0486124,-0.0457589,0.0542676\PG=C01 [X(
C2F6O2)]\\@

n.OCH2CH3-OCH2CH3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4H10O2\CYL509\21-Aug-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCH2CH3
.freq\\0,1\O,0.6087186266,-0.5181882417,0.3378727645\C,1.5907103176,0.
2292506343,-0.3727257217\C,2.7692075273,-0.708924637,-0.5944171828\H,1
.8873116529,1.1059380617,0.2184454739\H,1.1776972774,0.5831772549,-1.3
282407323\H,3.5646957233,-0.1841226462,-1.1342466217\H,2.4684314302,-1
.5814914982,-1.1831422212\H,3.1711118393,-1.0587023503,0.3616220326\O,
-0.4996793536,0.3965534899,0.5884387928\C,-1.6398914999,-0.1742085737,
-0.0457254786\C,-2.8093646107,0.7535358681,0.2540060937\H,-1.466604607
2,-0.2602802246,-1.1280684549\H,-1.8197291681,-1.1811181171,0.35396087
23\H,-3.7224985731,0.3596468539,-0.2049836027\H,-2.9713874482,0.836272
038,1.3332629312\H,-2.6253127162,1.7558388926,-0.1459283997\\Version=I
A64L-G03RevC.02\State=1-A\HF=-308.7992199\RMSD=9.854e-09\RMSF=1.007e-0
5\Dipole=-0.0657666,0.0733709,-0.5586533\PG=C01 [X(C4H10O2)]\\@

n.OCH3-OCH3
1\1\GINC-AC22\FOpt\RB3LYP\Gen\C2H6O2\CYL509\20-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.OCH3.fre
q\\0,1\O,-0.1419606567,-0.2867213957,0.7371362073\C,1.1598380764,0.000
6252547,1.2115195627\H,1.8736242254,-0.7800477136,0.9203079759\H,1.059
1041855,0.0158916623,2.3018688341\H,1.5167301834,0.9768846543,0.857906
6966\O,-0.0201211893,-0.3593463524,-0.7183721654\C,-1.0388772845,0.481
4610593,-1.2255081194\H,-0.8888820726,1.5281842012,-0.9299177377\H,-0.
9571184649,0.3886483731,-2.3136065555\H,-2.0325680402,0.1464629234,-0.
9027402083\\Version=IA64L-G03RevC.02\State=1-A\HF=-230.1611229\RMSD=3.
742e-09\RMSF=1.380e-05\Dipole=0.1242796,0.4949568,-0.0143433\PG=C01 [X
(C2H6O2)]\\@

n.OCHO-OCHO
1\1\GINC-AC18\FOpt\RB3LYP\Gen\C2H2O4\CYL509\22-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.OCHO-OCH
O.freq\\0,1\O,0.4975938721,0.8606454741,0.5445708995\C,1.4691179361,-0
.0743451079,0.2941711509\O,1.5270139821,-0.8314742432,-0.6262826062\H,
2.1829184716,0.0294102506,1.1274889284\O,-0.4875351776,0.8818099108,-0
.5177472104\C,-1.4693491692,-0.0492985565,-0.2963115398\O,-1.537096880

5,-0.8327497404,0.6009478146\H,-2.1813374414,0.0866005253,-1.126557775
5\\Version=IA64L-G03RevC.02\State=1-A\HF=-378.214001\RMSD=7.048e-09\RM
SF=1.051e-04\Dipole=0.0045547,0.5683532,0.0084061\PG=C01 [X(C2H2O4)]\\
@

n.OCOCH3-OCOCH3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H6O4\CYL509\21-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCOCH3.f
req\\0,1\O,-0.0687027902,0.7740822787,0.8472801942\C,0.9964638628,-0.0
723294791,1.1056263084\C,1.089068456,-0.2483230957,2.602282381\O,1.683
903481,-0.5758927278,0.2622109548\H,2.1058378562,-0.5533829934,2.85473
87286\H,0.3938233699,-1.0387443393,2.9057941013\H,0.8204005051,0.66686
71483,3.1351304682\O,-0.2401918134,0.968959017,-0.5702810039\C,-0.9720
192736,-0.0662417771,-1.1276469975\C,-1.0795417952,0.1956526881,-2.610
6749212\O,-1.4047795323,-1.0000143609,-0.5126273476\H,-1.9474498374,-0
.3410917226,-2.9970329255\H,-1.1612943664,1.2631286707,-2.8285957645\H
,-0.176979788,-0.1864004375,-3.1002176127\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-456.8691249\RMSD=4.040e-09\RMSF=1.021e-05\Dipole=-0.079141
2,0.4465202,0.0708747\PG=C01 [X(C4H6O4)]\\@

n.Si_CH3_3-Si_CH3_3
1\1\GINC-LC19\FOpt\RB3LYP\Gen\C6H18Si2\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Si_CH3
_3.freq\\0,1\H,0.8940428587,-1.5484853769,-2.949675075\C,0.8919393412,
-1.5445193805,-1.8521072453\H,1.9362017704,-1.5838627741,-1.5198981651
\H,0.4037213624,-2.4683985951,-1.5196587107\Si,-0.0000147484,0.0002603
901,-1.1842467067\C,-1.7838529887,0.0001252688,-1.8518756954\C,0.89170
40506,1.5454997873,-1.8512994436\H,-1.7884306409,0.0000458155,-2.94945
07547\H,-2.3399239583,0.8848602404,-1.5196025397\H,-2.339910388,-0.884
5714284,-1.5194232965\H,1.9361020651,1.5843688264,-1.5193614465\H,0.40
37846742,2.4692610714,-1.5180306951\H,0.8934502365,1.5501967696,-2.948
8712505\H,-0.8916733926,1.5499129333,2.9496143697\C,-0.8900932828,1.54
55892826,1.852046756\H,-1.9344813007,1.5858522758,1.5203207862\H,-0.40
11292089,2.4688736655,1.5190657648\Si,0.0000162773,-0.0002843077,1.184
2496175\C,1.7838523309,-0.0022374944,1.8518829465\C,-0.8935521571,-1.5
444294095,1.8513499056\H,1.7884277965,-0.0027684882,2.9494576435\H,2.3
39086021,-0.88730611,1.5191201932\H,2.3407493699,0.8821247953,1.519922
2391\H,-1.9378137561,-1.5823899848,1.5189015473\H,-0.4063596412,-2.468
7768972,1.5186234075\H,-0.8958490369,-1.5487702177,2.9489218884\\Versi
on=IA32L-G03RevC.02\State=1-A\HF=-818.5365514\RMSD=4.806e-09\RMSF=3.13
6e-05\Dipole=0.0000017,-0.0000155,0.000003\PG=C01 [X(C6H18Si2)]\\@

n.P_CH3_2-P_CH3_2
1\1\GINC-LC92\FOpt\RB3LYP\Gen\C4H12P2\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.P_CH3_2
.freq\\0,1\C,-1.5226667386,1.1006591668,1.3688466253\H,-0.915136076,0.
9395573931,2.2664322539\H,-2.3407615102,0.3731728305,1.3596345302\H,-1
.9703085871,2.0995029772,1.4208091546\P,0.5332148811,-0.9677261532,0.2
168754057\C,-0.8551674769,-2.1511442499,-0.2113434495\H,-0.4517455714,
-3.1695163143,-0.2422225322\H,-1.3240513683,-1.9283859493,-1.176351907
5\H,-1.6219971504,-2.1242215583,0.5695791232\C,1.5226667386,-1.1006591
668,-1.3688466253\H,0.915136076,-0.9395573931,-2.2664322539\H,2.340761
5102,-0.3731728305,-1.3596345302\H,1.9703085871,-2.0995029772,-1.42080
91546\P,-0.5332148811,0.9677261532,-0.2168754057\C,0.8551674769,2.1511
442499,0.2113434495\H,0.4517455714,3.1695163143,0.2422225322\H,1.32405
13683,1.9283859493,1.1763519075\H,1.6219971504,2.1242215583,-0.5695791
232\\Version=IA32L-G03RevC.02\State=1-AG\HF=-842.3722545\RMSD=2.672e-0
9\RMSF=2.743e-05\Dipole=0.,0.,0.\PG=CI [X(C4H12P2)]\\@

n.SC_CH3_2CN-SC_CH3_2CN
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H12N2S2\CYL509\21-Aug-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SC_CH
3_2CN.freq\\0,1\S,-0.4711486606,-0.4951182259,-1.2379535519\C,-2.01511
63425,-0.5225632385,-0.14234783\C,-1.7030507354,-0.7241426471,1.345472
8969\C,-2.8396190677,-1.6935490153,-0.717689569\C,-2.7365732501,0.7417
022541,-0.3408614302\H,-1.1645149248,-1.6627804502,1.4945472027\H,-1.0
94236186,0.0916373677,1.7398437575\H,-2.6412600211,-0.7557172067,1.911
4078174\H,-3.0518198978,-1.5548246788,-1.7816023566\H,-3.7924015295,-1
.7614238084,-0.1826937001\H,-2.2957635832,-2.6329766113,-0.5794175713\
N,-3.3181503908,1.7377397947,-0.4787368622\S,0.7019634402,1.0733770794
,-0.5582896767\C,2.1907715441,0.2939050523,0.3135423437\C,2.942909643,
-0.6596160674,-0.6291947016\C,3.058384265,1.5107035498,0.7004352079\C,
1.7741933756,-0.4223513562,1.5224812045\H,3.2686773731,-0.1130677019,-
1.5189276608\H,2.306745758,-1.4932724304,-0.937934086\H,3.8230983965,-
1.0686783117,-0.1203109299\H,2.5257392105,2.1864329562,1.3752497698\H,
3.9673606742,1.1646597375,1.2031853319\H,3.3472754271,2.0610596973,-0.
2002441903\N,1.4719598534,-1.0031285669,2.4824167964\\Version=IA64L-G0

3RevC.02\State=1-A\HF=-1217.9327178\RMSD=2.414e-09\RMSF=6.404e-06\Dipo
le=1.1515743,-0.8215004,-0.3422969\PG=C01 [X(C8H12N2S2)]\\@

n.SCH2COOCH3-SCH2COOCH3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C6H10O4S2\CYL509\21-Aug-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2C
OOCH3.freq\\0,1\S,-0.6425283571,-1.2447052639,1.303361518\C,1.13558924
58,-1.27459731,1.8197741814\C,2.0249342154,-0.6693039319,0.7531692241\
O,2.4000665716,0.485656326,0.7518046554\O,2.3043745302,-1.5612529278,-
0.2086181729\C,2.9694221656,-1.0284269358,-1.3719143904\H,1.2518791287
,-0.7292960061,2.7571454209\H,1.3628455592,-2.3349849391,1.9638244988\
H,3.9066998509,-0.5436242272,-1.0886388719\H,2.3108028262,-0.310837130
5,-1.8661922357\H,3.1577488518,-1.8881135904,-2.0151301183\S,-1.251009
4247,0.7159505937,1.6146671155\C,-0.6311836214,1.6756943275,0.15012987
57\C,-1.0108504379,1.066689766,-1.1803066061\O,-0.2516629955,0.4279293
225,-1.8794109944\O,-2.2987390849,1.3043597601,-1.4901153539\C,-2.7588
243508,0.710874968,-2.7165690088\H,0.4524809015,1.7616191734,0.2118811
333\H,-1.1037439223,2.6548749203,0.2765722595\H,-2.1846048207,1.091569
1101,-3.5653941255\H,-2.6570028886,-0.376552515,-2.6751576165\H,-3.807
3364487,0.9962947778,-2.8023492084\\Version=IA64L-G03RevC.02\State=1-A
\HF=-1331.9480343\RMSD=9.229e-09\RMSF=3.469e-06\Dipole=-0.0581964,-0.1
054325,-0.5620631\PG=C01 [X(C6H10O4S2)]\\@

n.SCH2Ph-SCH2Ph
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C14H14S2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2Ph
.freq\\0,1\S,0.9140753783,-0.4734094834,1.953231517\C,-0.7832793019,-1
.0196977046,2.500243639\C,-1.8265080496,-1.0578074488,1.4176201279\H,-
1.0895695174,-0.3772478039,3.3293128416\H,-0.5878112625,-2.0208785842,
2.9030154202\C,-2.7896037274,-0.0446766017,1.3232733353\C,-1.848076905
4,-2.0965390426,0.4742781618\C,-3.7465185756,-0.0623105333,0.305348942
4\C,-2.8040728705,-2.1181597103,-0.5398085571\C,-3.7557866598,-1.09784
8202,-0.6293120183\H,-4.5016306505,-1.1149922542,-1.4193316275\H,-2.81
05216941,-2.9332388241,-1.2587527702\H,-4.4864869859,0.73158835,0.2473
376282\H,-1.1070830136,-2.8903275752,0.5367723374\H,-2.7871204193,0.76
28266634,2.050926087\S,0.6822304205,1.5398687653,1.5048518741\C,0.2545
926904,1.5963225531,-0.3144213272\C,1.3144375373,1.0685011064,-1.23985
80056\H,-0.698628352,1.0834705293,-0.454867593\H,0.088189316,2.6697481
956,-0.4675827974\C,1.1689425153,-0.1899327863,-1.8371696325\C,2.46419
38525,1.8204509957,-1.5225964165\C,2.1493276365,-0.6861928069,-2.69899
81585\C,3.4426155883,1.3277261527,-2.3830445806\C,3.2878471109,0.07070
20869,-2.9745185799\H,4.0504579813,-0.3134385735,-3.6468094251\H,4.325
994736,1.924453618,-2.594887557\H,2.0211399277,-1.6643445031,-3.155281
9583\H,2.5921607147,2.79640178,-1.0597301994\H,0.2813513935,-0.7805978
776,-1.6256762259\\Version=IA64L-G03RevC.02\State=1-A\HF=-1338.3097624
\RMSD=4.538e-09\RMSF=4.045e-06\Dipole=-0.7684143,-0.2393808,-0.4801876
\PG=C01 [X(C14H14S2)]\\@

n.SCH3-SCH3
1\1\GINC-AC20\FOpt\RB3LYP\Gen\C2H6S2\CYL509\20-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.SCH3.fre
q\\0,1\S,-1.08208995,-0.0791053179,0.3920222043\C,-1.3138933607,1.5419
378611,-0.4395083416\H,-2.395715848,1.7044240575,-0.4872432429\H,-0.85
26524616,2.3435802558,0.1410033053\H,-0.9099393813,1.5310155392,-1.454
6431102\S,0.9879193145,-0.2507845199,0.5403546395\C,1.4655403246,-1.01
0717349,-1.0618953419\H,2.546730676,-1.1752819695,-1.0073353986\H,1.24
83451691,-0.3442792801,-1.9000623116\H,0.9600802299,-1.968544271,-1.20
13273125\\Version=IA64L-G03RevC.02\State=1-A\HF=-876.2075135\RMSD=4.43
7e-09\RMSF=7.211e-06\Dipole=0.0840578,0.2945252,-0.8323693\PG=C01 [X(C
2H6S2)]\\@

n.SO2CH3-SO2CH3
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C2H6O4S2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SO2CH3
.freq\\0,1\C,-1.291168118,-1.8558523648,0.3788945007\S,-0.8226673183,-
0.1534587274,0.7698684508\O,-1.9520576248,0.7468395621,0.5098297801\O,
-0.0903532737,-0.1334667271,2.04646906\H,-0.3946072196,-2.4761451979,0
.4049412197\H,-1.758839195,-1.8668902314,-0.607272355\H,-2.0037733915,
-2.158160715,1.1506481916\C,1.692061119,1.5454520359,-0.0480041003\S,0
.7616773049,0.200590046,-0.8201722481\O,1.582511841,-1.0212068061,-0.8
171414762\O,0.0998261851,0.6867821463,-2.0364144458\H,1.0422789806,2.4
199585518,0.0182500529\H,2.0237007943,1.2161774476,0.9373080518\H,2.54
23052184,1.7417756196,-0.7063001507\\Version=IA64L-G03RevC.02\State=1-
A\HF=-1176.9611361\RMSD=6.121e-09\RMSF=1.502e-05\Dipole=0.3333147,-0.2
583195,0.2753198\PG=C01 [X(C2H6O4S2)]\\@

n.SOCH3-SOCH3

1\1\GINC-LC95\FOpt\RB3LYP\Gen\C2H6O2S2\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SOCH3.
freq\\0,1\S,-0.3174340495,-0.961676029,0.6005272557\O,0.3014110007,-2.
1325375466,-0.1250292738\C,-2.0519226177,-0.7859733212,0.0336037767\H,
-2.6603194222,-1.5195519452,0.5686289032\H,-2.0923037467,-0.9778711509
,-1.042136198\H,-2.3886844413,0.2295640178,0.264548308\S,0.3174340495,
0.961676029,-0.6005272557\O,-0.3014110007,2.1325375466,0.1250292738\C,
2.0519226177,0.7859733212,-0.0336037767\H,2.6603194222,1.5195519452,-0
.5686289032\H,2.0923037467,0.9778711509,1.042136198\H,2.3886844413,-0.
2295640178,-0.264548308\\Version=IA32L-G03RevC.02\State=1-AG\HF=-1026.
5578495\RMSD=6.044e-09\RMSF=1.490e-05\Dipole=0.,0.,0.\PG=CI [X(C2H6O2S
2)]\\@

n.Ph-Ph
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C12H10\CYL509\21-Aug-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Ph.freq\
\0,1\C,-0.2535330755,-0.1317328582,-0.6857604922\C,-1.2162131794,-0.63
19075148,-3.2897513822\C,-0.523116221,0.9248587429,-1.5721831848\C,-0.
4773404609,-1.4446800651,-1.1339654262\C,-0.9537155681,-1.6923506276,-
2.4205427837\C,-0.9982620647,0.6781549403,-2.8594006942\H,-0.383097755
8,1.9493848016,-1.2386201786\H,-0.2505895369,-2.278654443,-0.475487655
7\H,-1.1115131528,-2.7169037402,-2.7474693192\H,-1.2071752606,1.512174
6026,-3.5244244433\H,-1.5870511013,-0.8245819956,-4.292846998\C,0.2535
273516,0.1317147095,0.6857660944\C,1.2162169766,0.6319195539,3.2897476
661\C,-0.182138716,-0.6379723544,1.7778213668\C,1.182590901,1.15777948
28,0.928331633\C,1.6581526085,1.4057967816,2.2151430952\C,0.2938294173
,-0.3915872382,3.0647960972\H,-0.9203370673,-1.4191623242,1.6186747221
\H,1.5540194255,1.7484164236,0.0954379155\H,2.3826002464,2.1998484411,
2.3768455711\H,-0.0639023859,-0.9950894002,3.8950389606\H,1.5870587713
,0.824606318,4.2928394897\\Version=IA64L-G03RevC.02\State=1-A\HF=-463.
306066\RMSD=2.336e-09\RMSF=5.028e-06\Dipole=0.0000016,0.000005,-0.0000
015\PG=C01 [X(C12H10)]\\@

n.C6H4CN-C6H4CN
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C14H8N2\CYL509\20-Aug-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4CN.
freq\\0,1\C,-0.2648221965,-0.1328821253,-0.6798564274\C,-1.2711771575,
-0.6378419635,-3.2632825528\C,-0.3127270734,0.8865616222,-1.6472062301
\C,-0.7320410869,-1.410792075,-1.0348264251\C,-1.2288548246,-1.6660822
851,-2.3072066773\C,-0.8083443534,0.6438813754,-2.9225174321\H,0.01654
48206,1.8882668211,-1.3885623553\H,-0.6798158694,-2.2210664593,-0.3140
917819\H,-1.5773280645,-2.6592363332,-2.5712990374\H,-0.8487536229,1.4
419108502,-3.6567172808\C,-1.7830192883,-0.8946858871,-4.5773075872\N,
-2.1982804123,-1.1031958339,-5.6438631552\C,0.2648190154,0.13287745,0.
6798375793\C,1.2711673216,0.637825362,3.263289629\C,-0.3169512757,-0.4
67433094,1.8105614193\C,1.3617066011,0.9916425509,0.8714803414\C,1.862
7782304,1.244088817,2.1427579919\C,0.1744001942,-0.2219230708,3.086981
077\H,-1.181990757,-1.112506744,1.6909070816\H,1.8452487724,1.44528502
83,0.0117563097\H,2.7159381856,1.9012935737,2.2759246429\H,-0.28988231
38,-0.6840122572,3.9521103636\C,1.7830127818,0.894674292,4.5773123871\
N,2.1983314865,1.1032815065,5.6438265124\\Version=IA64L-G03RevC.02\Sta
te=1-A\HF=-647.7920264\RMSD=1.304e-09\RMSF=3.507e-06\Dipole=-0.0000358
,-0.0000605,0.0000258\PG=C01 [X(C14H8N2)]\\@

n.C6H4NO2-C6H4NO2
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C12H8N2O4\CYL509\21-Aug-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4N
O2.freq\\0,1\C,-0.2523806564,-0.1313343775,-0.6849928857\C,-1.20061324
92,-0.6247626101,-3.2587211514\C,-0.9710584541,0.8530683874,-1.3877387
017\C,-0.0231351275,-1.3704217962,-1.306981167\C,-0.493511344,-1.6244
25277,-2.5942028029\C,-1.4468197339,0.6147344623,-2.6722633618\H,-1.13
5470256,1.8254881316,-0.9342977177\H,0.5053396783,-2.1533959384,-0.775
9964875\H,-0.3307710401,-2.578022846,-3.081035278\H,-1.9927235851,1.36
89466002,-3.225428392\N,-1.7013009652,-0.8853038932,-4.6177067421\O,-2
.3253563304,0.0152814811,-5.1777096578\O,-1.4652057592,-1.9877671964,-
5.110592364\C,0.2523690162,0.131319215,0.685000198\C,1.2006166839,0.62
476172,3.2587202139\C,-0.5111524114,0.8763311667,1.6022735595\C,1.5053
378568,-0.3589940279,1.0961696061\C,1.9855915738,-0.1165054498,2.37824
25697\C,-0.0452592494,1.1261891247,2.8882247245\H,-1.4923800155,1.2406
187904,1.3146507973\H,2.1225017088,-0.912728089,0.3956501537\H,2.95270
9804,-0.48119656,2.7015400682\H,-0.6292075996,1.6902714871,3.60492128\
N,1.7013124356,0.8853104763,4.6177012456\O,0.9873550793,1.5458836923,5
.3713656631\O,2.803208458,0.4266281756,4.9169302265\\Version=IA64L-G03
RevC.02\State=1-A\HF=-872.3081118\RMSD=3.861e-09\RMSF=2.106e-05\Dipole
=0.0000064,-0.0000098,0.0000005\PG=C01 [X(C12H8N2O4)]\\@

n.C6H4OCH3-C6H4OCH3

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C14H14O2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4OC
H3.freq\\0,1\C,-3.0724577871,0.030339441,0.5046183948\C,-3.0238896139,
-0.0588576325,1.9033400813\C,-1.7817191423,-0.1458471469,2.541100454\C
,-0.6112459071,-0.1398791503,1.7793976214\C,-0.6365531181,-0.053189235
4,0.3807269041\C,-1.8997097641,0.030474952,-0.2370235598\O,-4.23145773
76,-0.0538065468,2.5426183825\C,-4.2398446424,-0.1499744676,3.95707284
95\H,-1.9619661004,0.0710520969,-1.321022715\H,0.344783565,-0.17869644
35,2.2944438372\H,-1.7105332301,-0.2058463147,3.6212901979\H,-4.043415
517,0.0857497196,0.0219577298\H,-3.7814099484,-1.0866052049,4.30186299
36\H,-5.2905925456,-0.13338625,4.2527339757\H,-3.7193753007,0.69720316
11,4.4236781915\C,2.8958625499,-0.0313152217,-0.7864039045\C,3.0028439
729,-0.0365818175,-1.9369216709\C,1.915341133,0.7519470922,-2.32788539
57\C,0.7433853417,0.7392554614,-1.5685481867\C,0.6141354833,-0.0484687
758,-0.4164976724\C,1.7222803275,-0.8352313885,-0.0460930359\O,4.19676
14488,-0.1035425424,-2.5979816904\C,4.3554906764,0.674412201,-3.772541
7511\H,1.65120825,-1.4805562456,0.8251595804\H,-0.0798218219,1.3805257
93,-1.8716554782\H,1.9704132474,1.3846294146,-3.2066102355\H,3.7432865
563,-1.4470491674,-0.5008609009\H,4.2585016944,1.7482385338,-3.5632380
733\H,5.3644988036,0.468430254,-4.1348066211\H,3.6284756011,0.39259749
68,-4.5460727871\\Version=IA64L-G03RevC.02\State=1-A\HF=-692.3512891\R
MSD=9.250e-09\RMSF=9.972e-06\Dipole=0.0599826,0.2720087,0.0957116\PG=C
01 [X(C14H14O2)]\\@

n.C6H4OH-C6H4OH
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C12H10O2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4OH
.freq\\0,1\C,-3.0238085054,-0.5444879421,0.4825550173\C,-3.0927260951,
-0.0258060898,1.7797086348\C,-1.9425995992,0.5035870431,2.3724359845\C
,-0.7376352259,0.5096574422,1.6724605146\C,-0.643407684,-0.0031734883,
0.3690605684\C,-1.815854029,-0.5275548229,-0.2056259136\O,-4.304877665
9,-0.0638785531,2.4137840503\H,-1.7860626098,-0.9073281318,-1.22319215
2\H,0.1516561405,0.8984457556,2.1606926217\H,-1.9847996964,0.899700310
2,3.385896666\H,-3.9250339425,-0.943069597,0.0271835702\H,-4.210952357
3,0.3324664865,3.2938767834\C,2.7512773217,1.0980339196,-0.9473882656\
C,3.091525007,0.0282451717,-1.7817572269\C,2.211686352,-1.0501366937,-
1.913477597\C,1.006410782,-1.0555742199,-1.2140328912\C,0.6415444934,0
.0069604973,-0.3722384137\C,1.5432676213,1.0812055536,-0.2593015091\O,
4.2904000151,0.0932831467,-2.4384774079\H,1.280882798,1.9334148384,0.3
615499999\H,0.3492022863,-1.9157530602,-1.3064210117\H,2.4733907801,-1
.8920915733,-2.5525487079\H,3.436350416,1.9356471403,-0.8606892551\H,4
.3931047581,-0.7024611423,-2.9831950695\\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-613.7382482\RMSD=3.753e-09\RMSF=1.425e-05\Dipole=0.1165518,-
0.2367438,0.1987927\PG=C01 [X(C12H10O2)]\\@

n.CF2CF3-CF2CF3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4F10\CYL509\21-Aug-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF2CF3.fr
eq\\0,1\F,0.3727175063,0.5458781224,-1.6921575321\C,0.4097989774,0.569
6397573,-0.341211719\C,1.8984291954,0.6135666282,0.0945760529\F,-0.181
6988556,1.7059961972,0.0997688369\F,2.4951009131,-0.5575978494,-0.1655
717874\F,1.9971628323,0.8753391417,1.4020384928\F,2.522820229,1.579969
8912,-0.5884283024\F,-0.1224326502,-0.8056327767,1.5131123788\C,-0.381
7035636,-0.6529130364,0.1921063346\C,-1.9206152392,-0.5478338735,0.023
1392327\F,0.0351985338,-1.7539828035,-0.4718511774\F,-2.4207310166,0.3
797043226,0.8461276038\F,-2.2301395606,-0.2272708135,-1.2404783567\F,-
2.4719375116,-1.7307097488,0.3183665763\\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-1150.8139049\RMSD=8.772e-09\RMSF=4.162e-06\Dipole=-0.0016365
,0.004788,0.0085901\PG=C01 [X(C4F10)]\\@

n.CF2H-CF2H
1\1\GINC-LC69\FOpt\RB3LYP\Gen\C2H2F4\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF2H.fre
q\\0,1\C,-0.0142050539,-0.0161375781,-0.7617910786\H,0.9940534256,0.03
27246864,-1.1869555257\F,-0.7457428655,1.0408558311,-1.2038653591\F,-0
.6200865292,-1.1662183237,-1.1594479899\C,0.0142050539,0.0161375781,0.
7617910786\H,-0.9940534256,-0.0327246864,1.1869555257\F,0.7457428655,-
1.0408558311,1.2038653591\F,0.6200865292,1.1662183237,1.1594479899\\Ve
rsion=IA32L-G03RevC.02\State=1-AG\HF=-476.7604858\RMSD=6.532e-09\RMSF=
3.380e-04\Dipole=0.,0.,0.\PG=CI [X(C2H2F4)]\\@

n.CF3-CF3
1\1\GINC-LC99\FOpt\RB3LYP\Gen\C2F6\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF3.freq\\
0,1\F,0.3722442538,0.6429946437,-1.5925929648\C,0.378737505,0.62279447
44,-0.2545186873\F,1.6451926612,0.5919686897,0.1767919865\F,-0.2127867
337,1.7325959224,0.2030464515\F,-0.3722442538,-0.6429946437,1.59259296

48\C,-0.378737505,-0.6227944744,0.2545186873\F,-1.6451926612,-0.591968
6897,-0.1767919865\F,0.2127867337,-1.7325959224,-0.2030464515\\Version
=IA32L-G03RevC.02\State=1-AG\HF=-675.2549087\RMSD=5.320e-09\RMSF=1.437
e-05\Dipole=0.,0.,0.\PG=CI [X(C2F6)]\\@

n.CCl2H-CCl2H
1\1\GINC-LC95\FOpt\RB3LYP\Gen\C2H2Cl4\CYL509\19-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CCl2H.f
req\\0,1\C,-0.00119739,-0.0000001682,-0.7698959974\C,0.00119739,0.0000
001682,0.7698959974\Cl,0.8244651786,1.4689963454,1.3980854913\Cl,0.824
4636386,-1.4689967453,1.3980860573\Cl,-0.8244636386,1.4689967453,-1.39
80860573\Cl,-0.8244651786,-1.4689963454,-1.3980854913\H,1.0162972677,-
0.0000007394,-1.1566557522\H,-1.0162972677,0.0000007394,1.1566557522\\
Version=IA32L-G03RevC.02\State=1-AG\HF=-1918.1859928\RMSD=5.592e-09\RM
SF=1.489e-04\Dipole=0.,0.,0.\PG=CI [X(C2H2Cl4)]\\@

n.CCl3-CCl3
1\1\GINC-LC39\FOpt\RB3LYP\Gen\C2Cl6\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CCl3.freq
\\0,1\C,0.,0.,-0.7974998675\C,0.,0.,0.7974998675\Cl,0.8438872745,1.459
9354095,1.4070136025\Cl,0.8423975153,-1.4607955224,1.4070136025\Cl,-1.
6862847897,0.0008601129,1.4070136025\Cl,1.686284791,0.0008576657,-1.40
70136025\Cl,-0.8438851557,1.4599366342,-1.4070136025\Cl,-0.8423996352,
-1.4607942998,-1.4070136025\\Version=IA32L-G03RevC.02\State=1-A1\HF=-2
837.3350256\RMSD=1.068e-09\RMSF=7.448e-05\Dipole=0.,0.,0.\PG=D03 [C3(C
1.C1),X(Cl6)]\\@

n.CH2Cl-CH2Cl
1\1\GINC-LC120\FOpt\RB3LYP\Gen\C2H4Cl2\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Cl.
freq\\0,1\C,0.009109198,0.0185678912,-0.7591298697\C,-0.009109198,-0.0
185678912,0.7591298697\Cl,0.84113227,1.4502492354,1.4018612268\Cl,-0.8
4113227,-1.4502492354,-1.4018612268\H,1.0276026525,0.0010441058,-1.147
9331339\H,-1.0276026525,-0.0010441058,1.1479331339\H,-0.5157435102,0.8
930532252,-1.1445998231\H,0.5157435102,-0.8930532252,1.1445998231\\Ver
sion=IA32L-G03RevC.02\State=1-AG\HF=-999.0190105\RMSD=7.838e-09\RMSF=1
.334e-04\Dipole=0.,0.,0.\PG=CI [X(C2H4Cl2)]\\@

n.CH2F-CH2F
1\1\GINC-LC22\FOpt\RB3LYP\Gen\C2H4F2\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2F.fre
q\\0,1\C,0.1173701396,0.273625964,-0.6994470708\F,1.4872535847,0.35615
83197,-0.910419247\H,-0.3244310523,1.2714763444,-0.8013783002\H,-0.324
4318545,-0.3901733744,-1.4514211973\C,-0.1173701396,-0.273625964,0.699
4470708\F,-1.4872535847,-0.3561583197,0.910419247\H,0.3244310523,-1.27
14763444,0.8013783002\H,0.3244318545,0.3901733744,1.4514211973\\Versio
n=IA32L-G03RevC.02\State=1-AG\HF=-278.2779908\RMSD=1.705e-09\RMSF=1.32
8e-04\Dipole=0.,0.,0.\PG=C02H [SGH(C2F2),X(H4)]\\@

n.CH2OH-CH2OH
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C2H6O2\CYL509\20-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CH2OH.fr
eq\\0,1\C,-0.023959809,-0.0000001587,0.7597476616\O,1.3216095047,0.000
0000831,1.2204975054\H,-0.5767255984,-0.8890897698,1.1003667947\H,-0.5
767260404,0.8890890406,1.1003671522\H,1.3039109993,-0.0000001159,2.188
4919451\C,0.023959809,0.0000001587,-0.7597476616\O,-1.3216095047,-0.00
00000831,-1.2204975054\H,0.5767255984,0.8890897698,-1.1003667947\H,0.5
767260404,-0.8890890406,-1.1003671522\H,-1.3039109993,0.0000001159,-2.
1884919451\\Version=IA64L-G03RevC.02\State=1-AG\HF=-230.235715\RMSD=2.
278e-09\RMSF=7.716e-05\Dipole=0.,0.,0.\PG=C02H [SGH(C2H2O2),X(H4)]\\@

n.CH2Ph-CH2Ph
1\1\GINC-AC2\FOpt\RB3LYP\Gen\C14H14\CYL509\20-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CH2Ph.fre
q\\0,1\C,0.7719934193,0.076619868,0.\C,1.4912646618,-1.2547134436,0.\C
,1.8166655361,-1.8963839611,1.2028901701\C,1.8166655361,-1.8963839611,
-1.2028901701\C,2.4459337286,-3.1418366055,-1.206051423\C,2.4459337286,
-3.1418366055,1.206051423\C,2.7620054033,-3.7699228833,0.\H,3.2546978
579,-4.7385805445,0.\H,2.6935440309,-3.6194761686,2.1506666425\H,2.693
5440309,-3.6194761686,-2.1506666425\H,1.5794616285,-1.4103541352,2.147
293162\H,1.5794616285,-1.4103541352,-2.147293162\H,1.0660893357,0.6637
277558,-0.878992584\H,1.0660893357,0.6637277558,0.878992584\C,-0.77199
34193,-0.076619868,0.\C,-1.4912646618,1.2547134436,0.\C,-1.8166655361,
1.8963839611,-1.2028901701\C,-1.8166655361,1.8963839611,1.2028901701\C
,-2.4459337286,3.1418366055,-1.206051423\C,-2.4459337286,3.1418366055,
1.206051423\C,-2.7620054033,3.7699228833,0.\H,-3.2546978579,4.73858054
45,0.\H,-2.6935440309,3.6194761686,-2.1506666425\H,-2.6935440309,3.619

4761686,2.1506666425\H,-1.5794616285,1.4103541352,-2.147293162\H,-1.57
94616285,1.4103541352,2.147293162\H,-1.0660893357,-0.6637277558,0.8789
92584\H,-1.0660893357,-0.6637277558,-0.878992584\\Version=IA64L-G03Rev
C.02\State=1-AG\HF=-541.9303591\RMSD=4.486e-09\RMSF=4.187e-05\Dipole=0
.,0.,0.\PG=C02H [SGH(C6H2),X(C8H12)]\\@

n.CH_CH2_2-CH_CH2_2
1\1\GINC-LC95\FOpt\RB3LYP\Gen\C6H10\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH_CH2_2.
freq\\0,1\C,-1.733742743,-0.6662955878,-0.7408567606\C,-1.7242590191,-
0.6578899942,0.7698815434\C,-0.4209579353,-0.6203332594,0.0060772017\H
,0.1559150583,-1.545092106,0.0075991048\H,-2.0399970597,0.2514013539,1
.275939402\H,-1.9927618685,-1.5707303159,1.2951810601\H,-2.0558448916,
0.2373341446,-1.2530090714\H,-2.0087812438,-1.5849064067,-1.2525393208
\C,1.733742743,0.6662955878,0.7408567606\C,1.7242590191,0.6578899942,-
0.7698815434\C,0.4209579353,0.6203332594,-0.0060772017\H,-0.1559150583
,1.545092106,-0.0075991048\H,2.0399970597,-0.2514013539,-1.275939402\H
,1.9927618685,1.5707303159,-1.2951810601\H,2.0558448916,-0.2373341446,
1.2530090714\H,2.0087812438,1.5849064067,1.2525393208\\Version=IA32L-G
03RevC.02\State=1-AG\HF=-234.5932348\RMSD=9.295e-09\RMSF=2.256e-05\Dip
ole=0.,0.,0.\PG=CI [X(C6H10)]\\@

n.CH2CH=CH2-CH2CH=CH2
1\1\GINC-LC128\FOpt\RB3LYP\Gen\C6H10\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2CH=CH
2.freq\\0,1\C,-0.3277666278,0.5526000621,0.4317384366\C,0.3026424482,1
.9022289401,0.2223882928\H,-0.2393276792,0.2606339271,1.4882862228\H,-
1.401505269,0.6060917587,0.2087913041\H,1.3642628,1.9723734203,0.46776
69455\C,-0.3258370014,2.9824207952,-0.2427938503\H,0.1871831294,3.9309
028257,-0.3785726581\H,-1.3827170547,2.9609426766,-0.5024083189\C,0.32
77666278,-0.5526000621,-0.4317384366\C,-0.3026424482,-1.9022289401,-0.
2223882928\H,0.2393276792,-0.2606339271,-1.4882862228\H,1.401505269,-0
.6060917587,-0.2087913041\H,-1.3642628,-1.9723734203,-0.4677669455\C,0
.3258370014,-2.9824207952,0.2427938503\H,-0.1871831294,-3.9309028257,0
.3785726581\H,1.3827170547,-2.9609426766,0.5024083189\\Version=IA32L-G
03RevC.02\State=1-AG\HF=-234.6117105\RMSD=2.894e-09\RMSF=7.994e-06\Dip
ole=0.,0.,0.\PG=CI [X(C6H10)]\\@

n.CH2CH3-CH2CH3
1\1\GINC-LC95\FOpt\RB3LYP\Gen\C4H10\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2CH3.fr
eq\\0,1\C,-0.2795440659,0.5790345545,0.4182617103\H,0.3113481156,1.485
0836498,0.2205872128\C,-0.2867642822,0.2911749358,1.9227093611\H,-1.30
19325045,0.8057191639,0.0828620486\H,0.7269906311,0.0950969408,2.29368
9111\H,-0.8984203633,-0.5895874023,2.1548852412\H,-0.6912805878,1.1361
296721,2.4916536272\C,0.2795440659,-0.5790345545,-0.4182617103\H,-0.31
13481156,-1.4850836498,-0.2205872128\C,0.2867642822,-0.2911749358,-1.9
227093611\H,1.3019325045,-0.8057191639,-0.0828620486\H,-0.7269906311,-
0.0950969408,-2.293689111\H,0.8984203633,0.5895874023,-2.1548852412\H,
0.6912805878,-1.1361296721,-2.4916536272\\Version=IA32L-G03RevC.02\Sta
te=1-AG\HF=-158.4580441\RMSD=9.999e-09\RMSF=5.061e-05\Dipole=0.,0.,0.\
PG=CI [X(C4H10)]\\@

n.CH_CH3_2-CH_CH3_2
1\1\GINC-LC92\FOpt\RB3LYP\Gen\C6H14\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH_CH3_2.
freq\\0,1\C,-1.5298385233,1.1549090689,0.4532158066\H,-1.2526307314,1.
4050382845,1.4862239822\H,-2.6118643886,0.9787288039,0.4371035925\H,-1
.3328643736,2.0339296119,-0.1679345976\C,-0.7704410671,-0.0918137196,-
0.0325564178\H,-1.0334488961,-0.2541181784,-1.0906582894\C,-1.24799947
52,-1.3191956052,0.7626703323\H,-0.8446279192,-2.2567455687,0.36826237
48\H,-2.3413404801,-1.3960382028,0.7347415404\H,-0.9503724472,-1.24311
25159,1.8172479426\C,1.5298385233,-1.1549090689,-0.4532158066\H,1.2526
307314,-1.4050382845,-1.4862239822\H,2.6118643886,-0.9787288039,-0.437
1035925\H,1.3328643736,-2.0339296119,0.1679345976\C,0.7704410671,0.091
8137196,0.0325564178\H,1.0334488961,0.2541181784,1.0906582894\C,1.2479
994752,1.3191956052,-0.7626703323\H,0.8446279192,2.2567455687,-0.36826
23748\H,2.3413404801,1.3960382028,-0.7347415404\H,0.9503724472,1.24311
25159,-1.8172479426\\Version=IA32L-G03RevC.02\State=1-AG\HF=-237.08250
54\RMSD=3.012e-09\RMSF=3.441e-05\Dipole=0.,0.,0.\PG=CI [X(C6H14)]\\@

n.C_CH3_3-C_CH3_3
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H18\CYL509\21-Aug-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3.f
req\\0,1\C,0.1016681754,-0.0363947887,1.9767046785\C,0.3245355057,0.48
6367732,0.5387781876\C,-0.2872432553,1.9041663944,0.4592970735\H,0.658
1793572,0.5852306376,2.6885708876\H,0.4510474688,-1.0670114884,2.10398

S65

71662\H,-0.9527736518,0.0004944139,2.2692314267\C,1.8496259101,0.62525
02647,0.3256362353\H,2.2515723239,1.3885873857,1.0028714963\H,2.101047
7344,0.9328582137,-0.6954658748\H,2.381353118,-0.3082319653,0.53691678
61\H,0.0886531794,2.5181171633,1.2867257458\H,-1.3801419424,1.89090342
77,0.5357695463\H,-0.0207450151,2.4157794717,-0.4712666129\C,-0.363323
4947,0.1689998953,-1.9386518644\C,-0.3247482339,-0.4863645576,-0.53881
8892\C,0.4758716155,-1.8031261002,-0.6637223455\H,-0.7027646434,-0.562
280341,-2.6822186339\H,-1.0556033795,1.0163179482,-1.977379736\H,0.622
3762013,0.5238953145,-2.2593387065\C,-1.7765525486,-0.8589190268,-0.15
92842381\H,-2.2388414129,-1.4297370666,-0.9737473511\H,-1.8197676895,-
1.4828211971,0.7393848259\H,-2.4014210761,0.0243914496,0.013070625\H,-
0.0554233746,-2.5000431528,-1.3231915606\H,1.4690823594,-1.6414632549,
-1.0951848047\H,0.6051683979,-2.3048658385,0.3016317656\\Version=IA64L
-G03RevC.02\State=1-A\HF=-315.701357\RMSD=4.246e-09\RMSF=3.227e-05\Dip
ole=0.0000358,0.0000673,0.0000645\PG=C01 [X(C8H18)]\\@

n.CCH-CCH
1\1\GINC-LC39\FOpt\RB3LYP\Gen\C4H2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CCH.freq\\
0,1\C,-0.2457508885,-0.1227024082,-0.6269799923\C,-0.6810070316,-0.340
0240107,-1.7374414639\H,-1.0638578554,-0.5311798528,-2.7142021503\C,0.
2457508885,0.1227024082,0.6269799923\C,0.6810070316,0.3400240107,1.737
4414639\H,1.0638578554,0.5311798528,2.7142021503\\Version=IA32L-G03Rev
C.02\State=1-SGG\HF=-153.4816432\RMSD=4.924e-09\RMSF=7.907e-05\Dipole=
0.,0.,0.\PG=D*H [C*(H1C1C1.C1C1H1)]\\@

n.CH=C_CH3_2-CH=C_CH3_2
1\1\GINC-LC22\FOpt\RB3LYP\Gen\C8H14\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH=C_CH3_
2.freq\\0,1\C,-0.2045787358,-0.1903848545,-0.6711375784\C,0.5884345953
,-0.3497758647,-1.7540203671\H,-1.2681634208,-0.3668653588,-0.82140994
56\C,2.0837129559,-0.1565176461,-1.7683250213\C,-0.0004209392,-0.75106
82816,-3.0837965506\H,0.436722336,-1.6938487949,-3.4438345977\H,0.2134
528534,0.0016342928,-3.8566209951\H,-1.0860176137,-0.8807527233,-3.029
2786962\H,2.366663072,0.6152664925,-2.4983542614\H,2.5896868133,-1.079
7053527,-2.0851394854\H,2.4965480586,0.133879246,-0.8000484994\C,0.204
5787358,0.1903848545,0.6711375784\C,-0.5884345953,0.3497758647,1.75402
03671\H,1.2681634208,0.3668653588,0.8214099456\C,-2.0837129559,0.15651
76461,1.7683250213\C,0.0004209392,0.7510682816,3.0837965506\H,-0.43672
2336,1.6938487949,3.4438345977\H,-0.2134528534,-0.0016342928,3.8566209
951\H,1.0860176137,0.8807527233,3.0292786962\H,-2.366663072,-0.6152664
925,2.4983542614\H,-2.5896868133,1.0797053527,2.0851394854\H,-2.496548
0586,-0.133879246,0.8000484994\\Version=IA32L-G03RevC.02\State=1-AG\HF
=-313.2656567\RMSD=6.581e-09\RMSF=6.223e-05\Dipole=0.,0.,0.\PG=CI [X(C
8H14)]\\@

n.CH=CH2-CH=CH2
1\1\GINC-LC10\FOpt\RB3LYP\Gen\C4H6\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH=CH2.fre
q\\0,1\C,-0.2586689036,-0.1429780849,-0.6661603549\C,0.5064115581,-0.3
001164933,-1.7556103793\H,-1.3420823882,-0.2296128563,-0.7545853977\H,
1.5903701143,-0.2207272816,-1.705756052\H,0.0790418678,-0.5125294454,-
2.7308626872\C,0.2586689036,0.1429780849,0.6661603549\C,-0.5064115581,
0.3001164933,1.7556103793\H,1.3420823882,0.2296128563,0.7545853977\H,-
1.5903701143,0.2207272816,1.705756052\H,-0.0790418678,0.5125294454,2.7
308626872\\Version=IA32L-G03RevC.02\State=1-AG\HF=-155.9921396\RMSD=2.
651e-09\RMSF=5.355e-05\Dipole=0.,0.,0.\PG=CI [X(C4H6)]\\@

n.CH=CHCH3-CH=CHCH3
1\1\GINC-LC99\FOpt\RB3LYP\Gen\C6H10\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH=CHCH3.
freq\\0,1\C,-0.2583405636,-0.0866649406,-0.6745801852\C,0.470622017,-0
.5072262006,-1.7217929567\H,-1.3141256156,0.1468294138,-0.8247857663\H
,1.5255849822,-0.7386350514,-1.5635238126\C,-0.0464495549,-0.690818412
,-3.1173538105\H,0.501095033,-0.0614329106,-3.8328215151\H,-1.10977422
89,-0.4377833979,-3.189551988\H,0.0788800871,-1.7284644524,-3.45707155
04\C,0.2583405636,0.0866649406,0.6745801852\C,-0.470622017,0.507226200
6,1.7217929567\H,1.3141256156,-0.1468294138,0.8247857663\H,-1.52558498
22,0.7386350514,1.5635238126\C,0.0464495549,0.690818412,3.1173538105\H
,-0.501095033,0.0614329106,3.8328215151\H,1.1097742289,0.4377833979,3.
189551988\H,-0.0788800871,1.7284644524,3.4570715504\\Version=IA32L-G03
RevC.02\State=1-AG\HF=-234.6320327\RMSD=3.768e-09\RMSF=2.588e-05\Dipol
e=0.,0.,0.\PG=CI [X(C6H10)]\\@

n.CHO-CHO
1\1\GINC-LC111\FOpt\RB3LYP\Gen\C2H2O2\CYL509\19-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CHO.fre

q\\0,1\C,-0.2305831334,-0.1708979771,-0.7064653149\O,0.5603359091,-0.3
428220664,-1.6054264531\H,-1.3304437896,-0.2452315851,-0.8293970674\C,
0.2305831334,0.1708979771,0.7064653149\O,-0.5603359091,0.3428220664,1.
6054264531\H,1.3304437896,0.2452315851,0.8293970674\\Version=IA32L-G03
RevC.02\State=1-AG\HF=-227.8186306\RMSD=5.542e-09\RMSF=1.013e-04\Dipol
e=0.,0.,0.\PG=CI [X(C2H2O2)]\\@

n.CN-CN
1\1\GINC-LC61\FOpt\RB3LYP\Gen\C2N2\CYL509\19-Jun-2008\0\\#B3LYP/GEN 6D
 INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CN.freq\\0
,1\C,-0.2337396847,-0.117801629,-0.6388504595\N,-0.6277488869,-0.31637
69198,-1.7157448697\C,0.2337396847,0.117801629,0.6388504595\N,0.627748
8869,0.3163769198,1.7157448697\\Version=IA32L-G03RevC.02\State=1-SGG\H
F=-185.6546121\RMSD=3.376e-09\RMSF=4.767e-05\Dipole=0.,0.,0.\PG=D*H [C
*(N1C1.C1N1)]\\@

n.COCH3-COCH3
1\1\GINC-LC83\FOpt\RB3LYP\Gen\C4H6O2\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COCH3.fr
eq\\0,1\C,-0.0373353615,0.0100344105,0.7737647625\C,1.2590881969,0.256
8004917,1.5053322766\O,-1.1081594376,-0.1689257995,1.3219407267\H,1.68
93253635,1.2170058258,1.1988797968\H,1.0807888842,0.24832422,2.5818189
367\H,1.9965923974,-0.5078354465,1.2361948984\C,0.0373353615,-0.010034
4105,-0.7737647625\C,-1.2590881969,-0.2568004917,-1.5053322766\O,1.108
1594376,0.1689257995,-1.3219407267\H,-1.6893253635,-1.2170058258,-1.19
88797968\H,-1.0807888842,-0.24832422,-2.5818189367\H,-1.9965923974,0.5
078354465,-1.2361948984\\Version=IA32L-G03RevC.02\State=1-AG\HF=-306.4
760225\RMSD=3.168e-09\RMSF=9.680e-05\Dipole=0.,0.,0.\PG=CI [X(C4H6O2)]
\\@

n.CON_CH2CH3_2-CON_CH2CH3_2
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C10H20N2O2\CYL509\21-Aug-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CON_
CH2CH3_2.freq\\0,1\C,0.9310585923,0.0214690106,0.1180272761\O,1.823513
2603,0.2756748593,-0.6941666478\N,1.0619493675,-0.92383335,1.087933056
4\C,0.0325308871,-1.2605785516,2.0803706913\C,2.3367249862,-1.65218816
08,1.1518294826\H,0.5511179693,-1.4827837158,3.020339985\C,-0.83614265
84,-2.4517839335,1.6635811487\H,-0.5777152121,-0.3758402767,2.25753413
31\H,2.705871659,-1.7704430256,0.1305843818\H,2.1262726273,-2.64896094
67,1.5543470387\C,3.3848648964,-0.9332913483,2.0050388277\H,-1.4019078
63,-2.2218081237,0.7539218565\H,-1.5527137682,-2.6936769552,2.45701036
31\H,-0.2325472891,-3.3459626643,1.4701642408\H,3.6174083615,0.0428985
26,1.5703272643\H,4.3085077028,-1.5222218404,2.0472297259\H,3.03147043
21,-0.7816095201,3.0313172399\C,-0.3597780462,0.8660781341,0.097874138
9\O,-0.6806247984,1.5191883631,1.0930818799\N,-1.041592565,0.923714732
1,-1.0782644453\C,-0.7186019056,0.1433646617,-2.2789771455\C,-2.194998
3175,1.8312628655,-1.1465141619\H,-1.6677401824,-0.2167458547,-2.69620
64387\C,0.0653033506,0.9361171273,-3.327326679\H,-0.1482515458,-0.7391
830269,-1.9836825376\H,-1.965265501,2.7074231664,-0.5364965996\H,-2.29
52965767,2.1595457804,-2.1861891038\C,-3.4923586703,1.1802954977,-0.65
93623334\H,1.0305248544,1.2342841326,-2.9121788798\H,0.2370445758,0.31
54798552,-4.2145801507\H,-0.4791705977,1.8322174822,-3.6461708592\H,-3
.4014632652,0.9011460273,0.3943254331\H,-4.3291854533,1.8813254,-0.757
8505962\H,-3.7341849279,0.2823683086,-1.2399961034\\Version=IA64L-G03R
evC.02\State=1-A\HF=-653.0909253\RMSD=5.776e-09\RMSF=3.697e-06\Dipole=
-0.6723281,-1.0988535,-0.2089039\PG=C01 [X(C10H20N2O2)]\\@

n.CON_CH3_2-CON_CH3_2
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H12N2O2\CYL509\21-Aug-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CON_C
H3_2.freq\\0,1\H,-1.8820911491,2.6170274372,-1.9720831936\C,-2.1430447
906,1.6951909856,-1.4360473304\N,-1.07595571,1.3272525209,-0.515099276
5\H,-2.2810814972,0.8850095048,-2.1506899686\H,-3.0765921977,1.8673912
589,-0.8855842193\C,-0.4176821421,0.1505963536,-0.7169572371\O,-0.7063
426219,-0.6467865524,-1.6091406644\C,-0.7799409458,2.3013129412,0.5261
85293\H,-0.4378300692,3.2434396695,0.0789414591\H,0.003541759,1.940271
4676,1.1872509192\H,-1.6881430492,2.5055906138,1.108025264\H,1.8883212
345,-1.9403722844,2.5304749404\C,2.1088493458,-1.6973101964,1.48334277
91\N,0.8839895939,-1.3392286545,0.7806822873\H,2.7957568453,-0.8533507
952,1.4380947167\H,2.5737162866,-2.5745493752,1.0147859959\C,0.8177562
668,-0.1254362274,0.1634493794\O,1.7202776496,0.7104620485,0.206331646
6\C,-0.1544401743,-2.3600910601,0.7665712436\H,-0.4106238566,-2.638635
8353,1.7970352899\H,-1.0438921526,-2.0052533696,0.2525985982\H,0.20221
50774,-3.2577161053,0.2452764988\\Version=IA64L-G03RevC.02\State=1-A\H
F=-495.8266781\RMSD=5.936e-09\RMSF=7.102e-06\Dipole=-0.7428886,-0.0467
56,1.0278868\PG=C01 [X(C6H12N2O2)]\\@

n.CONH2-CONH2
1\1\GINC-LC61\FOpt\RB3LYP\Gen\C2H4N2O2\CYL509\19-Jun-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CONH2.
freq\\0,1\C,-0.0310487488,0.0046131236,0.7727642591\N,1.1701113417,0.2
868584087,1.3154515219\O,-1.0712282221,-0.2233256796,1.3800226434\H,1.
2796702022,0.3265880208,2.3176292426\H,1.9506480197,0.4552263262,0.694
5738108\C,0.0310487488,-0.0046131236,-0.7727642591\N,-1.1701113417,-0.
2868584087,-1.3154515219\O,1.0712282221,0.2233256796,-1.3800226434\H,-
1.2796702022,-0.3265880208,-2.3176292426\H,-1.9506480197,-0.4552263262
,-0.6945738108\\Version=IA32L-G03RevC.02\State=1-AG\HF=-338.6012987\RM
SD=3.501e-09\RMSF=3.448e-05\Dipole=0.,0.,0.\PG=CI [X(C2H4N2O2)]\\@

n.CONHCH3-CONHCH3
1\1\GINC-LC128\FOpt\RB3LYP\Gen\C4H8N2O2\CYL509\19-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CONHC
H3.freq\\0,1\C,0.3173422784,-0.5732997806,-0.4083647121\O,1.4841926959
,-0.5242439564,-0.7951504304\N,-0.5579466,-1.575437779,-0.6173596905\H
,-1.4779814179,-1.4284443668,-0.2165638818\C,-0.2366991571,-2.78068244
49,-1.3539287274\H,0.8018428655,-2.7034585696,-1.6803846083\H,-0.88274
08231,-2.8883973022,-2.2328932136\H,-0.3498655699,-3.6694428829,-0.722
3880889\C,-0.3173422784,0.5732997806,0.4083647121\O,-1.4841926959,0.52
42439564,0.7951504304\N,0.5579466,1.575437779,0.6173596905\H,1.4779814
179,1.4284443668,0.2165638818\C,0.2366991571,2.7806824449,1.3539287274
\H,-0.8018428655,2.7034585696,1.6803846083\H,0.8827408231,2.8883973022
,2.2328932136\H,0.3498655699,3.6694428829,0.7223880889\\Version=IA32L-
G03RevC.02\State=1-AG\HF=-417.2264496\RMSD=5.946e-09\RMSF=8.987e-05\Di
pole=0.,0.,0.\PG=CI [X(C4H8N2O2)]\\@

n.COOC_CH3_3-COOC_CH3_3
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H18O4\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOC_C
H3_3.freq\\0,1\C,0.7347958534,-0.1447771873,-0.2655378792\O,1.34430610
29,0.5594074762,-1.0386575614\O,1.2109414903,-1.1342384148,0.489102286
\C,2.6395620213,-1.5233689846,0.4491485477\C,3.0023058719,-2.003632008
2,-0.9592573466\C,2.6944359198,-2.6757992144,1.4535171117\C,3.50872389
74,-0.3493084145,0.9100870613\H,3.7153423576,-3.0664776486,1.519596500
6\H,2.0288484668,-3.4881134132,1.1455861302\H,2.3863477901,-2.33716503
46,2.4477379733\H,4.0220979023,-2.4044317349,-0.954354096\H,2.95186798
73,-1.1885571618,-1.6832212071\H,2.3244003392,-2.8036287967,-1.2755215
263\H,4.549844692,-0.6801570243,0.9950337102\H,3.1835290506,0.00267849
71,1.8950906049\H,3.463114205,0.4814055562,0.2038628958\C,-0.793492078
4,-0.0235067442,-0.0348422896\O,-1.4780166303,-0.9427574077,0.35438412
68\O,-1.184842559,1.2090635412,-0.3555372729\C,-2.6073347335,1.6157649
078,-0.2842233833\C,-3.1040504041,1.5095327768,1.160876391\C,-2.555414
2563,3.0743748701,-0.7420705209\C,-3.4344613547,0.7646191908,-1.252342
8208\H,-3.5628223509,3.5037535339,-0.7390738276\H,-1.9225110096,3.6670
014343,-0.0740183154\H,-2.1479693227,3.1465783647,-1.7552130522\H,-4.1
153886415,1.9257693907,1.2283398475\H,-3.1306311443,0.4718522157,1.497
6714663\H,-2.4555083477,2.0845966991,1.8306324265\H,-4.4601399129,1.14
85417374,-1.2873745782\H,-3.0158077885,0.8213229565,-2.2628316462\H,-3
.4641459253,-0.2801662857,-0.9384051611\\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-692.8321244\RMSD=4.184e-09\RMSF=6.920e-07\Dipole=0.049101,0.
1407737,0.2512811\PG=C01 [X(C10H18O4)]\\@

n.COOCH2CH3-COOCH2CH3
1\1\GINC-LC95\FOpt\RB3LYP\Gen\C6H10O4\CYL509\19-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOCH2C
H3.freq\\0,1\C,0.7256234723,-0.2549472433,-0.0626047277\O,1.3932371116
,-0.1704616071,-1.0665717509\O,1.1174988713,-0.7942988467,1.0954428853
\C,2.4698167187,-1.3161240805,1.1173470261\H,3.1596571082,-0.503407351
3,0.8681191686\H,2.5602147188,-2.0791320148,0.3375010131\C,2.717111226
6,-1.8771109951,2.5038929968\H,3.7328582859,-2.2831042975,2.5617785215
\H,2.0096930804,-2.6802434834,2.7323088405\H,2.6117753086,-1.097938275
7,3.2650958386\C,-0.7256234723,0.2549472433,0.0626047277\O,-1.39323711
16,0.1704616071,1.0665717509\O,-1.1174988713,0.7942988467,-1.095442885
3\C,-2.4698167187,1.3161240805,-1.1173470261\H,-3.1596571082,0.5034073
513,-0.8681191686\H,-2.5602147188,2.091320148,-0.3375010131\C,-2.7171
112266,1.8771109951,-2.5038929968\H,-3.7328582859,2.2831042975,-2.5617
785215\H,-2.0096930804,2.6802434834,-2.7323088405\H,-2.6117753086,1.09
79382757,-3.2650958386\\Version=IA32L-G03RevC.02\State=1-AG\HF=-535.56
81905\RMSD=7.000e-09\RMSF=7.284e-05\Dipole=0.,0.,0.\PG=CI [X(C6H10O4)]
\\@

n.COOCH3-COOCH3
1\1\GINC-LC61\FOpt\RB3LYP\Gen\C4H6O4\CYL509\19-Jun-2008\0\\#B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOCH3.f
req\\0,1\C,0.4200229747,-0.63425011,-0.124402361\O,1.6148191611,-0.639

7662476,-0.3016605316\O,-0.3730016564,-1.7108840954,-0.1128424472\C,0.
2990145883,-2.9637449831,-0.3353084237\H,0.790031998,-2.9636328138,-1.
3119657336\H,-0.4821244967,-3.722265197,-0.294783599\H,1.0485961923,-3
.1362725693,0.4414343404\C,-0.4200229747,0.63425011,0.124402361\O,-1.6
148191611,0.6397662476,0.3016605316\O,0.3730016564,1.7108840954,0.1128
424472\C,-0.2990145883,2.9637449831,0.3353084237\H,-0.790031998,2.9636
328138,1.3119657336\H,0.4821244967,3.722265197,0.294783599\H,-1.048596
1923,3.1362725693,-0.4414343404\\Version=IA32L-G03RevC.02\State=1-AG\H
F=-456.9295614\RMSD=9.453e-09\RMSF=2.991e-05\Dipole=0.,0.,0.\PG=CI [X(
C4H6O4)]\\@

n.COOH-COOH
1\1\GINC-LC86\FOpt\RB3LYP\Gen\C2H2O4\CYL509\19-Jun-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOH.fre
q\\0,1\C,-0.0090939132,0.0252491585,0.7686928745\O,0.9598780859,0.2249
606681,1.4576672978\O,-1.2545758665,-0.1843456322,1.22338752\H,-1.2011
786115,-0.1405219784,2.1968870615\C,0.0090939132,-0.0252491585,-0.7686
928745\O,-0.9598780859,-0.2249606681,-1.4576672978\O,1.2545758665,0.18
43456322,-1.22338752\H,1.2011786115,0.1405219784,-2.1968870615\\Versio
n=IA32L-G03RevC.02\State=1-AG\HF=-378.3134401\RMSD=5.842e-09\RMSF=1.29
2e-04\Dipole=0.,0.,0.\PG=CI [X(C2H2O4)]\\@

n.COPh-COPh
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C14H10O2\CYL509\21-Aug-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COPh.f
req\\0,1\C,-4.2485703452,-0.548973554,0.2111137101\C,-4.2782797936,-0.
1976928713,1.5648423562\C,-3.0856302178,-0.0290307366,2.2709083375\C,-
1.860300962,-0.2109234488,1.6315584177\C,-1.8233500599,-0.5629372384,0
.2720811728\C,-3.0290668791,-0.7283317703,-0.4315428416\C,-0.556636046
7,-0.7323257243,-0.4902941205\O,-0.5386382936,-1.0167409306,-1.6809595
06\H,-2.9807135366,-0.9971941907,-1.4817922378\H,-0.9384289074,-0.0965
875622,2.1890734377\H,-3.1090670033,0.2404666847,3.3230365998\H,-5.176
6621055,-0.6803332368,-0.3383173403\H,-5.2312118084,-0.0560403089,2.06
79325205\C,4.1713207043,0.9904268996,-0.1312828915\C,4.0018315705,1.77
23617644,-1.2787542697\C,2.7799983843,1.7689042633,-1.9544284781\C,1.7
241299352,0.9859373351,-1.490345191\C,1.8873306041,0.1990817135,-0.338
0537104\C,3.1202515932,0.2106019088,0.3371991886\C,0.7955735855,-0.628
4155435,0.2428704459\O,0.9435026266,-1.2913148517,1.2615799907\H,3.226
5805343,-0.4011250441,1.2272141081\H,0.7843159288,0.9730773727,-2.0291
682774\H,2.6498139144,2.3736865889,-2.8474182915\H,5.1222170384,0.9930
227045,0.3943377488\H,4.822628845,2.3833752652,-1.6450949016\\Version=
IA64L-G03RevC.02\State=1-A\HF=-689.9529555\RMSD=6.911e-09\RMSF=2.596e-
05\Dipole=-0.1857453,1.0622678,0.1927348\PG=C01 [X(C14H10O2)]\\@