

A Comparison of Methods for Measuring Relative Radical Stabilities of Carbon-Centred Radicals

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SUPPORTING INFORMATION

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Table S1. Experimental Data Corresponding to the R–H, R–CH₃, R–Cl and R–R BDEs in Table 1

X	R-H BDE			R-Cl BDE			R-CH ₃ BDE			R-R BDE		
	P	S	T	P	S	T	P	S	T	P	S	T
H	439.3±4 440.6±2.9 438.5±8 440.6±2.5 439.28±13	420.5±2.1 420.5±2.1 421.7±2.9 422.6±1.7 420.5±1.3	410.5±2.9 413.8±2.5 412.5±1.7 409.2±2.1 407.5±4.2	350.2±1.7	352.3±3.3	354.0±6.3	377.4±0.8	370.3±2.1	369.0±3.8	377.4±8	363.2±2.5	353.5±4.6
BH ₂												
CH ₃	420.5±2.1 420.5±2.1 421.7±2.9 422.6±1.7 420.5±1.3	410.5±2.9 413.8±2.5 412.5±1.7 409.2±2.1 407.5±4.2	400.0±2.9 397.5 399.6±2.9 399.6±1.3 400.4±2.9	352.3±3.3	354.0±6.3	351.9±6.3	370.3±2.1	369.0±3.8	363.6±2.9	363.2±2.5	353.5±4.6	322.6±4.2
NH ₂	392.9±8.4	377.0±8.4	372.0±8.4				344.1	347.7±9.6	307.1±10.5 ^d 337.5±9.4 ^d	286.2±12.6^g 319.0		
OH	401.9±0.6	396.6	396.5				364.8±4.2	367.8±5.0	349.4±5.0	358.2±6.3	378.7±6.3	
F	423.8±4.2	410.9±8.4		354.4±11.7			389.9±8.4			368.2±8.4		
SiH ₃												
PH ₂												
SH	392.9±8.4						345.2±9.2			313.4±11.7		
Cl	419.0±2.3	406.6±1.5		331.8 338.5 325.9 338.1 328.4			375.7±9.2			364.8±13.8 360.7±8.4 364.6±5.3		
Br	425.1±4.2	406.7±4.2										
N(CH ₃) ₂	389.8											
NHCH ₃	394.1											
NHCHO												
NHCOCH ₃			389.5									
NO ₂	415.4	410.5	394.9				364.4	376.6		211.3 ^b		
OCF ₃	426.8±4.2											
OCH ₂ CH ₃	389.1	389.1										

Table S1. (Continued)

X	R-H BDE			R-Cl BDE			R-CH ₃ BDE			R-R BDE		
	P	S	T	P	S	T	P	S	T	P	S	T
OCHO												
OCOCH ₃	404.6		392.3									
Si(CH ₃) ₃	418±6.3											
P(CH ₃) ₂												
SC(CH ₃) ₂ CN												
SCH ₂ COOCH ₃												
SCH ₂ Ph												
SCH ₃	392.0±5.9			301.2±2.5			343.1±8.4					
SO ₂ CH ₃	414.2											
SOCH ₃	393.3 ^f											
Ph	370.3±6.3	357.3±6.3	348.1±4.2	305.0±8.4	292.4±4.4	292.8±6.3	310	308.8	303.3±8.4			
				299.6			317.1	312.1±6.3				
				299.9±4.3			319.7±7.1	318.8±8.4		272.8±9.2		
C ₆ H ₄ -pCN	368.0			280.3								
C ₆ H ₄ -pNO ₂	383.4											
C ₆ H ₄ -pOCH ₃	362.5											
C ₆ H ₄ -pOH												
CF ₂ CF ₃												
CF ₂ H	433.0±14.6											
CF ₃	446.4±4.5											
CCl ₂ H												
CCl ₃												
CH ₂ Cl	423.1±2.4	409.3±3.9		331								
				348.1±9.6								
				345.1±5.0								
CH ₂ F	433.5±8.4											
CH ₂ OH	423.8	394.6±8.4										
CH ₂ Ph				319.8								
CH(CH ₂) ₂	407.5±6.7											
CH ₂ CH=CH ₂	410.9			342.7								

Table S1. (Continued)

X	R-H BDE			R-Cl BDE			R-CH ₃ BDE			R-R BDE		
	P	S	T	P	S	T	P	S	T	P	S	T
OCH ₃	402.1						363.2±5.0			338.9±10.5		
CH ₂ CH ₃	418.0±4.2	414.6±1.7	383.3±8.4	352.7±4.2	350.2±6.3	352.7±6.3	372.0±2.9	368.2±2.9		366.1±3.3	348.5±3.3	
	417.6±8.4	411.1±2.2	403.8±4.2									
	422.2±2.1	412.5±2.1	387.4									
	423.4±2.1	411.3±2.1	400.8									
CH(CH ₃) ₂		407.5±4.2										
	419.2±4.2		399.2±13.0	350.6±6.3						356.9±5.4		
	415.5±8.4											
	425.1±2.1											
C(CH ₃) ₃	422.0±4.2											
	415.9±4.2			352.1								
	419.7±4.2											
	415.9±4.2											
CCH	422.6±8.4											
	423											
	373.2±10.0	355.6	345.2±8.4				318.0±8.4	305.4±8.4	295.8±6.3			
	364.8±8.4	365.3	338.9±9.6				320.5±5.0					
	377.8±12.6	347.7±9.2										
CH=C(CH ₃) ₂	372.0±4.2	346.8										
	384.1±4.2	373.0										
		331.9										
CH=CH ₂	362.8±6.3	344.3	332.6±7.1	298.3±5.0	300.0±6.3		320.1±9.2	302.5±6.3	284.9±6.3	257.3±4.2		
	364.8±2.1	341.0±6.3	319.7				317.6±3.8		282.4±6.3			
	371.5±2.9	345.6±5.4	347.7									
	368.6±2.9	350.6	339.6									
CH=CHCH ₃	364.0±4.6	349.2										
	356.8	341.8±6.3		310.5±5								
CHO	394.6±9.2						343.1±10.0					

Table S1. (Continued)

X	R-H BDE			R-Cl BDE			R-CH ₃ BDE			R-R BDE		
	P	S	T	P	S	T	P	S	T	P	S	T
CN	401.7	393.3±12.6	384.5	267.4 277.9±2.9 295.0			348.1±12.6	332.6±8.4	340.6±16.7	295.8±16.7		256.1±12.6 ^c 279.8±14.4 ^e
COCH ₃	401.2±2.9	386.2±7.1					361.9±12.6					
CON(CH ₂ CH ₃) ₂				324.2								
CON(CH ₃) ₂				322.3								
CONH ₂				337.7								
CONHCH ₃												
COOC(CH ₃) ₃	399.5			301.7								
COOCH ₂ CH ₃	401.7		387.4									
COOCH ₃	406.3±10.5			301.7								
COOH	398.7±12.1	398.8	389.0	278.7 ^c 310.9±2.2	298.0±3.2		353.5±12.6			342.7±4.3		
COPh	405 389.1 390.4 402.8±3.6	388.7	376.1	309								

^a All data from Luo, Y.-R., *Comprehensive Handbook of Chemical Bond Energies*. CRC Press: Boca Raton, FL, 2007, unless otherwise noted. Boldface values are those recommended by Luo.

^b This value, according to its original reference, actually refers to CH₂NHNO₂, not CH₂NO₂ as stated in Luo. (G3(MP2)-RAD gives 364.8)

^c This value comes from a semi-empirical correlation not a direct measurement and is very different from the other value. (G3(MP2)-RAD gives 318.3)

^d $\Delta_f H^0(R)$ is 69.9±8.4 from Luo, $\Delta_f H^0(R-CH_3)$ is -120.9±0.7 from the reference therein and $\Delta_f H^0(CH_3)$ is 146.7 from Luo, so this gives BDE(R-CH₃) 337.5±9.4. (G3(MP2)-RAD gives 346.4)

^e $\Delta_f H^0(R)$ is 190.4±12.6 from Luo, $\Delta_f H^0(R-R)$ is 101.0±1.8, so this gives BDE(R-R) 279.8±14.4. (G3(MP2)-RAD gives 291.1)

^f Exp value estimated from acidities and oxidation potential empirical fitting. (G3(MP2)-RAD gives 426.8)

^g $\Delta_f H^0(R)$ is 151.9±8.4 from Luo book and $\Delta_f H^0(R-R)$ is -17.6±0.6 from the reference therein, so this gives BDE(R-R) 321.4±9.0. (G3(MP2)-RAD gives 318.2)

Table S2. Electronegativity $\chi[\text{CH}_2\text{X}]$ obtained by equation (10), with the known $\chi[\text{Cl}] = 3.18$ and the G3(MP2)-RAD values of BDE[Cl–Cl] and BDE[XCH₂–CH₂X].
BDE[CH₃–CH₂X] obtained by equation (9), with the known $\chi[\text{CH}_3] = 2.52$, $\chi[\text{CH}_2\text{X}]$ calculated by equation (10) and the G3(MP2)-RAD value of BDE[XCH₂–CH₂X].^a

X	χ	CH ₃ –CH ₂ X, G3(MP2)-RAD	CH ₃ –CH ₂ X, eq. (9)	abs(difference)
H	2.520	370.7	370.7	0.0
BH ₂	2.490	331.4	331.4	0.0
CH ₃	2.460	368.5	369.1	0.6
NH ₂	2.360	344.4	346.8	2.4
OH	2.432	362.7	360.6	2.1
F	2.518	384.6	377.1	7.5
SiH ₃	2.525	358.0	359.1	1.1
PH ₂	2.538	356.8	357.9	1.1
SH	2.596	347.9	346.8	1.1
Cl	2.632	370.7	369.3	1.4
Br	2.656	373.4	373.8	0.4
N(CH ₃) ₂	2.278	333.9	336.6	2.7
NHCH ₃	2.500	343.6	341.9	1.7
NHCHO	2.532	347.4	350.6	3.2
NHCOCH ₃	2.513	347.8	351.7	3.9
NO ₂	2.667	379.1	369.8	9.3
OCF ₃	2.582	383.8	375.4	8.4
OCH ₂ CH ₃	2.536	363.8	360.7	3.1
OCH ₃	2.539	364.0	360.6	3.4
OCHO	2.592	377.4	371.4	6.0
OCOCH ₃	2.575	376.0	371.2	4.8
Si(CH ₃) ₃	2.472	358.2	361.0	2.8
P(CH ₃) ₂	2.447	348.8	351.8	3.0
SC(CH ₃) ₂ CN	2.635	348.8	349.6	0.8
SCH ₂ COOCH ₃	2.521	349.1	350.0	0.9
SCH ₂ Ph	2.599	346.1	347.4	1.3
SCH ₃	2.589	343.2	343.0	0.2
SO ₂ CH ₃	2.794	389.3	394.2	4.9
SOCH ₃	2.588	354.8	357.8	3.0
Ph	2.515	322.0	323.8	1.8
C ₆ H ₄ - <i>p</i> CN	2.546	321.0	322.3	1.3
C ₆ H ₄ - <i>p</i> NO ₂	2.550	322.0	323.3	1.3
C ₆ H ₄ - <i>p</i> OCH ₃	2.495	319.9	321.5	1.6
C ₆ H ₄ - <i>p</i> OH	2.501	320.2	321.9	1.7
CF ₂ CF ₃	2.681	388.8	387.7	1.1
CF ₂ H	2.639	384.4	385.2	0.8
CF ₃	2.662	390.7	388.2	2.5
CCl ₂ H	2.609	379.4	379.5	0.1
CCl ₃	2.606	385.8	383.6	2.2

Table S2. (*Continue*)

X	χ	CH ₃ –CH ₂ X, G3-RAD	CH ₃ –CH ₂ X, eq. (9)	abs(difference)
CH ₂ Cl	2.489	372.3	371.2	1.1
CH ₂ F	2.508	375.1	374.0	1.1
CH ₂ OH	2.483	371.7	371.8	0.1
CH ₂ Ph	2.467	373.5	375.1	1.6
CH(CH ₂) ₂	2.461	360.0	360.8	0.8
CH ₂ CH=CH ₂	2.468	371.7	372.3	0.6
CH ₂ CH ₃	2.456	370.3	370.8	0.5
CH(CH ₃) ₂	2.414	366.2	367.4	1.2
C(CH ₃) ₃	2.418	370.5	371.9	1.4
CCH	2.614	326.9	327.0	0.1
CH=C(CH ₃) ₂	2.474	304.0	305.4	1.4
CH=CH ₂	2.495	308.6	308.1	0.5
CH=CHCH ₃	2.480	307.3	308.1	0.8
CHO	2.640	347.6	348.0	0.4
CN	2.686	347.4	342.9	4.5
COCH ₃	2.635	351.1	352.2	1.1
CON(CH ₂ CH ₃) ₂	2.695	360.1	367.3	7.2
CON(CH ₃) ₂	2.703	361.4	368.8	7.4
CONH ₂	2.535	359.4	361.4	2.0
CONHCH ₃	2.461	355.2	354.3	0.9
COOC(CH ₃) ₃	2.639	360.0	361.3	1.3
COOCH ₂ CH ₃	2.654	359.9	361.1	1.2
COOCH ₃	2.658	360.0	361.1	1.1
COOH	2.677	360.6	362.0	1.4
COPh	2.663	353.0	357.4	4.4

^a The absolute average deviation for the 64 entries is ± 2.18 kJ mol^{–1}. Only two entries have a deviation greater than 8 kJ mol^{–1}: X = NO₂, 9.3 and X = OCF₃, 8.4. This demonstrates the validity of Pauling's scheme, the accuracy of the G3(MP2)-RAD values, and the assumption that any steric strain in BDE[XCH₂–CH₂X] is the same as in BDE[CH₃–CH₃]; the latter is generally considered to be strain-free.

Table S3. Correlation between B3LYP/6-31G(d) and G3(MP2)-RAD for Vertical ionization potentials (IP, eV) and Electron Affinities (EA, eV) for •CH₂X radicals [ΔH 0 K]

X	EA (eV)		IP (eV)	
	B3LYP/6-31G(d)	G3(MP2)-RAD	B3LYP/6-31G(d)	G3(MP2)-RAD
H	-0.10	-0.08	9.81	9.88
BH ₂	1.69	1.91	10.52	10.54
CH ₃	-0.51	-0.40	8.42	8.63
NH ₂	-1.15	-0.87	7.13	7.19
OH	-0.87	-0.79	8.11	8.21
F	-0.36	-0.36	9.44	9.61
SiH ₃	0.63	0.86	9.21	9.44
PH ₂	0.13	0.33	8.04	8.07
SH	-0.31	-0.14	7.82	7.77
Cl	-0.01	0.12	8.99	8.94
Br	0.22	0.35	8.83	8.80
N(CH ₃) ₂	-0.66	-0.36	6.34	6.37
NHCH ₃	-0.89	-0.58	6.66	6.71
NHCHO	0.02	0.06	7.49	7.53
NHCOCH ₃	-0.09	-0.02	7.17	7.25
NO ₂	2.33	2.29	11.36	11.21
OCF ₃	0.03	0.08	9.07	9.22
OCH ₂ CH ₃	-0.60	-0.44	7.54	7.61
OCH ₃	-0.61	-0.47	7.68	7.74
OCHO	0.26	0.19	8.59	8.62
OCOCH ₃	0.08	0.04	8.22	8.29
Si(CH ₃) ₃	0.52	0.78	8.37	8.79
P(CH ₃) ₂	0.40	0.65	7.23	7.29
SC(CH ₃) ₂ CN	0.41	0.63	7.66	7.67
SCH ₂ COOCH ₃	-0.07	0.16	7.31	7.33
SCH ₂ Ph	0.03	0.26	7.02	7.07
SCH ₃	-0.23	-0.02	7.29	7.26
SO ₂ CH ₃	1.50	1.68	9.82	9.94
SOCH ₃	1.07	1.26	8.41	8.38
Ph	0.77	0.88	7.02	7.39
C ₆ H ₄ - <i>p</i> CN	1.72	1.78	7.57	7.93
C ₆ H ₄ - <i>p</i> NO ₂	2.07	2.05	7.81	8.07
C ₆ H ₄ - <i>p</i> OCH ₃	0.52	0.65	6.42	6.76
C ₆ H ₄ - <i>p</i> OH	0.53	0.65	6.56	6.92
CF ₂ CF ₃	1.28	1.35	10.32	10.78
CF ₂ H	0.70	0.74	9.87	10.16
CF ₃	1.02	1.08	10.46	10.85
CCl ₂ H	1.20	1.28	9.36	9.52
CCl ₃	1.49	1.58	9.55	9.67
CH ₂ Cl	0.94	1.01	9.18	9.31
CH ₂ F	0.07	0.14	8.99	9.27
CH ₂ OH	-0.22	-0.13	8.43	8.72

Table S3. (*Continue*)

X	EA (eV)		IP (eV)	
	B3LYP/6-31G(d)	G3(MP2)-RAD	B3LYP/6-31G(d)	G3(MP2)-RAD
CH ₂ Ph	0.00	0.12	7.83	8.30
CH(CH ₂) ₂	-0.27	-0.09	7.32	7.60
CH ₂ CH=CH ₂	-0.07	0.04	8.19	8.55
CH ₂ CH ₃	-0.17	-0.01	8.25	8.51
CH(CH ₃) ₂	-0.13	0.05	8.10	8.37
C(CH ₃) ₃	-0.13	0.09	7.99	8.29
CCH	0.68	0.73	8.50	8.76
CH=C(CH ₃) ₂	0.20	0.31	6.93	7.29
CH=CH ₂	0.37	0.42	7.95	8.27
CH=CHCH ₃	0.15	0.24	7.30	7.66
CHO	1.65	1.72	10.28	10.37
CN	1.51	1.55	10.15	10.31
COCH ₃	1.43	1.54	9.81	9.96
CON(CH ₂ CH ₃) ₂	1.18	1.34	8.63	8.68
CON(CH ₃) ₂	1.17	1.31	8.81	8.89
CONH ₂	1.20	1.31	9.52	9.77
CONHCH ₃	1.09	1.21	9.05	9.26
COOC(CH ₃) ₃	1.34	1.46	9.29	9.60
COOCH ₂ CH ₃	1.35	1.46	9.48	9.79
COOCH ₃	1.37	1.47	9.64	9.91
COOH	1.50	1.58	10.11	10.32
COPh	1.79	1.92	8.94	9.38
Correlation Coefficient R	1.00	1	0.99	1

Table S4. Comparison of alternative RSE_V values for $\bullet CH_2X$ radicals^{a,b}

X	RSE_V old fit RH	RSE_V old fit RCH_3	RSE_V old fit RCl	RSE_V old fit average	RSE_V refit
H	206.3	188.5	163.2	186.0	185.7
BH ₂	157.6	139.6	149.2	148.8	147.3
CH ₃	195.4	189.6	159.7	181.6	180.9
NH ₂	166.8	169.0	137.0	157.6	157.9
OH	177.8	185.3	150.7	171.3	172.6
F	194.6	203.9	169.0	189.2	191.1
SiH ₃	192.6	173.6	156.6	174.2	173.6
PH ₂	183.8	176.0	145.5	168.5	168.5
SH	172.8	169.1	125.3	155.7	157.2
Cl	186.6	189.3	151.0	175.6	177.1
Br	190.9	191.3	154.5	178.9	180.1
N(CH ₃) ₂	165.4	158.2	135.1	152.9	154.1
NHCH ₃	165.0	168.1	121.5	151.5	153.1
NHCHO	165.9	167.9	135.5	156.4	156.5
NHCOCH ₃	166.0	169.1	136.0	157.0	157.1
NO ₂	182.0	182.3	186.5	183.6	184.3
OCF ₃	194.0	202.2	164.1	186.8	188.9
OCH ₂ CH ₃	178.5	186.3	142.1	169.0	170.7
OCH ₃	178.4	186.4	142.1	169.0	170.8
OCHO	189.2	195.4	159.3	181.3	183.2
OCOCH ₃	189.0	195.3	157.3	180.5	182.3
Si(CH ₃) ₃	193.5	175.3	158.8	175.9	174.9
P(CH ₃) ₂	182.4	168.0	147.1	165.9	164.8
SC(CH ₃) ₂ CN	171.2	167.3	130.4	156.3	157.1
SCH ₂ COOCH ₃	171.8	170.2	135.1	159.0	159.1
SCH ₂ Ph	170.2	167.1	125.5	154.3	155.3
SCH ₃	168.3	164.9	121.0	151.4	152.5
SO ₂ CH ₃	202.5	199.5	179.0	193.7	194.7
SOCH ₃	195.0	169.1	152.0	172.0	172.0
Ph	145.1	139.6	117.0	133.9	134.4
C ₆ H ₄ - <i>p</i> CN	138.7	132.0	128.3	133.0	133.0
C ₆ H ₄ - <i>p</i> NO ₂	137.4	130.1	135.9	134.5	134.1
C ₆ H ₄ - <i>p</i> OCH ₃	144.4	139.6	111.9	132.0	132.5
C ₆ H ₄ - <i>p</i> OH	144.4	139.6	112.3	132.1	132.6
CF ₂ CF ₃	206.8	199.6	183.0	196.5	197.3
CF ₂ H	206.6	198.8	175.3	193.6	193.9
CF ₃	209.5	202.8	182.8	198.4	199.4
CCl ₂ H	197.3	191.9	177.0	188.7	188.7
CCl ₃	200.0	196.3	186.5	194.3	194.6
CH ₂ Cl	192.9	186.3	175.9	185.1	185.0
CH ₂ F	200.8	193.3	167.2	187.1	187.7
CH ₂ OH	198.4	191.8	162.6	184.3	184.3
CH ₂ Ph	197.7	193.5	167.0	186.0	185.4
CH(CH ₂) ₂	186.0	181.7	149.6	172.4	171.9
CH ₂ CH=CH ₂	196.8	191.6	164.9	184.4	183.7
CH ₂ CH ₃	196.0	190.5	163.7	183.4	182.6
CH(CH ₃) ₂	197.6	186.4	163.8	182.6	181.3

Table S4. (*Continue*)

X	RSE _V old fit RH	RSE _V old fit RCH ₃	RSE _V old fit RCl	RSE _V old fit average	RSE _V refit
C(CH ₃) ₃	201.1	190.9	167.4	186.5	185.3
CCH	152.1	143.2	115.3	136.9	137.4
CH=C(CH ₃) ₂	131.0	124.5	95.9	117.1	116.6
CH=CH ₂	134.7	127.0	102.1	121.3	121.5
CH=CHCH ₃	134.3	127.5	98.9	120.2	119.7
CHO	162.3	155.5	151.0	156.3	155.5
CN	167.2	157.1	141.3	155.2	156.4
COCH ₃	168.0	161.7	152.2	160.6	160.6
CON(CH ₂ CH ₃) ₂	180.1	173.5	152.7	168.8	169.9
CON(CH ₃) ₂	181.6	174.7	153.9	170.1	171.3
CONH ₂	178.3	171.6	165.3	171.8	170.8
CONHCH ₃	179.6	168.6	163.0	170.4	170.1
COOC(CH ₃) ₃	177.8	171.7	157.4	169.0	168.4
COOCH ₂ CH ₃	177.7	171.3	156.7	168.6	168.4
COOCH ₃	177.7	171.1	157.0	168.6	168.6
COOH	177.2	170.5	159.1	168.9	168.9
COPh	168.9	162.3	156.2	162.5	162.7
MAD	11.0	6.5	18.0	0.8	0
MAX	23.0	15.6	31.9	2.2	0
R	0.975	0.968	0.929	0.999	1

^aIn this and in Tables S5 and S6, the “old fit” data was obtained using values of RSE_V[H•] = 235.8, RSE_V[CH₃•] = 190.6, RSE_V[Cl•] = 145.2, $a = -12.88 \text{ kJ mol}^{-1} \text{ eV}^{-2}$ and $b = -216.50 \text{ kJ mol}^{-1}$; these are the originally published values, taken from de Vleeschouwer, F.; Van Speybroeck, V.; Waroquier, M.; Geerlings, P.; de Proft, F., *J. Org. Chem.* **2008**, 73, 9109–9120.

^bThe refit values were obtained by refitting the RSE_V scheme to our set high-level ab initio BDE data. This fitting was performed separately for the primary, secondary and tertiary radicals. In each case, the RSE_V values for all R• species, along with values of the other unknown parameters, were obtained via a 69 parameter fit to all of the corresponding R-H, R-Cl and R-CH₃ BDE data. For the primary radicals, the additional parameters obtained were RSE_V[H•] = 241.8, RSE_V[CH₃•] = 190.3, RSE_V[Cl•] = 126.7, $a = -2.62 \text{ kJ mol}^{-1} \text{ eV}^{-2}$ and $b = -420.80 \text{ kJ mol}^{-1}$. The mean absolute deviation (MAD), maximum absolute deviation (MAX) and correlation coefficients between these values and each of the alternative estimates are provided in the Table.

Table S5. Comparison of alternative RSEV values for $\bullet\text{CH}(\text{CH}_3)\text{X}$ radicals^a

X	RSEV old fit RH	RSEV old fit RCH ₃	RSEV old fit RCl	RSEV old fit average	RSEV refit
H	195.4	189.6	159.7	181.6	179.9
BH ₂	136.2	124.2	127.3	129.2	125.8
CH ₃	187.3	190.4	159.1	178.9	176.8
NH ₂	162.6	173.6	140.0	158.7	155.7
OH	173.8	185.2	150.9	170.0	167.8
F	189.7	204.5	166.2	186.8	186.5
SiH ₃	177.8	170.9	151.0	166.6	164.4
PH ₂	177.8	175.8	143.9	165.8	164.6
SH	168.4	175.2	131.7	158.5	158.7
Cl	181.5	190.4	150.5	174.1	174.7
Br	184.7	191.4	153.2	176.5	177.1
N(CH ₃) ₂	157.6	163.3	138.8	153.2	148.7
NHCH ₃	162.1	169.2	140.4	157.3	153.4
NHCHO	164.0	172.3	138.4	158.2	157.0
NHCOCH ₃	165.2	173.6	130.8	156.6	156.6
NO ₂	165.1	172.8	169.6	169.2	169.1
OCF ₃	187.7	198.2	153.1	179.7	181.2
OCH ₂ CH ₃	174.7	182.3	146.0	167.7	165.9
OCH ₃	174.7	182.3	152.2	169.7	166.8
OCHO	184.4	195.2	152.7	177.4	178.7
OCOCH ₃	184.5	195.8	160.5	180.3	179.6
Si(CH ₃) ₃	178.7	172.8	153.9	168.5	165.4
P(CH ₃) ₂	170.9	174.6	148.9	164.8	162.5
SC(CH ₃) ₂ CN	166.0	166.8	132.1	155.0	154.8
SCH ₂ COOCH ₃	168.9	169.1	137.7	158.6	156.7
SCH ₂ Ph	166.0	172.8	132.4	157.1	156.9
SCH ₃	164.6	169.4	131.8	155.3	154.3
SO ₂ CH ₃	188.1	191.3	177.3	185.6	184.7
SOCH ₃	160.8	164.9	137.3	154.3	153.1
Ph	138.7	138.8	117.8	131.8	129.5
C ₆ H ₄ - <i>p</i> CN	131.0	129.9	127.2	129.4	126.6
C ₆ H ₄ - <i>p</i> NO ₂	126.6	125.0	131.9	127.8	124.7
C ₆ H ₄ - <i>p</i> OCH ₃	138.5	138.7	113.7	130.3	128.1
C ₆ H ₄ - <i>p</i> OH	138.8	139.5	114.1	130.8	128.7
CF ₂ CF ₃	191.9	187.8	166.6	182.1	182.0
CF ₂ H	195.7	197.6	169.3	187.5	187.2
CF ₃	196.7	198.0	172.8	189.1	189.2
CCl ₂ H	184.2	186.6	173.6	181.5	179.8
CCl ₃	186.4	186.1	175.0	182.5	181.3
CH ₂ Cl	179.6	181.9	170.0	177.2	174.5
CH ₂ F	191.9	195.2	164.8	183.9	182.7
CH ₂ OH	192.1	195.7	163.1	183.6	182.2
CH ₂ Ph	189.2	193.6	165.4	182.7	180.6
CH(CH ₂) ₂	181.6	186.4	150.2	172.7	171.2
CH ₂ CH=CH ₂	188.5	192.0	163.3	181.3	179.1
CH ₂ CH ₃	190.4	191.2	162.0	181.2	178.9
CH(CH ₃) ₂	185.1	186.2	160.7	177.3	174.3

Table S5. (*Continue*)

X	RSE _V old fit RH	RSE _V old fit RCH ₃	RSE _V old fit RCl	RSE _V old fit average	RSE _V refit
C(CH ₃) ₃	189.8	183.9	159.4	177.7	174.5
CCH	142.8	143.1	113.3	133.1	132.6
CH=C(CH ₃) ₂	123.1	125.8	89.2	112.7	111.9
CH=CH ₂	123.6	125.7	98.6	115.9	114.2
CH=CHCH ₃	126.0	128.5	96.5	117.0	115.5
CHO	144.9	142.5	138.8	142.0	139.9
CN	153.8	152.8	133.1	146.5	146.8
COCH ₃	148.7	144.9	138.2	143.9	141.6
CON(CH ₂ CH ₃) ₂	164.6	163.2	142.2	156.6	155.8
CON(CH ₃) ₂	165.9	162.7	142.7	157.1	156.1
CONH ₂	161.9	161.4	151.0	158.1	155.6
CONHCH ₃	159.2	163.8	151.0	158.0	155.5
COOC(CH ₃) ₃	161.7	160.6	144.3	155.6	154.4
COOCH ₂ CH ₃	161.4	159.6	142.6	154.5	153.6
COOCH ₃	161.3	159.4	142.3	154.3	153.5
COOH	160.5	157.8	143.7	154.0	153.1
COPh	151.1	147.0	139.8	146.0	144.5
MAD	8.4	10.6	14.7	1.6	0
MAX	15.4	18.0	28.0	4.5	0
R	0.987	0.977	0.926	0.998	1

^AThe refit values were obtained by refitting the RSE_V scheme to our set high-level ab initio BDE data. This fitting was performed separately for the primary, secondary and tertiary radicals. In each case, the RSE_V values for all R• species, along with values of the other unknown parameters, were obtained via a 69 parameter fit to all of the corresponding R-H, R-Cl and R-CH₃ BDE data. For the secondary radicals, the additional parameters obtained RSE_V[H•] = 237.2, RSE_V[CH₃•] = 191.9, RSE_V[Cl•] = 125.9, $a = -1.05 \text{ kJ mol}^{-1} \text{ eV}^{-2}$ and $b = -494.96 \text{ kJ mol}^{-1}$. The mean absolute deviation (MAD), maximum absolute deviation (MAX) and correlation coefficients between these values and each of the alternative estimates are provided in the Table.

Table S6. Comparison of alternative RSE_V values for $\bullet C(CH_3)_2X$ radicals^a

X	RSE_V old fit RH	RSE_V old fit RCH ₃	RSE_V old fit RCl	RSE_V old fit average	RSE_V refit
H	187.3	190.4	159.1	178.9	176.4
BH ₂	111.2	112.7	131.9	118.6	110.8
CH ₃	182.3	191.2	159.9	177.8	174.9
NH ₂	161.1	172.1	140.8	158.0	153.9
OH	170.5	186.4	152.0	169.6	166.8
F	186.5	203.6	165.3	185.1	184.1
SiH ₃	165.9	168.6	148.6	161.0	157.8
PH ₂	169.5	175.9	143.9	163.1	161.2
SH	165.9	174.9	134.2	158.3	157.8
Cl	178.3	190.1	150.2	172.9	173.0
Br	180.5	190.3	152.2	174.3	174.4
N(CH ₃) ₂	162.9	164.2	140.4	155.8	150.3
NHCH ₃	161.5	167.2	141.3	156.7	151.6
NHCHO	172.3	179.3	141.5	164.3	163.2
NHCOCH ₃	175.2	181.5	143.2	166.6	165.3
NO ₂	157.2	164.7	156.7	159.5	159.1
OCF ₃	187.8	192.0	152.5	177.4	177.5
OCH ₂ CH ₃	175.1	183.0	153.9	170.7	166.8
OCH ₃	175.3	183.0	153.8	170.7	166.9
OCHO	191.2	195.9	161.5	182.9	182.1
OCOCH ₃	191.7	195.9	159.9	182.5	181.6
Si(CH ₃) ₃	166.8	170.6	151.6	163.0	158.9
P(CH ₃) ₂	170.8	171.7	149.3	163.9	160.1
SC(CH ₃) ₂ CN	163.8	163.0	141.3	156.0	153.5
SCH ₂ COOCH ₃	161.8	168.7	141.4	157.3	154.9
SCH ₂ Ph	169.5	172.9	139.2	160.5	159.0
SCH ₃	164.7	172.1	138.6	158.4	156.3
SO ₂ CH ₃	176.1	184.1	169.9	176.7	175.1
SOCH ₃	154.0	161.6	136.1	150.6	148.3
Ph	137.9	139.1	118.2	131.8	128.8
C ₆ H ₄ - <i>p</i> CN	129.1	129.7	127.2	128.7	125.0
C ₆ H ₄ - <i>p</i> NO ₂	127.3	127.1	133.9	129.4	125.3
C ₆ H ₄ - <i>p</i> OCH ₃	138.1	140.2	116.2	131.5	128.3
C ₆ H ₄ - <i>p</i> OH	138.6	140.6	116.4	131.9	128.9
CF ₂ CF ₃	177.2	177.2	153.8	169.4	168.6
CF ₂ H	189.6	197.4	168.0	185.0	184.0
CF ₃	188.6	195.8	168.6	184.3	183.7
CCl ₂ H	174.3	179.2	165.5	173.0	170.5
CCl ₃	178.9	181.5	168.0	176.1	174.3
CH ₂ Cl	170.1	178.0	166.0	171.4	167.9
CH ₂ F	185.6	194.1	163.8	181.2	179.2
CH ₂ OH	186.4	194.8	171.6	184.3	180.4
CH ₂ Ph	181.6	188.7	162.5	177.6	174.4
CH(CH ₂) ₂	179.9	182.8	151.6	171.4	168.1
CH ₂ CH=CH ₂	183.7	190.1	163.7	179.2	175.7
CH ₂ CH ₃	184.9	191.1	163.1	179.7	176.2
CH(CH ₃) ₂	181.9	184.6	158.0	174.8	170.9

Table S6. (*Continue*)

X	RSE _V old fit RH	RSE _V old fit RCH ₃	RSE _V old fit RCl	RSE _V old fit average	RSE _V refit
C(CH ₃) ₃	182.4	181.0	154.2	172.5	168.7
CCH	135.6	142.0	112.3	130.0	128.8
CH=C(CH ₃) ₂	132.0	120.4	99.0	117.1	112.9
CH=CH ₂	119.7	125.4	101.1	115.4	112.6
CH=CHCH ₃	122.3	127.9	99.6	116.6	113.9
CHO	128.9	135.0	130.9	131.6	128.3
CN	145.5	151.1	129.6	142.0	141.6
COCH ₃	139.4	142.1	135.9	139.1	135.6
CON(CH ₂ CH ₃) ₂	167.0	150.3	139.0	152.1	148.0
CON(CH ₃) ₂	161.4	145.5	135.1	147.3	143.2
CONH ₂	154.4	156.9	147.7	153.0	149.1
CONHCH ₃	156.4	158.4	147.8	154.2	150.1
COOC(CH ₃) ₃	150.8	155.9	140.2	148.9	146.7
COOCH ₂ CH ₃	149.8	154.5	138.3	147.5	145.5
COOCH ₃	149.8	154.2	137.9	147.3	145.4
COOH	147.9	152.1	137.5	145.8	144.1
COPh	143.8	131.5	133.1	136.2	131.7
MAD	7.6	11.7	12.3	2.7	0
MAX	19.1	19.5	25.0	7.8	0
R	0.980	0.986	0.917	0.998	1

^aThe refit values were obtained by refitting the RSE_V scheme to our set high-level ab initio BDE data. This fitting was performed separately for the primary, secondary and tertiary radicals. In each case, the RSE_V values for all R• species, along with values of the other unknown parameters, were obtained via a 69 parameter fit to all of the corresponding R-H, R-Cl and R-CH₃ BDE data. For the tertiary radicals, the additional parameters obtained were RSE_V[H•] = 235.4, RSE_V[CH₃•] = 191.6, RSE_V[Cl•] = 126.5 $a = -0.28 \text{ kJ mol}^{-1} \text{ eV}^{-2}$ and $b = -524.91 \text{ kJ mol}^{-1}$. The mean absolute deviation (MAD), maximum absolute deviation (MAX) and correlation coefficients between these values and each of the alternative estimates are provided in the Tables.

Table S7. B3-LYP/6-31G(d) Optimized Geometries of All Species

r.CH2-H

```
1\1\GINC-AC26\FOpt\UB3LYP\Gen\C1H3(2)\CYL509\07-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-H.freq
q\0,2\C,0.0001306759,-0.0002263373,0.0000924018\H,-0.1806991463,0.312
9798271,1.0205249217\H,0.9019270919,0.3129800721,-0.5105395821\H,-0.72
20120012,-0.6246018754,-0.5105397505\Version=IA64L-G03RevC.02\State=2
-A1\HF=-39.8382918\S2=0.753763\S2-1=0.\S2A=0.750007\RMSD=7.619e-09\RMS
F=4.401e-05\Dipole=-0.0003492,0.0006049,-0.0002469\PG=C03V [C3(C1),3SG
V(H1)]\@
```

r.CH2-BH2

```
1\1\GINC-AC24\FOpt\UB3LYP\Gen\C1H4B1(2)\CYL509\07-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-BH2
.a2.freq\0,2\H,-0.7209361012,0.,-1.601996078\B,-0.7089367594,0.,-0.40
50969317\C,0.6216810162,0.,0.3554263943\H,-1.7468278907,0.,0.191117595
5\H,1.5930046028,0.,-0.1396837943\H,0.689357089,0.,1.4434885694\Versi
on=IA64L-G03RevC.02\State=2-A\HF=-65.2889331\S2=0.752239\S2-1=0.\S2A=
0.750003\RMSD=4.302e-09\RMSF=8.006e-05\Dipole=0.4438491,0.,0.2537044\PG
=CS [SG(C1H4B1)]\@
```

r.CH2-CH3

```
1\1\GINC-AC25\FOpt\UB3LYP\Gen\C2H5(2)\CYL509\07-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH3.f
req\0,2\H,0.1074003772,-0.2545598811,-1.4786668365\C,0.1598875097,-0.
5304406965,-0.4180619694\H,1.1914474844,-0.885156083,-0.2400720999\H,-
0.4953492395,-1.3961091701,-0.2601594361\C,-0.2046679109,0.6089732983,
0.4693261846\H,0.0536841473,1.6285774495,0.2016220847\H,-0.5885003624,
0.436052074,1.4696909963\Version=IA64L-G03RevC.02\State=2-A\HF=-79.15
78677\S2=0.753923\S2-1=0.\S2A=0.75001\RMSD=6.275e-09\RMSF=9.548e-05\Di
pole=0.0670585,-0.0670456,-0.0291779\PG=C01 [X(C2H5)]\@
```

r.CH2-NH2

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C1H4N1(2)\CYL509\08-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-NH2
.freq\0,2\H,-1.2846814137,0.357125054,-0.4893762938\N,-0.2704425663,0
.3924852644,-0.4653621097\C,0.3075448276,-0.4139656835,0.5247795453\H,
0.0996677384,0.2346705042,-1.3973752729\H,-0.1572676756,-0.3594778836,
1.504979471\H,1.390110349,-0.4959204249,0.4906295919\Version=IA64L-G0
3RevC.02\State=2-A\HF=-95.1956132\S2=0.752852\S2-1=0.\S2A=0.750006\RMS
D=3.467e-09\RMSF=5.491e-05\Dipole=-0.2606904,-0.042382,-0.391633\PG=C0
1 [X(C1H4N1)]\@
```

r.CH2-OH

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C1H3O1(2)\CYL509\07-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OH.
freq\0,2\C,0.1106398254,0.0569512135,-0.6795123821\O,-0.1914071212,0.
0128080668,0.6561407744\H,1.0087069959,-0.4515268754,-1.0266745698\H,-
0.7733091749,0.0724077704,-1.3064243047\H,0.6320201967,-0.06505271,1.1
610469719\Version=IA64L-G03RevC.02\State=2-A\HF=-115.0520322\S2=0.752
931\S2-1=0.\S2A=0.750006\RMSD=5.074e-09\RMSF=3.420e-05\Dipole=0.562274
9,-0.2206395,0.075964\PG=C01 [X(C1H3O1)]\@
```

r.CH2-F

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C1H2F1(2)\CYL509\07-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-F.f
req\0,2\H,0.1116846938,-0.3484851126,-1.4363565642\C,0.282410658,-0.4
640804249,-0.3707604674\H,1.2053526578,-0.8617580552,0.0391605493\F,-0
```

```
.3346112555,0.443858413,0.4024176466\\Version=IA64L-G03RevC.02\\State=2-A'\\HF=-139.0642653\\S2=0.753039\\S2-1=0.\\S2A=0.750006\\RMSD=2.849e-09\\RMSF=1.096e-05\\Dipole=0.3214173,-0.203413,-0.3089969\\PG=CS [SG(C1F1),X(H2)]\\@
```

r.CH2-SiH3

```
1\\1\\GINC-AC28\\FOpt\\UB3LYP\\Gen\\C1H5Si1(2)\\CYL509\\07-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-SiH3.freq\\0,2\\H,-0.8010849429,-0.0000002202,-1.6007382325\\Si,-0.561547062,0.0000000723,-0.1262087726\\C,1.2442908638,-0.0000001621,0.2858913467\\H,-1.2223828389,1.2130664535,0.4292986449\\H,-1.2223833572,-1.2130657874,0.4292991503\\H,1.8208823427,-0.9158775028,0.396857312\\H,1.8208824816,0.9158770011,0.3968578617\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-330.5397094\\S2=0.75373\\S2-1=0.\\S2A=0.750009\\RMSD=5.804e-09\\RMSF=7.022e-05\\Dipole=0.2953433,0.,0.0495055\\PG=C01 [X(C1H5Si1)]\\@
```

r.CH2-PH2

```
1\\1\\GINC-AC25\\FOpt\\UB3LYP\\Gen\\C1H4P1(2)\\CYL509\\07-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-PH2.freq\\0,2\\H,-1.3233587167,-0.8999578828,-0.1439881133\\P,-0.5320580425,0.2666753488,0.0608075604\\H,-0.5744809581,0.2229567758,1.4839801095\\C,1.1024160705,-0.4019513226,-0.2298680271\\H,1.9593006817,0.0349043822,0.2748303589\\H,1.3049132069,-0.9463255708,-1.1477275982\\Version=IA64L-G03RevC.02\\State=2-A'\\HF=-381.7900041\\S2=0.754914\\S2-1=0.\\S2A=0.750018\\RMSD=5.941e-09\\RMSF=4.894e-05\\Dipole=0.1236564,-0.2019903,0.0824429\\PG=CS [SG(C1P1),X(H4)]\\@
```

r.CH2-SH

```
1\\1\\GINC-AC29\\FOpt\\UB3LYP\\Gen\\C1H3S1(2)\\CYL509\\07-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-SH.freq\\0,2\\H,-0.7745611673,0.0516164395,-1.2888878107\\S,-0.0056449699,0.5207112331,-0.2831102115\\C,0.0645740821,-0.9357335354,0.6660664268\\H,-0.1253299825,-1.9033727761,0.2197753672\\H,0.6027661753,-0.8652221798,1.6024772676\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-438.0341151\\S2=0.753958\\S2-1=0.\\S2A=0.750012\\RMSD=2.330e-09\\RMSF=1.625e-05\\Dipole=-0.1024562,-0.3569473,-0.1990203\\PG=C01 [X(C1H3S1)]\\@
```

r.CH2-Cl

```
1\\1\\GINC-AC29\\FOpt\\UB3LYP\\Gen\\C1H2Cl1(2)\\CYL509\\08-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-Cl.freq\\0,2\\Cl,-0.0765088803,0.03524678,-0.5828350523\\C,0.135831355,-0.0799738855,1.1148214487\\H,0.9691749048,-0.6648539499,1.4774017939\\H,-0.48351207,0.5455020026,1.7418654026\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-499.4383238\\S2=0.754062\\S2-1=0.\\S2A=0.750011\\RMSD=3.255e-09\\RMSF=4.949e-05\\Dipole=0.092837,0.0096899,0.4664736\\PG=C01 [X(C1H2Cl1)]\\@
```

r.CH2-Br

```
1\\1\\GINC-AC24\\FOpt\\UB3LYP\\Gen\\C1H2Br1(2)\\CYL509\\07-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-Br.freq\\0,2\\Br,-0.0229788898,0.1332836283,-0.3457210239\\C,0.0843573436,-0.5153654142,1.4060951769\\H,1.0498709565,-0.4795171953,1.8902564296\\H,-0.7517538765,-1.0932173111,1.7734083442\\Version=IA64L-G03RevC.02\\State=2-A'\\HF=-2613.1236075\\S2=0.754354\\S2-1=0.\\S2A=0.750013\\RMSD=8.668e-09\\RMSF=4.625e-05\\Dipole=0.0519107,-0.2259276,0.3862134\\PG=CS [SG(C1Br1),X(H2)]\\@
```

r.CH2-N_CH3_2

```
1\\1\\GINC-AC1\\FOpt\\UB3LYP\\Gen\\C3H8N1(2)\\CYL509\\07-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2-N_CH
```

3_2.freq\0,2\C,0.5698257945,-0.0228208525,1.2667579461\H,1.6643806807
,0.0103773169,1.2351430223\H,0.2685801126,-0.8602390582,1.9036891151\H
,0.2060517646,0.9108862103,1.7299400855\N,0.0466173999,-0.2233285042,-
0.0740692376\C,-1.2839819621,-0.6157506129,-0.176971701\C,0.525038833,
0.7374272457,-1.0537529142\H,-1.632621702,-1.3117291856,0.5804548864\H
, -1.666728968,-0.7327524173,-1.1866597672\H,1.6203131022,0.7583757136,
-1.0462887324\H,0.1555743634,1.7599213547,-0.8621998916\H,0.1928328541
,0.4353249134,-2.0517940405\Version=IA64L-G03RevC.02\State=2-A\HF=-17
3.8171353\S2=0.753011\S2-1=0.\S2A=0.750006\RMSD=3.842e-09\RMSF=4.013e-
05\Dipole=0.3902836,0.1641793,0.0463006\PG=C01 [X(C3H8N1)]\@

r.CH2-NHCH3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C2H6N1(2)\CYL509\07-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-NH
CH3.freq\0,2\C,0.9171466646,0.0649663476,0.7789658539\H,1.9909701362,0
.0849039463,0.5683603176\H,0.700011807,-0.8507249269,1.3403650974\H,0.
6649760032,0.9237250854,1.4225269963\N,0.1746362123,0.0389816212,-0.47
14002489\C,-1.2095979305,-0.1142931682,-0.4185184175\H,-1.5729161191,-
0.8450930201,0.2996421084\H,-1.7287085292,-0.0438277023,-1.3699059764\H
,0.4779208114,0.7541061923,-1.123871419\Version=IA64L-G03RevC.02\Sta
te=2-A\HF=-134.5056116\S2=0.752884\S2-1=0.\S2A=0.750006\RMSD=3.125e-09
\RMSF=1.202e-05\Dipole=0.4055181,0.2110202,0.0122498\PG=C01 [X(C2H6N1)]\@

r.CH2-NHCHO

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C2H4N1O1(2)\CYL509\08-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-N
HCHO.freq\0,2\H,0.671305094,-0.129763781,-1.8117874377\C,0.5549186255
,0.0502346592,-0.7276432011\O,1.4325933132,0.5090310613,-0.0166652276\N
, -0.6984997208,-0.3056302998,-0.2763053791\C,-1.116075322,-0.18888748
48,1.0299101639\H,-1.3450333886,-0.6766875293,-0.9613462823\H,-0.41280
87457,0.2057899152,1.7453830818\H,-2.1177712401,-0.5002580429,1.281608
3362\Version=IA64L-G03RevC.02\State=2-A\HF=-208.5409695\S2=0.756344\S
2-1=0.\S2A=0.750025\RMSD=4.318e-09\RMSF=5.783e-05\Dipole=-1.2815155,-0
.5753885,-0.5612492\PG=C01 [X(C2H4N1O1)]\@

r.CH2-NHCOCH3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H6N1O1(2)\CYL509\07-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-N
HCOCH3.freq\0,2\H,-0.5347779547,2.1301930267,-1.2120424453\C,0.104688
6551,1.2524195969,-1.3512267882\C,0.1245506498,0.4456316294,-0.0648818
277\H,1.1156211596,1.618342813,-1.5584507188\H,-0.2517736359,0.6922022
079,-2.222056777\N,-0.306582378,-0.8667982585,-0.1793014155\O,0.493299
2852,0.9088414467,1.0061363518\C,-0.3588467642,-1.7497379498,0.8756220
723\H,-0.5988061849,-1.1911850061,-1.0910993481\H,-0.0438792265,-1.389
0530378,1.841554276\H,-0.7090570369,-2.7535234274,0.69103337\Version=
IA64L-G03RevC.02\State=2-A\HF=-247.8643916\S2=0.755475\S2-1=0.\S2A=0.7
5002\RMSD=7.169e-09\RMSF=8.533e-06\Dipole=-0.4731401,-0.6916758,-1.230
8479\PG=C01 [X(C3H6N1O1)]\@

r.CH2-NO2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C1H2N1O2(2)\CYL509\07-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-N
O2.freq\0,2\O,-0.1036357482,0.2960757251,-1.2522775028\N,-0.091746568
8,-0.0004381995,-0.0479187553\C,1.1595710086,0.0061187849,0.6058221312
\O,-1.0846442189,-0.3023307576,0.6314611224\H,2.0232492039,0.269108682
7,0.0121861753\H,1.167790467,-0.2527137326,1.6548433586\Version=IA64L
-G03RevC.02\State=2-A\HF=-244.3393225\S2=0.756296\S2-1=0.\S2A=0.750027
\RMSD=8.469e-09\RMSF=3.637e-05\Dipole=1.3096093,0.0068014,0.6841764\PG

=C01 [X(C1H2N1O2)]\@

r.CH2-OCF3

1\1\GINC-AC22\FOpt\UB3LYP\Gen\C2H2F3O1(2)\CYL509\08-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OCF3.freq\0,2\C,1.9673353746,-0.1424287783,0.082179597\O,0.7803381465,-0.5895732424,-0.4657639589\C,-0.3647962161,-0.0022804325,-0.0230881087\F,-0.3617655025,1.3289428028,-0.2355062196\F,-0.5554754397,-0.1949402882,1.2929658376\F,-1.3808798312,-0.5410352137,-0.6914082439\H,2.0023381158,0.8809874159,0.4370396421\H,2.822808722,-0.6328519199,-0.3599392673\Version=IA64L-G03RevC.02\State=2-A\HF=-452.0950668\S2=0.753009\S2-1=0.\S2A=0.750006\RMSD=4.683e-09\RMSF=2.806e-06\Dipole=0.585771,0.1616606,-0.0046338\PG=C01 [X(C2H2F3O1)]\@

r.CH2-OCH2CH3

1\1\GINC-AC2\FOpt\UB3LYP\Gen\C3H7O1(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OCH2CH3.freq\0,2\H,-0.1642570143,-2.1810303628,1.5132047817\C,-0.1149394976,-1.7148648479,0.5231208442\C,0.0068815243,-0.2075841495,0.6590146364\O,0.072184578,0.3584455256,-0.6510574659\C,0.1190228957,1.7160568764,-0.6952588733\H,0.1046220398,2.1067307066,-1.7067267122\H,-0.3638069829,2.2692951309,0.1107185271\H,-0.8597073428,0.2124112829,1.1928717205\H,0.9110864412,0.0688251158,1.2194601886\H,0.7488282021,-2.1241779964,-0.0102794227\H,-1.0200315008,-1.9812653565,-0.0320489994\Version=IA64L-G03RevC.02\State=2-A\HF=-193.6811985\S2=0.752876\S2-1=0.\S2A=0.750006\RMSD=9.991e-09\RMSF=1.246e-05\Dipole=-0.1801712,-0.1086938,0.4704357\PG=C01 [X(C3H7O1)]\@

r.CH2-OCH3

1\1\GINC-AC13\FOpt\UB3LYP\Gen\C2H5O1(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OCH3.freq\0,2\C,-0.5868137744,0.1805443982,-0.9728610811\O,-0.3313784912,-0.266250232,0.3507094221\C,0.8951241197,0.0608719608,0.8378447329\H,0.1630757752,-0.2150687333,-1.6729753484\H,-1.5740856658,-0.1947812813,-1.2499300816\H,-0.5820897739,1.2769768908,-1.0256981957\H,1.0782303334,-0.3463290077,1.8259076049\H,1.7160351892,0.1607058332,0.1271187337\Version=IA64L-G03RevC.02\State=2-A\HF=-154.361818\S2=0.752854\S2-1=0.\S2A=0.750006\RMSD=1.851e-09\RMSF=4.448e-05\Dipole=0.1126662,0.0762611,-0.5111519\PG=C01 [X(C2H5O1)]\@

r.CH2-OCHO

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C2H3O2(2)\CYL509\08-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OCHO.a4.freq\0,2\C,-0.8642876238,0.0015556494,-1.1866197928\O,-0.8496437027,0.0135802828,0.181978068\C,0.3563180851,0.0184024234,0.8152884054\H,0.1778550578,0.0430352993,1.8979294944\O,1.4311661578,-0.0021457474,0.2743406889\H,0.0685448072,-0.1349331185,-1.7137259327\H,-1.8507622738,-0.1193269004,-1.6067652923\Version=IA64L-G03RevC.02\State=2-A\HF=-228.3941012\S2=0.753919\S2-1=0.\S2A=0.750011\RMSD=8.888e-09\RMSF=3.552e-05\Dipole=-0.640719,-0.072987,0.026719\PG=C01 [X(C2H3O2)]\@

r.CH2-OCOCH3

1\1\GINC-AC21\FOpt\UB3LYP\Gen\C3H5O2(2)\CYL509\08-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-OCOCH3.freq\0,2\C,-1.905114131,-0.1763642249,0.0368443064\O,-0.6370604526,-0.6896001766,0.0021608039\C,0.4200720707,0.1906873363,-0.0007645477\C,1.724156888,-0.5638126627,-0.0041346673\O,0.2798916124,1.3897791853,0.0007450983\H,-2.0316910455,0.8886815224,-0.0933007903\H,-2.67314157,-0.9205091033,-0.1121097795\H,2.5512016717,0.1459801217,-0.036290697\

H,1.7734990768,-1.2344354161,-0.8683303947\H,1.802793623,-1.1842118864
,0.8951138953\\Version=IA64L-G03RevC.02\State=2-A\HF=-267.7202613\S2=0
.753536\S2-1=0.\S2A=0.750008\RMSD=8.223e-09\RMSF=1.604e-05\Dipole=0.10
58213,-0.713767,-0.0885621\PG=C01 [X(C3H5O2)]\\@

r.CH2-Si_CH3_3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C4H11Si1(2)\CYL509\07-Apr-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-S
i_CH3_3.freq\0,2\H,0.8288341648,-1.5873111441,-1.7557552759\C,0.80276
9826,-1.5686941027,-0.6593599998\H,1.8387705545,-1.6326822016,-0.30446
01927\H,0.2802348166,-2.472477944,-0.3248142613\Si,-0.0446369748,-0.00
0457738,-0.0155009096\C,-1.785675749,0.0726156995,-0.6758007078\C,-0.0
94696763,-0.0142380584,1.8790493774\C,0.9449513912,1.5152602816,-0.593
8160289\H,-2.0756011484,-0.343624311,-1.6404162271\H,-2.6021756539,0.5
683588351,-0.1510511612\H,1.9722203832,1.4798893358,-0.2089687541\H,0.
489406368,2.4486095524,-0.2428472694\H,1.00020358,1.563868877,-1.68762
84534\H,0.9174658585,-0.0369453979,2.3013726914\H,-0.6333424362,-0.890
1244184,2.2591453566\H,-0.5951910715,0.8791842293,2.2720004371\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-448.5215463\S2=0.753497\S2-1=0.\S2A=0
.750007\RMSD=6.356e-09\RMSF=1.585e-05\Dipole=0.0040991,0.0129701,-0.00
64929\PG=C01 [X(C4H11Si1)]\\@

r.CH2-P_CH3_2

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C3H8P1(2)\CYL509\07-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-P_C
H3_2.freq\0,2\C,-0.6043728577,1.3581271762,0.7725432939\H,0.109584763
8,2.1376672468,1.0579490898\H,-1.2624975541,1.1772631757,1.6287700074\
H,-1.2019287669,1.7171638069,-0.0720691284\P,0.3247766219,-0.207605221
8,0.3656290714\C,-1.0246344648,-1.278092013,-0.3510044696\C,1.27634798
14,0.248851217,-1.0613045797\H,-0.5787818245,-2.1803222678,-0.78236356
08\H,-1.5967809057,-0.759666652,-1.1276859396\H,-1.7036634297,-1.59008
45043,0.4493357317\H,1.8729083427,1.1581762153,-1.0423923202\H,1.60546
61002,-0.5194369267,-1.7573853983\\Version=IA64L-G03RevC.02\State=2-A\
HF=-460.4328518\S2=0.756236\S2-1=0.\S2A=0.750024\RMSD=8.621e-09\RMSF=8
.251e-06\Dipole=-0.3586176,0.1250715,-0.1593189\PG=C01 [X(C3H8P1)]\\@

r.CH2-SC_CH3_2CN

1\1\GINC-SC117\FOpt\UB3LYP\6-31G(d)\C5H8N1S1(2)\MLC501\23-Sep-2002\0\#\n
UB3LYP/6-31G(D) OPT=(MAXCYC=100) FREQ MAXDISK=52428800 GEOM=CHECK\
ch2scme2cn-clb-6dub3\0,2\C,2.216203809,-0.0104805434,-0.1549408816\H,
2.2124891486,-0.0104815977,0.9305891576\H,3.1568671101,-0.0197233775,-
0.6925761048\S,0.8286229278,-0.5339169106,-1.0366526174\C,-0.599969057
1,0.1901463328,-0.0522060574\C,-0.5915749507,1.7270808565,-0.146789857
3\C,-1.8833176522,-0.4115520613,-0.6559343429\C,-0.4582679961,-0.22442
8565,1.3499281472\H,0.3497812116,2.1362691642,0.2283017181\H,-0.712347
3903,2.0280941129,-1.1915585968\H,-1.4165004748,2.1450622339,0.4414051
552\H,-1.9564943352,-0.1369539714,-1.7131055672\H,-2.7597863423,-0.015
4848027,-0.133271841\H,-1.8901665774,-1.5015087304,-0.5724657191\N,-0.
3343220162,-0.5295997971,2.4641116613\\Version=DEC-AXP-OSF/1-G98RevA.1
1.3\HF=-648.2151962\S2=0.755015\S2-1=0.\S2A=0.750017\RMSD=7.231e-09\RM
SF=2.917e-06\Dipole=-0.3235252,0.5904565,-1.0178268\PG=C01 [X(C5H8N1S1
)\\@

r.CH2-SCH2COOCH3

1\1\GINC-SC123\FOpt\UB3LYP\6-31G(d)\C4H7O2S1(2)\MLC501\20-Sep-2002\1\#\n
UB3LYP/6-31G(D) OPT=(Z-MATRIX,MAXCYC=100) FREQ MAXDISK=52428800 GEO
M=CHECK\ch2sch2co2ch3-clp-6dub3\0,2\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,B
7,5,A6,7,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\
B1=1.73218229\B2=1.08339889\B3=1.08374008\B4=1.84209974\B5=1.51467098\
B6=1.21315793\B7=1.34658231\B8=1.43874406\B9=1.09170656\B10=1.09162575
\B11=1.09303436\B12=1.09303538\B13=1.09003054\A1=115.86996819\A2=120.0
2408378\A3=101.45128476\A4=111.37524829\A5=124.40766091\A6=111.3920199
9\A7=115.34855438\A8=108.87789335\A9=105.81007532\A10=110.50131068\A11
=110.36047466\A12=105.48128035\D1=-159.27059229\D2=183.88538086\D3=-67
.25514346\D4=86.64066542\D5=-178.52626952\D6=176.73687142\D7=120.66718
891\D8=-120.75782314\D9=60.16144943\D10=-120.73140431\D11=119.69454139
\\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-705.2213851\S2=0.754133\S2-1=
0.\S2A=0.750013\RMSD=5.196e-09\RMSF=3.766e-05\Dipole=-0.320091,-0.3251
822,-0.5102612\PG=C01 [X(C4H7O2S1)]\\@
```

r.CH2-SCH2Ph

```
1\1\GINC-SC90\FOpt\UB3LYP\6-31G(d)\C8H9S1(2)\MLC501\24-Jan-2003\0\#N
B3LYP/6-31G(D) OPT FREQ MAXDISK=39321600 GEOM=CHECK GUESS=READ\CH2SB2
(based on c1cy)//B3LYP\0,2\C,2.2890243412,1.1042155784,-0.9968097515
\S,2.4682148589,-0.3907221864,-0.1509036442\C,1.1225379022,-0.28621318
16,1.1225476215\H,1.3107207601,1.5610575659,-1.102603258\H,3.075599949
2,1.3512283071,-1.7000127755\C,-0.2711493981,-0.1551745282,0.564326655
8\H,1.3608755879,0.5488633714,1.7871423637\H,1.2376766027,-1.214308172
2,1.6915234601\C,-0.95329325,1.0657421787,0.6394616707\C,-0.9121192978
,-1.2480730672,-0.0376886\C,-2.2464469979,1.1946439378,0.1265252273\C,
-2.2022041354,-1.1226946014,-0.5478815353\C,-2.8740810671,0.1007283115
,-0.4679674561\H,-3.8807489186,0.1974088184,-0.8655582935\H,-2.6863783
19,-1.9804336061,-1.007245593\H,-2.7612133853,2.1493477275,0.194971213
4\H,-0.39086816,-2.1998103758,-0.1093106115\H,-0.4707104422,1.91915357
78,1.1104688062\\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-708.4022103\S2
=0.754322\S2-1=0.\S2A=0.750014\RMSD=3.796e-09\RMSF=2.003e-06\Dipole=-0
.5920659,0.0932405,0.1849989\PG=C01 [X(C8H9S1)]\\@
```

r.CH2-SCH3

```
1\1\GINC-SC40\FOpt\UB3LYP\6-31G(d)\C2H5S1(2)\ROOT\09-Aug-2001\1\#P UB
3LYP/6-31G* GEOM=CHECK GUESS=READ FOPT=Z-MATRIX FREQ MAXDISK=393216000
0\CH3-S-CH2* rad c1\0,2\S\C,1,cs1\H,2,hc1,1,hcs1\H,2,hc2,1,hcs2,3,dh
1,0\C,1,cs2,2,csc,3,dh2,0\H,5,hc3,1,hcs3,2,dh3,0\H,5,hc4,1,hcs4,2,dh4,
0\H,5,hc5,1,hcs5,2,dh5,0\cs1=1.72792339\hc1=1.08323195\hc2=1.08486743
\cs2=1.82757399\hc3=1.09259995\hc4=1.09284674\hc5=1.09379903\hcs1=116.
54833307\hcs2=120.61117155\csc=101.38957243\hcs3=107.21472595\hcs4=110
.5393542\hcs5=110.59047311\dh1=-159.93202602\dh2=-173.68441562\dh3=-17
7.97662667\dh4=62.80681521\dh5=-59.18214036\\Version=DEC-AXP-OSF/1-G98
RevA.9\HF=-477.3516401\S2=0.754164\S2-1=0.\S2A=0.750013\RMSD=3.903e-09
\RMSF=1.827e-05\Dipole=-0.5687768,-0.0455824,0.0333926\PG=C01 [X(C2H5S
1)]\\@
```

r.CH2-SO2CH3

```
1\1\GINC-AC1\FOpt\UB3LYP\Gen\C2H5O2S1(2)\CYL509\25-Nov-2008\0\#B3LYP/
gen 6D INT(grid=ultrafine) OPT Freq=noraman maxdisk=2684354560\r.CH2-
SO2CH3.freq\0,2\S,0.,0.0263902971,0.103205553\O,-1.2826590543,-0.0304
262637,0.819284335\O,1.2826590543,-0.0304262637,0.819284335\C,0.,1.531
7256768,-0.8983703118\C,0.,-1.2830647712,-1.0857837081\H,0.,2.36688178
66,-0.1922078501\H,0.902252617,1.5598155217,-1.5128679086\H,-0.9022526
17,1.5598155217,-1.5128679086\H,-0.9506986716,-1.6964717527,-1.4021262
675\H,0.9506986716,-1.6964717527,-1.4021262675\\Version=IA64L-G03RevE.
01\State=2-A'\HF=-627.7231727\S2=0.754024\S2-1=0.\S2A=0.750009\RMSD=8.
285e-09\RMSF=9.170e-05\Thermal=0.\Dipole=0.,0.1840419,-1.7790757\PG=CS
[SG(C2H1S1),X(H4O2)]\\@
```

r.CH2-SOCH3

```
1\1\GINC-AC15\FOpt\UB3LYP\Gen\C2H5O1S1(2)\CYL509\11-Apr-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-S
OCH3.b1.freq\0,2\H,0.4254157175,1.5282474227,-1.3039167574\C,0.535719
5274,1.4977751506,-0.2178495389\H,1.5768366713,1.6720027941,0.06361677
49\H,-0.1134194819,2.2338365172,0.2644805838\S,0.0986119212,-0.1913795
365,0.3819289922\O,0.8843230669,-1.2052240907,-0.4092792316\C,-1.58645
95135,-0.1903827584,-0.0851196916\H,-2.2312849037,0.5676570016,0.35151
52988\H,-2.0054833607,-1.1422327799,-0.3945105394\Version=IA64L-G03Re
vC.02\State=2-A\HF=-552.514987\S2=0.756064\S2-1=0.\S2A=0.750025\RMSD=3
.442e-09\RMSF=1.875e-05\Dipole=-0.7751986,1.198574,0.3433886\PG=C01 [X
(C2H5O1S1)]\@
```

r.CH2-Ph

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C7H7(2)\CYL509\07-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-Ph.fr
eq\0,2\H,-2.8725642252,-0.5568568989,-0.0120559536\C,-1.8061543165,-0
.3501619097,-0.0076192594\C,-0.9376655693,-1.137735774,0.7621397366\C,
0.4237959691,-0.8786501128,0.7717926964\C,0.9770888867,0.189683467,0.0
044268863\C,0.0710202969,0.9745294627,-0.769767181\C,-1.2886534559,0.7
060523254,-0.7716078836\H,-1.3342124359,-1.9574732665,1.3558077377\C,2
.3580617241,0.457115827,0.0098931596\H,3.0447185471,-0.1417746275,0.59
93170184\H,2.7759707435,1.2699949623,-0.5750576268\H,0.4666617655,1.79
45843656,-1.3640866038\H,1.0924167729,-1.49259348,1.370338891\H,-1.957
9523764,1.3191192171,-1.369812381\Version=IA64L-G03RevC.02\State=2-A\
HF=-270.9151377\S2=0.783681\S2-1=0.\S2A=0.750769\RMSD=2.560e-09\RMSF=2
.875e-05\Dipole=-0.0516376,-0.0100317,-0.0002428\PG=C01 [X(C7H7)]\@
```

r.CH2-C6H4CN

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C8H6N1(2)\CYL509\08-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C6H
4CN.freq\0,2\N,-3.5924728454,-0.6500322132,0.0041792086\C,-2.44594465
92,-0.4426650501,0.0027746374\C,-1.0412915687,-0.1885388576,0.00111722
55\C,-0.1694286534,-1.001999337,0.7606688401\C,1.1880016846,-0.7560052
514,0.7588960852\C,1.7491725837,0.3165163637,-0.0020450627\C,0.8460047
536,1.1240202696,-0.7613558586\C,-0.5115009705,0.878619182,-0.76006575
55\H,-0.5799239589,-1.8202965373,1.3436907111\C,3.1271028144,0.5660516
911,-0.0033965294\H,3.8104550895,-0.048244089,0.5736057659\H,3.5505179
375,1.3814418165,-0.5805650815\H,1.2458290289,1.946002087,-1.348804232
3\H,1.8518137403,-1.3855153563,1.3451373614\H,-1.1840778265,1.50084350
92,-1.3418804766\Version=IA64L-G03RevC.02\State=2-A\HF=-363.1606183\S
2=0.78767\S2-1=0.\S2A=0.750949\RMSD=5.919e-09\RMSF=4.294e-05\Dipole=1.
8774124,0.3398618,-0.0019635\PG=C01 [X(C8H6N1)]\@
```

r.CH2-C6H4NO2

```
1\1\GINC-AC25\FOpt\UB3LYP\Gen\C7H6N1O2(2)\CYL509\08-Apr-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C
6H4NO2.freq\0,2\O,-2.474238831,1.1688431828,-0.9960222701\N,-1.254567
8663,1.3400527936,-1.0700058402\C,-0.3924827106,0.4191814984,-0.334809
2879\O,-0.7138426006,2.2367674126,-1.7226180012\C,-0.9771110144,-0.610
3822825,0.4165821326\C,-0.160454432,-1.479856602,1.1109897442\C,1.2635
512821,-1.3498991533,1.0772990364\C,1.81143704,-0.2836311581,0.2971003
187\C,0.9981428131,0.5878828926,-0.3986950867\H,1.4048908722,1.3974994
854,-0.991871779\C,2.090574722,-2.233149242,1.7828423538\H,3.170798566
,-2.1339488644,1.7577125796\H,1.6747015465,-3.0415390248,2.3752199642\
H,-0.6001736256,-2.2818430058,1.6971981018\H,2.8904559193,-0.164292456
8,0.256456303\H,-2.0559929605,-0.70200617,0.4365926158\Version=IA64L-
G03RevC.02\State=2-A\HF=-475.4191201\S2=0.784042\S2-1=0.\S2A=0.75074\R
MSD=6.327e-09\RMSF=9.623e-05\Dipole=1.2348313,-1.3190121,1.0531129\PG=
C01 [X(C7H6N1O2)]\@
```

r.CH2-C6H4OCH3

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C8H9O1(2)\CYL509\08-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C6H
4OCH3.freq\0,2\C,-0.9114236212,-0.0262059222,-1.0372487714\C,-0.86757
00882,-0.0351033645,0.3716302319\C,0.3749184918,0.0063847132,1.0249856
946\C,1.5458878931,0.0555521345,0.2808574979\C,1.537431792,0.065960223
2,-1.1434665394\C,0.2538091979,0.0228160322,-1.7724224669\C,2.72553548
03,0.115740288,-1.8916379132\O,-2.0777266456,-0.084718232,0.9993457184
\C,-2.1005128634,-0.0967740505,2.417766926\H,3.6953013669,0.1482799361
,-1.4059388255\H,2.7068983921,0.1233820959,-2.9765192637\H,0.203259764
,0.0290284902,-2.8584161447\H,2.5017658423,0.0873319058,0.7979094389\H
,0.4335436281,0.0004416232,2.1077956981\H,-1.8829209091,-0.0587807049,
-1.521202861\H,-1.5819188805,-0.9760615499,2.8222994552\H,-3.154094252
6,-0.1382247366,2.7000610622\H,-1.6484794796,0.812128473,2.8364577361\
\Version=IA64L-G03RevC.02\State=2-A\HF=-385.4384015\S2=0.781086\S2-1=0
.\S2A=0.750638\RMSD=3.112e-09\RMSF=2.114e-05\Dipole=-0.0987668,-0.0086
197,0.6313801\PG=C01 [X(C8H9O1)]\@
```

r.CH2-C6H4OH

```
1\1\GINC-AC14\FOpt\UB3LYP\Gen\C7H7O1(2)\CYL509\08-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C6H
4OH.freq\0,2\C,-1.1836206233,-0.0430038903,-0.7369934028\C,-1.2029894
697,-0.0674429184,0.667887595\C,0.0045088458,-0.0229273617,1.382435797
\C,1.2115735878,0.0448123738,0.7065275009\C,1.2704663578,0.0713493167,
-0.7184128765\C,0.0208863271,0.024583753,-1.4102740192\C,2.4936141862,
0.1401631555,-1.4060504917\O,-2.4233625038,-0.134713303,1.2797672378\H
,3.4377909312,0.1755064992,-0.8725555598\H,2.5285432322,0.1600626172,-
2.4902851166\H,0.0259831243,0.0430404608,-2.4971887098\H,2.1400104186,
0.0788351542,1.2708161857\H,-0.0104753882,-0.0418401394,2.4713096837\H
,-2.1277199527,-0.0781972189,-1.2719580043\H,-2.2938676053,-0.14490752
08,2.2410030022\Version=IA64L-G03RevC.02\State=2-A\HF=-346.1318436\S2
=0.781585\S2-1=0.\S2A=0.750661\RMSD=3.812e-09\RMSF=8.450e-06\Dipole=0.
0756949,-0.0060813,0.5720519\PG=C01 [X(C7H7O1)]\@
```

r.CH2-CF2CF3

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H2F5(2)\CYL509\08-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CF2
CF3.a4.freq\0,2\F,-0.8441701187,0.0227636633,-1.548605658\C,-0.763843
0594,0.013499976,-0.1873667526\C,0.734270158,-0.0383093384,0.184267086
9\C,-1.5641272408,-1.0970381528,0.3752518083\F,-1.2272560176,1.2315460
314,0.2576661525\F,1.2946136609,-1.1558000033,-0.3066597166\F,0.872785
4741,-0.0476399193,1.5235832128\F,1.3879047333,1.0202066318,-0.3062464
904\H,-2.3682500137,-1.5145190018,-0.2170141859\H,-1.42444872,-1.39408
35426,1.4064638283\Version=IA64L-G03RevC.02\State=2-A\HF=-614.6575332
\S2=0.753618\S2-1=0.\S2A=0.750008\RMSD=9.386e-09\RMSF=2.279e-05\Dipole
=-0.4816376,-0.5745817,0.2723021\PG=C01 [X(C3H2F5)]\@
```

r.CH2-CF2H

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C2H3F2(2)\CYL509\07-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CF2
H.freq\0,2\C,0.2947990909,0.0000418249,-0.1677514333\C,0.5296378967,0
.0758148471,1.2933643028\H,0.6695806823,1.0419263013,1.762557062\H,1.2
171687969,-0.0032157668,-0.7688678458\F,-0.4500273387,1.0739821108,-0.
5859632172\F,-0.3893524576,-1.1474697235,-0.4805752039\H,0.7210467623,
-0.8324620523,1.8514793575\Version=IA64L-G03RevC.02\State=2-A\HF=-277
.623617\S2=0.753592\S2-1=0.\S2A=0.750007\RMSD=4.861e-09\RMSF=1.724e-05
\Dipole=0.6781382,0.0390979,0.4372995\PG=C01 [X(C2H3F2)]\@
```

r.CH2-CF3

```
1\1\GINC-AC25\FOpt\UB3LYP\Gen\C2H2F3(2)\CYL509\07-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CF3
.freq\0,2\F,0.0128718406,-0.0761290671,-1.3473602125\C,-0.0033142933,
-0.016775884,0.0023435378\F,1.2745943601,-0.0761315492,0.4369829283\C,
-0.82649078,-1.1008174964,0.5844163377\F,-0.4739087643,1.2144801475,0.
3351061555\H,-1.7149401238,-1.4272066627,0.0600327873\H,-0.6282463677,
-1.4272088355,1.5968481138\Version=IA64L-G03RevC.02\State=2-A\HF=-376
.8760983\S2=0.753512\S2-1=0.\S2A=0.750007\RMSD=9.340e-09\RMSF=6.425e-0
5\Dipole=-0.4635179,-0.5564104,0.3277563\PG=C01 [X(C2H2F3)]\@
```

r.CH2-CCl2H

```
1\1\GINC-AC22\FOpt\UB3LYP\Gen\C2H3Cl2(2)\CYL509\08-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CC
l2H.a4.freq\0,2\C,0.5095527229,-0.2269209121,0.2021195085\C,0.5359824
681,-0.1786953978,1.6629291909\H,1.4373695836,-0.57964637,-0.241811478
6\Cl,0.2909105106,1.4811316249,-0.4906636264\Cl,-0.8090944618,-1.29618
07993,-0.4116235266\H,1.4863040747,-0.064257586,2.1727124635\H,-0.3877
576337,-0.0665622199,2.2176884192\Version=IA64L-G03RevC.02\State=2-A\
HF=-998.3437945\S2=0.754674\S2-1=0.\S2A=0.750016\RMSD=6.518e-09\RMSF=5
.103e-05\Dipole=0.5753676,-0.2478011,0.6420243\PG=C01 [X(C2H3Cl2)]\@
```

r.CH2-CCl3

```
1\1\GINC-AC14\FOpt\UB3LYP\Gen\C2H2Cl3(2)\CYL509\08-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CC
l3.freq\0,2\C,0.0131146588,0.0000028361,0.3001322278\C,0.2361393025,-
0.0139099809,1.7489984486\Cl,1.6368650673,-0.1448972532,-0.5678060874\
Cl,-0.7587844138,1.5465431133,-0.2158537947\Cl,-1.0151424191,-1.393469
4418,-0.2046241202\H,0.4990091114,0.9097163755,2.2494411326\H,0.335517
1343,-0.9652726198,2.2566028477\Version=IA64L-G03RevC.02\State=2-A\HF
=-1457.9250766\S2=0.754527\S2-1=0.\S2A=0.750015\RMSD=4.639e-09\RMSF=7.
707e-05\Dipole=0.0899082,-0.0048857,0.7733678\PG=C01 [X(C2H2Cl3)]\@
```

r.CH2-CH2Cl

```
1\1\GINC-AC22\FOpt\UB3LYP\Gen\C2H4Cl1(2)\CYL509\08-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH
2Cl.a4.freq\0,2\C,-0.8608636142,0.2542549076,-1.4371263922\C,-0.85282
73657,0.2611192524,0.023633441\Cl,0.8439815135,-0.2539382074,0.6779200
076\H,-0.4904498474,1.1098067293,-1.9918097922\H,-1.0339747468,-0.6685
878128,-1.9804878509\H,-1.5326297764,-0.4645580187,0.4697116958\H,-1.0
0848548,1.2480436675,0.4589035254\Version=IA64L-G03RevC.02\State=2-A\
HF=-538.7554678\S2=0.755332\S2-1=0.\S2A=0.75002\RMSD=5.477e-09\RMSF=5.
819e-06\Dipole=-0.7919534,0.239627,-0.4282809\PG=C01 [X(C2H4Cl1)]\@
```

r.CH2-CH2F

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C2H4F1(2)\CYL509\08-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH2
F.a4.freq\0,2\C,-1.2183971455,-0.2565797597,0.0943929104\C,0.05220982
98,0.5038501164,0.1352939683\F,1.1263602561,-0.3103226424,-0.218303652
9\H,-1.3428654135,-1.0523334375,-0.6317418427\H,-2.0831706974,0.090098
9824,0.6495768721\H,0.2401767657,0.9158447083,1.1376736359\H,0.0457409
343,1.3556713876,-0.5688970613\Version=IA64L-G03RevC.02\State=2-A\HF=
-178.3812331\S2=0.753776\S2-1=0.\S2A=0.750009\RMSD=7.510e-09\RMSF=3.20
8e-05\Dipole=-0.5439651,0.4058386,0.1201605\PG=C01 [X(C2H4F1)]\@
```

r.CH2-CH2OH

```
1\1\GINC-AC6\FOpt\UB3LYP\Gen\C2H5O1(2)\CYL509\21-Nov-2008\0\#B3LYP/ge
n 6D INT(grid=ultrafine) OPT Freq=noraman maxdisk=2684354560\r.CH2-CH
2OH.freq\0,2\H,-1.2963719937,-1.1861126263,0.5691712718\C,-1.23615722
```

56,-0.2704677618,-0.0117371384\H,-2.1411051232,0.1108737304,-0.4741525
794\C,0.0113298481,0.5394611783,0.0323816443\H,0.0713153796,1.13109121
16,0.9602590242\H,0.024845133,1.2669289981,-0.7973382794\O,1.193784792
6,-0.2606379228,0.0433137521\H,1.1388101892,-0.8499088075,-0.725674695
2\\Version=IA64L-G03RevE.01\State=2-A\HF=-154.3613802\S2=0.753813\S2-1
=0.\S2A=0.750009\RMSD=9.119e-09\RMSF=2.221e-05\Thermal=0.\Dipole=-0.48
14178,-0.0208429,-0.4033036\PG=C01 [X(C2H5O1)]\@

r.CH2-CH2Ph

1\1\GINC-SC109\FOpt\UB3LYP\6-31G(d)\C8H9(2)\MLC501\11-Sep-2002\0\#N U
B3LYP/6-31G(D) OPT=(MAXCYC=100,TIGHT) FREQ SCF=(TIGHT,MAXCYC=100) MAXD
ISK=52428800\etbz_rad-cla-6dub3\0,2\C,-2.03452684,-2.0512941126,0.33
24478083\C,-0.6420304454,-1.9399542889,-0.2000743247\C,-0.0508558132,-
0.5429243693,-0.1134582342\C,0.4913398018,0.0842541701,-1.2410059535\C
, -0.0274801177,0.1457417281,1.1080457068\C,1.046074949,1.3631473884,-1
.1547761696\C,0.5252915484,1.4226125461,1.1993467209\C,1.0649541968,2.
036857646,0.0665065029\H,1.4951343558,3.0324663079,0.136287752\H,1.460
3795209,1.8325247546,-2.0434783758\H,0.5352032701,1.9393156892,2.15579
3481\H,0.4781960201,-0.4336517467,-2.1977738577\H,-0.449973448,-0.3270
655114,1.9916602032\H,0.00765341,-2.6500255972,0.3352581197\H,-0.60835
41106,-2.2704429873,-1.2545284257\H,-2.4241734132,-3.0089567382,0.6633
438848\H,-2.7306692819,-1.2248084189,0.2312448771\\Version=DEC-AXP-OSF
/1-G98RevA.11.3\HF=-310.2072089\S2=0.753928\S2-1=0.\S2A=0.75001\RMSD=8
.145e-09\RMSF=1.629e-06\Dipole=0.0104278,-0.1026318,-0.0496021\PG=C01
[X(C8H9)]\@

r.CH2-CH_CH2_2

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\14-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH_CH
2_2.freq\0,2\C,-0.862972115,0.32664052,-0.7477537525\C,-0.8628032954,
0.3266181334,0.7479568054\C,0.4758378598,0.2897496685,-0.0000479244\H,
-1.1623860357,-0.5815090212,-1.2640477004\H,-1.1187015804,1.2443529683
, -1.2712575958\H,-1.1621018917,-0.5815468278,1.2642907201\H,-1.1184165
638,1.2443144985,1.2715455853\H,1.0229838682,1.230010332,-0.0000973516
\C,1.3014599832,-0.9111245385,-0.0001582896\H,0.8459595603,-1.89697578
06,-0.000106584\H,2.3835280475,-0.8499488695,-0.0003081071\\Version=IA
64L-G03RevC.02\State=2-A\HF=-156.5443598\S2=0.754799\S2-1=0.\S2A=0.750
017\RMSD=5.281e-09\RMSF=8.995e-05\Dipole=-0.1013687,0.1195534,0.000008
7\PG=C01 [X(C4H7)]\@

r.CH2-CH2CH=CH2

1\1\GINC-AC14\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\08-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH2CH
=CH2.a2.freq\0,2\C,0.6630562256,0.4906872302,0.1601801795\C,0.6180369
951,0.3884705124,1.6528335913\H,1.7107982721,0.4500782595,-0.17421657\H,
0.2834776429,1.4739453552,-0.1734978789\C,-0.1309388306,-0.591899207
3,-0.5316117704\H,1.4599796051,0.6995715936,2.2629833806\H,-0.30886690
32,0.1307409094,2.1557191858\C,-1.1677520859,-0.3809785555,-1.34275206
71\H,0.1837008651,-1.6142724684,-0.3189354281\H,-1.7062736522,-1.20135
03757,-1.8097802969\H,-1.5172296551,0.6236068479,-1.5741719925\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-156.5479905\S2=0.753926\S2-1=0.\S2A=0
.75001\RMSD=5.747e-09\RMSF=2.990e-06\Dipole=0.0804532,0.059887,0.00945
75\PG=C01 [X(C4H7)]\@

r.CH2-CH2CH3

1\1\GINC-AC\FOpt\UB3LYP\Gen\C3H7(2)\CYL509\21-Nov-2008\0\#B3LYP/gen 6
D INT(grid=ultrafine) OPT Freq=noraman\\r.CH2-CH2CH3.freq\0,2\H,0.066
3316757,-0.0307119651,0.0072924518\C,0.0009153142,0.0009680722,1.10061
75388\H,1.0225583435,0.0730250172,1.4930138252\H,-0.5310146716,0.91637

04097,1.3831639257\C,-0.7089575196,-1.246786598,1.6460694159\H,-1.7407
409841,-1.2839154445,1.2672339276\H,-0.8139958635,-1.1396598447,2.7428
681827\C,-0.0060496712,-2.522447892,1.3223376904\H,1.0768733286,-2.551
0842564,1.2370849644\H,-0.533913952,-3.4711644983,1.3293180775\\Versio
n=IA64L-G03RevE.01\State=2-A\HF=-118.4713708\S2=0.753881\S2-1=0.\S2A=0
.75001\RMSD=4.066e-09\RMSF=7.835e-06\Thermal=0.\Dipole=-0.0433494,0.05
65398,0.0685421\PG=C01 [X(C3H7)]\@

r.CH2-CH_CH3_2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C4H9(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH_CH
3_2.freq\0,2\C,-0.8252754363,1.1660309895,0.2244362588\H,-0.588243666
,1.3105481031,1.2854297128\H,-1.913497604,1.0670403255,0.1345888722\H,
-0.5237953655,2.0705499239,-0.3166826645\C,-0.1055223427,-0.0764847157
, -0.3306992497\C,1.4239228405,0.0744441122,-0.2407929989\H,-0.35873857
95,-0.1391433976,-1.4078802441\C,-0.5763009344,-1.3303050748,0.3351648
64\H,0.0420668577,-2.2235237022,0.3420992901\H,-1.601388996,-1.4259174
077,0.68203527\H,1.9340392463,-0.8002564886,-0.6612443066\H,1.74319359
28,0.1790488305,0.8031899546\H,1.7654197523,0.9595419451,-0.79018913\\
Version=IA64L-G03RevC.02\State=2-A\HF=-157.7856453\S2=0.753865\S2-1=0.
\S2A=0.750009\RMSD=2.915e-09\RMSF=2.300e-05\Dipole=-0.0011788,0.034164
9,-0.0858614\PG=C01 [X(C4H9)]\@

r.CH2-C_CH3_3

1\1\GINC-AC24\FOpt\UB3LYP\Gen\C5H11(2)\CYL509\07-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C_CH
3_3.freq\0,2\C,-0.2413260543,-0.5213207338,1.4117340814\C,-0.01873229
07,-0.0269419818,-0.0438571605\C,-0.6562744657,1.3694193788,-0.2016797
647\C,-0.6572216223,-0.9926083017,-1.0012414584\H,0.2181537448,0.17106
5253,2.1297753561\H,0.2028386775,-1.511750962,1.5634192646\H,-1.310010
5401,-0.5918777242,1.6444952342\C,1.4975115385,0.0598041763,-0.3171153
776\H,-0.1307474695,-1.8900918291,-1.3150296009\H,-1.7175370597,-0.925
2608444,-1.2299560597\H,1.9847537866,0.7439099787,0.388469077\H,1.6941
195387,0.4223971579,-1.3325988458\H,1.9731005346,-0.9231774451,-0.2130
878023\H,-0.2177657487,2.0831674145,0.5065073465\H,-1.7364422057,1.332
4238804,-0.0142545155\H,-0.504205891,1.7590798937,-1.2147813747\\Versi
on=IA64L-G03RevC.02\State=2-A\HF=-197.0993032\S2=0.753812\S2-1=0.\S2A=
0.750009\RMSD=3.721e-09\RMSF=6.816e-05\Dipole=0.0057012,0.0025665,0.07
72368\PG=C01 [X(C5H11)]\@

r.CH2-CCH

1\1\GINC-AC23\POpt\UB3LYP\Gen\C3H3(2)\CYL509\08-Apr-2008\1\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT(Z-MATRIX) FREQ=NORAMAN MAXDISK=1342177280\
\CH2-CCH.freq\0,2\C\H,1,hc2\H,1,hc3,2,hch3\C,1,cc4,3,cch4,2,dih4,0\C,
4,cc5,1,ccc5,2,dih5,0\H,5,hc6,4,hcc6,1,dih6,0\\hc2=1.08576992\hc3=1.08
57708\hch3=117.84032417\cc4=1.36968328\cch4=121.06134711\dih4=180.0446
2481\cc5=1.22843414\dih5=-154.8644291\hc6=1.06594062\dih6=181.07588692
\ccc5=179.546\hcc6=179.954\\Version=IA64L-G03RevC.02\State=2-A\HF=-116
.0012791\S2=0.772666\S2-1=0.\S2A=0.750218\RMSD=7.103e-09\RMSF=1.677e-0
4\Dipole=-0.0053817,-0.0009716,-0.0058218\PG=C01 [X(C3H3)]\@

r.CH2-CH=C_CH3_2

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C5H9(2)\CYL509\08-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH=C_
CH3_2.freq\0,2\H,2.3641217248,-0.5282665255,-0.7155309404\C,1.6930978
358,-0.7741085859,0.1219203413\C,0.3984446286,-0.0170022113,0.02732281
32\C,0.5130815716,1.4809606556,0.0221559555\C,-0.8188310411,-0.6985026
711,-0.0496924465\C,-2.0929593615,-0.1661172269,-0.1410652869\H,-2.284
0073185,0.9019715366,-0.1633456463\H,-2.9600382973,-0.8159191654,-0.19

```
44339564\H,-0.7504791549,-1.7874984343,-0.0356479353\H,1.5374130125,-1
.8577994025,0.1204556379\H,2.2446364815,-0.5134581563,1.0383791383\H,1
.1319271615,1.8242935725,-0.8202756183\H,1.0126311616,1.8394948175,0.9
34507574\H,-0.453206572,1.9858019949,-0.0479565129\Version=IA64L-G03R
evC.02\State=2-A\HF=-195.8989799\S2=0.778444\S2-1=0.\S2A=0.750172\RMSD
=4.812e-09\RMSF=4.584e-06\Dipole=0.2295504,0.0648892,0.0150514\PG=C01
[X(C5H9)]\@
```

r.CH2-CH=CH2

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H5(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH=CH
2.freq\0,2\H,-1.0121737191,-1.3257011473,0.7401238019\C,0.0380542932,
-1.0593138931,0.6541732347\H,0.7584804386,-1.7253703615,1.1172038728\C
,0.4341907012,0.0850962109,-0.02022515\C,-0.422367136,0.9840044586,-0.
6362538551\H,1.5032491034,0.2945508068,-0.0699892483\H,-0.0500981772,1
.8641360645,-1.1500144656\H,-1.4987247964,0.8336639785,-0.6234893384\
Version=IA64L-G03RevC.02\State=2-A\HF=-117.260351\S2=0.781809\S2-1=0.\
S2A=0.750195\RMSD=7.567e-09\RMSF=1.929e-05\Dipole=0.0296075,0.0057573,
-0.0014034\PG=C01 [X(C3H5)]\@
```

r.CH2-CH=CHCH3

```
1\1\GINC-AC25\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CH=CH
CH3.freq\0,2\C,0.2297836246,0.328676913,1.8385615486\H,1.268702405,0.
6610307604,1.7362713339\H,0.2141783936,-0.5140970565,2.5456074257\H,-0
.3373988687,1.1402879484,2.3182076132\C,-0.3610303934,-0.0497692213,0.
5178096742\C,0.3132829263,0.0091644325,-0.6948767693\H,-1.3951872323,-
0.3951262326,0.5162663615\H,1.3477607188,0.3573170977,-0.6715063936\C,
-0.2189034673,-0.3367917312,-1.9262518034\H,0.3655037375,-0.2663115942
,-2.8374380991\H,-1.242355295,-0.6907832813,-2.0188641416\Version=IA6
4L-G03RevC.02\State=2-A\HF=-156.5806348\S2=0.78002\S2-1=0.\S2A=0.75018
4\RMSD=6.625e-09\RMSF=9.031e-06\Dipole=0.0140011,0.029499,0.1801192\PG
=C01 [X(C4H7)]\@
```

r.CH2-CHO

```
1\1\GINC-AC23\FOpt\UB3LYP\Gen\C2H3O1(2)\CYL509\07-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CHO
.a2.freq\0,2\O,0.4538196396,0.,-1.1127350944\C,0.4104456558,0.,0.1253
805822\H,1.3465715536,0.,0.7183225854\C,-0.8110876316,0.,0.8601826063\
H,-1.7550872658,0.,0.3241038271\H,-0.8181895499,0.,1.9460752117\Versi
on=IA64L-G03RevC.02\State=2-A\HF=-153.1715339\S2=0.76935\S2-1=0.\S2A=
0.750095\RMSD=4.629e-09\RMSF=8.200e-05\Dipole=-0.3361437,0.,1.0494631\
PG=CS [SG(C2H3O1)]\@
```

r.CH2-CN

```
1\1\GINC-AC23\POpt\UB3LYP\Gen\C2H2N1(2)\CYL509\08-Apr-2008\1\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT=(Z-MATRIX) FREQ=NORAMAN MAXDISK=13421772
80\CH2-CN.freq\0,2\N\C,1,cn2\C,2,cc3,1,ccn3\H,3,hc4,2,hcc4,1,dih4,0\
H,3,hc5,4,hch5,2,dih5,0\cn2=1.17682823\cc3=1.3825195\hc4=1.08404901\h
cc4=120.31513682\dih4=-6.51089417\hc5=1.08404608\hch5=119.3668224\dih5
=180.00235492\ccn3=179.993\Version=IA64L-G03RevC.02\State=2-A\HF=-132
.0946697\S2=0.768754\S2-1=0.\S2A=0.750144\RMSD=9.734e-09\RMSF=2.903e-0
6\Dipole=0.0000861,0.0000099,1.3178436\PG=C01 [X(C2H2N1)]\@
```

r.CH2-COCH3

```
1\1\GINC-AC22\FOpt\UB3LYP\Gen\C3H5O1(2)\CYL509\08-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-COC
H3.a2.freq\0,2\C,-0.1024868845,0.0118179324,-1.4031692771\C,-0.083249
1399,-0.0036891679,0.1191790388\C,1.1913077662,0.0265038501,0.78827755
```

67\O,-1.1331842785,-0.0413102288,0.7762636103\H,-1.1364390592,-0.01481
91592,-1.7522995641\H,0.4388704186,-0.8511692825,-1.8100063995\H,0.387
1492293,0.9133872428,-1.7914300257\H,2.1314001016,0.0595790123,0.24506
22284\H,1.2110630869,0.0157083289,1.8728409684\\Version=IA64L-G03RevC.
02\State=2-A\HF=-192.4950196\S2=0.766403\S2-1=0.\S2A=0.750084\RMSD=3.5
66e-09\RMSF=8.643e-06\Dipole=1.0184735,0.0351047,-0.5063764\PG=C01 [X(
C3H5O1)]\@

r.CH2-CON_CH2CH3_2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C6H12N1O1(2)\CYL509\07-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-
CON_CH2CH3_2.freq\0,2\H,0.5753759619,-2.4878589701,2.4346783139\C,0.2
565687139,-2.1259380008,1.4500795599\C,0.4876791963,-0.6148986234,1.33
01496684\N,0.1335750391,-0.0674625473,0.0219596187\C,1.1749723188,-0.0
28006215,-1.0080162922\C,1.9735526422,1.2794356766,-1.0054052206\C,-1
.1010940882,0.4643479315,-0.2982286004\O,-1.305521132,0.9968278964,-1.
3996527825\C,-2.1851839929,0.368122164,0.6718805222\H,-3.116257939,0.8
467768201,0.395565122\H,-2.1414605978,-0.1892917013,1.5997840014\H,1.5
457450424,-0.3870791781,1.5060800693\H,-0.0639776634,-0.0803209236,2.1
091227699\H,0.6878542474,-0.159353442,-1.9765517287\H,1.8389431982,-0.
884936109,-0.8439926204\H,-0.8024897115,-2.3730114846,1.3187375323\H,0
.8239384353,-2.6712682499,0.6879135831\H,1.3090814842,2.1219457521,-1.
2164816409\H,2.7529459896,1.2518822075,-1.7760208324\H,2.4604765946,1.
4517187797,-0.0380874642\\Version=IA64L-G03RevC.02\State=2-A\HF=-365.7
966826\S2=0.756685\S2-1=0.\S2A=0.750029\RMSD=4.438e-09\RMSF=8.440e-06\
Dipole=0.5717548,-0.6783787,1.1476374\PG=C01 [X(C6H12N1O1)]\@

r.CH2-CON_CH3_2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C4H8N1O1(2)\CYL509\08-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C
ON_CH3_2.a3.freq\0,2\C,1.9307681805,0.0113999319,-0.2898176134\C,0.56
57271058,0.5226398516,-0.2561561339\N,-0.4600642843,-0.3338124156,0.10
58311281\O,0.3554045028,1.7114131468,-0.5353125309\H,2.2530338483,-0.9
288675766,0.1407936299\H,2.6792418123,0.6829011126,-0.6911198094\C,-0.
2786133052,-1.7300177578,0.4621771516\C,-1.789411733,0.2185977588,0.31
11862377\H,-1.1820801167,-2.286141887,0.1890786018\H,0.5536376825,-2.1
716472354,-0.0887024815\H,-0.1081100119,-1.8736946903,1.5403377695\H,-
2.5312918532,-0.3475258628,-0.2664047992\H,-2.0755229999,0.1782354653,
1.372316764\H,-1.7825158825,1.2564037011,-0.0189551767\\Version=IA64L-
G03RevC.02\State=2-A\HF=-287.164222\S2=0.757078\S2-1=0.\S2A=0.750031\R
MSD=8.837e-09\RMSF=6.888e-06\Dipole=-0.0741048,-1.3761826,0.4304253\PG
=C01 [X(C4H8N1O1)]\@

r.CH2-CONH2

1\1\GINC-AC22\FOpt\UB3LYP\Gen\C2H4N1O1(2)\CYL509\08-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C
ONH2.freq\0,2\C,1.3400019584,-0.4400627753,-0.0630641142\C,-0.0007109
638,0.1264479725,-0.0064586047\N,-1.0437407552,-0.7811721963,0.0493469
084\O,-0.2000140432,1.3419182878,-0.0442037294\H,1.529510149,-1.509330
7937,-0.0686540537\H,2.1761700712,0.2453273241,-0.1168434257\H,-0.8816
719727,-1.7301837352,0.3546847584\H,-1.9534565831,-0.3912649068,0.2561
505104\\Version=IA64L-G03RevC.02\State=2-A\HF=-208.5467873\S2=0.757523
\S2-1=0.\S2A=0.750034\RMSD=1.766e-09\RMSF=1.421e-05\Dipole=0.0149025,-
1.400156,0.343957\PG=C01 [X(C2H4N1O1)]\@

r.CH2-CONHCH3

1\1\GINC-AC24\FOpt\UB3LYP\Gen\C3H6N1O1(2)\CYL509\08-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-C
ONHCH3.freq\0,2\H,-1.473868694,0.7158564406,-2.1019391299\C,-1.470773

3623,0.7166472677,-1.0046122368\N,-0.1208129479,0.7197864468,-0.478938
8858\C,0.3644903572,-0.2942354057,0.319219248\C,1.7444680245,-0.133904
0922,0.761658554\O,-0.3160625869,-1.2729126444,0.6403550503\H,2.358782
8856,0.7196803458,0.4891160784\H,2.1669331566,-0.9074380016,1.39015121
5\H,0.4868804555,1.4931289904,-0.7059105878\H,-1.9535489991,-0.1937757
34,-0.6463825622\H,-2.0400975908,1.5862973677,-0.652896606\Version=IA
64L-G03RevC.02\State=2-A\HF=-247.8580498\S2=0.756035\S2-1=0.\S2A=0.750
025\RMSD=3.388e-09\RMSF=4.187e-05\Dipole=0.5298123,1.2557201,-0.546861
9\PG=C01 [X(C3H6N1O1)]\@

r.CH2-COOC_CH3_3

1\1\GINC-AC14\FOpt\UB3LYP\Gen\C6H11O2(2)\CYL509\08-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-CO
OC_CH3_3.a2.freq\0,2\H,-1.2775163508,-1.0687102901,-2.2721576131\C,-1
.2401730879,-0.7587125483,-1.2216340596\C,0.219587021,-0.5575062782,-0
.7984234558\C,0.896292656,0.5811918311,-1.5703635437\O,0.2945072038,-0
.3005069088,0.6487531596\C,-0.2954477077,0.7850355553,1.2083575653\O,-
0.9314830642,1.6417422332,0.6057955056\C,-0.0798694062,0.8146635156,2.
642881604\C,1.0115856198,-1.8591628084,-0.9479173956\H,-0.5034819079,1
.6361659673,3.206760786\H,0.4880567163,0.0404783293,3.144747204\H,1.03
4346758,-2.1681306641,-1.9982981764\H,0.5523349366,-2.6607686317,-0.36
03394608\H,2.0421456206,-1.7263301778,-0.6029036485\H,-1.8152849616,0.
1614365579,-1.1074605701\H,-1.7058670178,-1.5459771427,-0.6186041473\H
,0.9433810143,0.3245550636,-2.6347898719\H,1.9207899448,0.7280764941,-
1.2109895149\H,0.3450515612,1.516266296,-1.4597585955\Version=IA64L-G
03RevC.02\State=2-A\HF=-385.6742053\S2=0.757336\S2-1=0.\S2A=0.750033\R
MSD=5.593e-09\RMSF=1.036e-05\Dipole=0.3918114,-0.5950329,0.1118899\PG=
C01 [X(C6H11O2)]\@

r.CH2-COOCH2CH3

1\1\GINC-AC15\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\07-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-COO
CH2CH3.freq\0,2\C,-2.3140256859,0.2515332062,0.\C,-1.0204293314,-0.39
84156156,0.\O,-0.8542361441,-1.6110604011,0.\O,-0.0004160078,0.4999967
425,0.\C,1.3268658829,-0.0668569681,0.\C,2.3156459406,1.0839043466,0.\
H,-2.400752609,1.3314150833,0.\H,-3.2004876827,-0.3696304993,0.\H,1.43
96349199,-0.7059287643,0.8823636954\H,1.4396349199,-0.7059287643,-0.88
23636954\H,2.1855790446,1.7114312902,-0.8875093379\H,3.3396887409,0.69
47298182,0.\H,2.1855790446,1.7114312902,0.8875093379\Version=IA64L-G0
3RevC.02\State=2-A\HF=-307.0427322\S2=0.757625\S2-1=0.\S2A=0.750034\R
MSD=5.121e-09\RMSF=1.344e-04\Dipole=0.1291744,0.7435132,0.\PG=CS [SG(C
4H3O2),X(H4)]\@

r.CH2-COOCH3

1\1\GINC-AC24\FOpt\UB3LYP\Gen\C3H5O2(2)\CYL509\08-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-COO
CH3.freq\0,2\C,0.36130853,0.,-1.8450211878\C,0.362599517,0.,-0.397602
4171\O,1.369095091,0.,0.2976801671\O,-0.8992238609,0.,0.1112197602\C,-
0.9732584986,0.,1.5430162251\H,-2.0373556885,0.,1.7822262241\H,-0.5651
297961,0.,-2.4065928814\H,1.3139381921,0.,-2.3588823365\H,-0.487159919
2,-0.8890937059,1.9548469275\H,-0.4871599192,0.8890937059,1.9548469275
\Version=IA64L-G03RevC.02\State=2-A\HF=-267.7237414\S2=0.757602\S2-1
=0.\S2A=0.750034\RMSD=3.639e-09\RMSF=1.208e-04\Dipole=-0.6427842,0.,-0
.2455588\PG=CS [SG(C3H3O2),X(H2)]\@

r.CH2-COOH

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C2H3O2(2)\CYL509\07-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-COO
H.freq\0,2\C,0.0396022322,-0.125938903,-1.4003660796\C,0.0760805056,0

.0729910823,0.0314303372\O,0.8369589679,0.834519573,0.6116803126\O,-0.8416044522,-0.6876654747,0.6937008763\H,0.7326750747,0.4351016965,-2.0135992968\H,-0.6606386769,-0.8167824935,-1.8542237628\H,-0.7289689501,-0.4754650651,1.638388003\Version=IA64L-G03RevC.02\State=2-A\HF=-228.4166642\S2=0.758171\S2-1=0.\S2A=0.750037\RMSD=9.073e-09\RMSF=4.141e-05\Dipole=-0.3772441,-0.3810101,-0.3182947\PG=C01 [X(C2H3O2)]\@

r.CH2-COPh

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C8H7O1(2)\CYL509\07-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2-COPh.freq\0,2\C,-2.2087322643,-0.0475957419,-0.175423818\C,-2.2475487791,-0.1266528324,1.2195868433\C,-1.0567334541,-0.1320602824,1.947722922\C,0.1687531534,-0.0628616617,1.285473365\C,0.2182111985,0.0147238721,-0.114836122\C,-0.9859423424,0.024569168,-0.8359309858\C,1.4980537362,0.0964437176,-0.8968706738\O,1.4681791948,0.2554657523,-2.1315974696\C,2.7743604174,-0.0195751302,-0.2430629911\H,2.9005994017,-0.2024665563,0.8176043886\H,3.6599092853,0.060804182,-0.8634031641\H,-0.9340008876,0.0899714041,-1.9175554243\H,1.0815153468,-0.0609635454,1.873053709\H,-1.08079426,-0.1891496593,3.0325615312\H,-3.1334358662,-0.0415895026,-0.7461848347\H,-3.2017565712,-0.182278995,1.7367523129\Version=IA64L-G03RevC.02\State=2-A\HF=-384.2346644\S2=0.767445\S2-1=0.\S2A=0.750092\RMSD=3.597e-09\RMSF=1.356e-06\Dipole=-0.0942202,-0.1565799,1.1428683\PG=C01 [X(C8H7O1)]\@

r.CHCH3-H

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C2H5(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-H.freq\0,2\C,-0.6516454881,-0.2569068694,0.3770572448\H,-0.7498789345,-0.1525344384,1.4530041959\C,0.5765777961,0.2047637875,-0.3280446202\H,-1.5354937841,-0.5538416301,-0.1786812733\H,1.4759083045,0.0616806927,0.2835992056\H,0.5354701342,1.2814297219,-0.5741279959\H,0.7244004315,-0.3238758547,-1.2778698799\Version=IA64L-G03RevC.02\State=2-A\HF=-79.1578682\S2=0.753921\S2-1=0.\S2A=0.75001\RMSD=1.487e-09\RMSF=8.249e-06\Dipole=0.0508547,0.0744713,-0.0428201\PG=C01 [X(C2H5)]\@

r.CHCH3-BH2

1\1\GINC-AC12\FOpt\UB3LYP\Gen\C2H6B1(2)\CYL509\10-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-BH2.freq\0,2\H,-1.4692274098,0.,-1.4567429364\B,-1.4526476738,0.,-0.2572486307\C,-0.1212367888,0.,0.4913769835\H,-2.4880466034,0.,0.3438285229\C,1.2226679351,0.,-0.1682265895\H,-0.107538771,0.,1.5833367285\H,2.0596601464,0.,0.5367209089\H,1.3299020644,0.8730554688,-0.8299012174\H,1.3299020644,-0.8730554688,-0.8299012174\Version=IA64L-G03RevC.02\State=2-A\HF=-104.6107478\S2=0.75248\S2-1=0.\S2A=0.750005\RMSD=3.672e-09\RMSF=5.749e-06\Dipole=0.644354,0.,0.1837523\PG=CS [SG(C2H4B1),X(H2)]\@

r.CHCH3-CH3

1\1\GINC-AC4\FOpt\UB3LYP\Gen\C3H7(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CH3.freq\0,2\H,-0.1372002171,-1.0031454541,-1.4991599933\C,0.0671973818,-1.236862582,-0.4445663857\H,1.1402635565,-1.5000410827,-0.3922377292\H,-0.4926676276,-2.1422038338,-0.1834797575\C,-0.2779093682,-0.0907393613,0.4472375643\C,0.1106397474,1.3076661548,0.0985979962\H,-0.5861914643,-0.3033601657,1.4685281399\H,1.1913397531,1.4913726488,0.2462835526\H,-0.4211589239,2.0452564716,0.7104951942\H,-0.0939516429,1.5317361471,-0.9580444558\Version=IA64L-G03RevC.02\State=2-A\HF=-118.4781563\S2=0.754002\S2-1=0.\S2A=0.750011\RMSD=9.217e-09\RMSF=2.275e-05\Dipole=0.0799348,-0.0008523,-0.0024437\PG=C01 [X(C3H7)]\@

r.CHCH3-NH2

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C2H6N1(2)\CYL509\11-Apr-2008\0\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-N
H2.freq\0,2\H,-1.1736331815,0.0128501953,-1.2291132979\N,-0.220604924
8,0.3639565262,-1.1763674233\C,0.5083203558,-0.1573878451,-0.091469272
9\H,0.2365966872,0.2374028205,-2.0741434361\C,-0.1752467687,-0.2075081
748,1.2362018013\H,1.5714701638,0.0728703908,-0.1239881761\H,0.4505479
433,-0.7214568498,1.9735856305\H,-1.129164868,-0.7536327185,1.17800188
96\H,-0.4100237939,0.7936465974,1.6418341833\Version=IA64L-G03RevC.02
\State=2-A\HF=-134.5159116\S2=0.753022\S2-1=0.\S2A=0.750007\RMSD=8.755
e-09\RMSF=3.332e-05\Dipole=-0.1530215,-0.2104331,-0.3357615\PG=C01 [X(
C2H6N1)]\@
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r.CHCH3-OH

```
1\1\GINC-AC27\FOpt\UB3LYP\Gen\C2H5O1(2)\CYL509\21-Nov-2008\0\B3LYP/g
en 6D INT(grid=ultrafine) OPT Freq=noraman maxdisk=2684354560\r.CHCH3
-OH.freq\0,2\C,0.0132479473,-0.0039473455,1.0975130245\H,0.9972564452
,-0.1007713334,1.5924657793\H,-0.6100616678,-0.8354080877,1.4615930184
\H,-0.4438998235,0.9247813505,1.4547762726\C,0.1071002213,0.000889562,
-0.3916084275\H,0.4011503836,0.8989130068,-0.927025629\O,0.5580938773,
-1.1253927605,-1.0420501977\H,0.3231116167,-1.9034073922,-0.5114308407
\Version=IA64L-G03RevE.01\State=2-A\HF=-154.3753149\S2=0.753078\S2-1=
0.\S2A=0.750007\RMSD=4.169e-09\RMSF=6.045e-06\Thermal=0.\Dipole=-0.106
4176,-0.1962603,0.5899288\PG=C01 [X(C2H5O1)]\@
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r.CHCH3-F

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C2H4F1(2)\CYL509\11-Apr-2008\0\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-F
.freq\0,2\C,0.1345491783,-0.0197216234,-1.2002244462\C,0.4453680983,-
0.1815679004,0.2413673419\H,1.42686276,0.0161115049,0.6668777772\F,-0.
5624331393,0.125178175,1.0934012994\H,0.9678980773,-0.3871856261,-1.80
78102953\H,-0.0447151742,1.0341820187,-1.4754119604\H,-0.7676510686,-0.
5819743294,-1.4711245906\Version=IA64L-G03RevC.02\State=2-A\HF=-178.
3909889\S2=0.753093\S2-1=0.\S2A=0.750007\RMSD=9.893e-09\RMSF=6.888e-05
\Dipole=0.3499928,0.0526283,-0.448163\PG=C01 [X(C2H4F1)]\@
```

r.CHCH3-SiH3

```
1\1\GINC-AC26\FOpt\UB3LYP\Gen\C2H7Si1(2)\CYL509\11-Apr-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
SiH3.freq\0,2\H,-1.1173211775,-0.5227663377,-1.8024312936\Si,-1.06742
01534,-0.372824576,-0.315121225\C,0.6636949601,-0.2906344256,0.3410346
626\H,-1.8066535436,0.8803088495,0.0122701414\H,-1.7898380123,-1.53567
44318,0.2708104641\H,1.1335024911,-1.2031093508,0.7106406\C,1.53237180
29,0.9303420573,0.350844551\H,2.3909081811,0.8157648653,-0.330981791\H
,1.9611375272,1.1096279739,1.3485662343\H,0.995746103,1.8371467065,0.0
515475126\Version=IA64L-G03RevC.02\State=2-A\HF=-369.858529\S2=0.7538
78\S2-1=0.\S2A=0.750011\RMSD=7.135e-09\RMSF=1.466e-06\Dipole=0.4179913
,0.0786068,0.1156337\PG=C01 [X(C2H7Si1)]\@
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r.CHCH3-PH2

```
1\1\GINC-AC4\FOpt\UB3LYP\Gen\C2H6P1(2)\CYL509\11-Apr-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-PH
2.freq\0,2\H,-1.5284479478,-0.8110113763,0.537656386\P,-0.9279742972,
0.4832096758,0.5068434909\H,-0.7945786605,0.6058480067,1.9200516691\C,
0.7629941247,0.0204897254,0.089180859\H,1.5528008187,0.6428304528,0.50
71248215\C,1.0917026761,-0.794462129,-1.1234721776\H,2.0647340846,-1.2
89096406,-1.0099889701\H,1.1557259628,-0.1810989941,-2.0386790035\H,0.
3411993946,-1.5717823989,-1.3130693541\Version=IA64L-G03RevC.02\State
```

=2-A\HF=-421.1084255\S2=0.7548\S2-1=0.\S2A=0.750018\RMSD=4.894e-09\RMSF=1.064e-05\Dipole=0.2822675,-0.2265215,0.0158779\PG=C01 [X(C2H6P1)]\@

r.CHCH3-SH

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C2H5S1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-SH.freq\0,2\H,-1.014446352,0.2144366027,-1.8031639674\S,-0.2373854175,0.7212394708,-0.82263958\C,-0.149540853,-0.7209189353,0.1757728548\H,-0.3063929441,-1.677322727,-0.3126762204\C,0.601819433,-0.64426911,1.4634024013\H,1.6960997893,-0.6850114522,1.3255030533\H,0.3281745423,-1.4846038878,2.1119115141\H,0.3810601638,0.283798203,2.0056073636\Version=IA64L-G03RevC.02\State=2-A\HF=-477.3535172\S2=0.753983\S2-1=0.\S2A=0.750012\RMSD=3.060e-09\RMSF=1.810e-05\Dipole=-0.0536048,-0.4358635,-0.053748\PG=C01 [X(C2H5S1)]\@

r.CHCH3-Cl

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C2H4Cl1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-Cl.freq\0,2\Cl,-0.4607641184,0.2723861003,-0.9939921578\C,-0.1964280312,0.1340075262,0.7169308066\C,0.9752150414,-0.6352177075,1.2096575237\H,-0.7002881646,0.8946619351,1.301155247\H,1.9310514059,-0.1327737554,0.9859649875\H,1.0216089584,-1.6319658392,0.7543129967\H,0.9078957514,-0.7532249575,2.2969034704\Version=IA64L-G03RevC.02\State=2-A\HF=-538.7611963\S2=0.753952\S2-1=0.\S2A=0.750011\RMSD=6.876e-09\RMSF=5.511e-05\Dipole=0.2717097,-0.0301457,0.5907446\PG=C01 [X(C2H4Cl1)]\@

r.CHCH3-Br

1\1\GINC-AC14\FOpt\UB3LYP\Gen\C2H4Br1(2)\CYL509\10-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-Br.freq\0,2\Br,-0.3188129531,0.2718034652,-0.656681023\C,-0.0209174812,-0.6943616694,0.9470365261\C,1.2455867188,-0.4943537424,1.6971431939\H,-0.9352320577,-1.0466516312,1.4092642816\H,2.1214803956,-0.5818164474,1.043783262\H,1.3266754235,-1.2492964759,2.488396438\H,1.2975141705,0.4969357442,2.1773135039\Version=IA64L-G03RevC.02\State=2-A\HF=-2652.4463004\S2=0.754252\S2-1=0.\S2A=0.750013\RMSD=2.969e-09\RMSF=3.070e-05\Dipole=0.1789199,-0.1697691,0.6132898\PG=C01 [X(C2H4Br1)]\@

r.CHCH3-N_CH3_2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C4H10N1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-N_CH3_2.freq\0,2\C,0.9352192491,0.1174004628,1.6013175197\H,2.0261833869,0.2180663968,1.5939680215\H,0.6767601362,-0.768313659,2.1900979202\H,0.5081350905,1.00220803,2.1055146361\N,0.4483333032,-0.0455389997,0.2406586755\C,-0.8618611116,-0.5255097639,0.1187957685\C,0.8812427345,1.0135234683,-0.6570909165\H,-1.1256909221,-1.2421326524,0.8935363681\C,-1.4910782545,-0.6934134417,-1.2285540785\H,1.967496421,1.1302048756,-0.5802542716\H,0.412857323,1.9876427681,-0.4258390334\H,0.6417176131,0.755911337,-1.6914591516\H,-0.9115600931,-1.3496597682,-1.9047672741\H,-1.6338292876,0.2583585726,-1.7593945438\H,-2.4815384951,-1.145517256,-1.1128231594\Version=IA64L-G03RevC.02\State=2-A\HF=-213.134297\S2=0.753172\S2-1=0.\S2A=0.750007\RMSD=2.501e-09\RMSF=8.622e-06\Dipole=0.2665933,0.1732558,0.0570481\PG=C01 [X(C4H10N1)]\@

r.CHCH3-NHCH3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H8N1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-NHCH3.freq\0,2\C,1.3808295183,0.1028770992,1.2751793597\H,2.4270164731,0.3838028529,1.118419773\H,1.3620330271,-0.9285264622,1.6448733402\H,

0.9536868526,0.7498058718,2.0593307358\N,0.6642015905,0.1657870242,0.0
102363073\C,-0.6670812285,-0.2634301871,-0.0176731082\H,-0.8516026774,
-1.1634099737,0.5672873178\C,-1.44188336,-0.0528158729,-1.2788711811\H
,0.8032984243,1.0493659411,-0.472087601\H,-1.0696212238,-0.6552255651,
-2.1279299485\H,-1.4103944252,0.9986476769,-1.6024571522\H,-2.49501716
34,-0.3147557465,-1.1309010387\Version=IA64L-G03RevC.02\State=2-A\HF=
-173.8254835\S2=0.753032\S2-1=0.\S2A=0.750007\RMSD=7.196e-09\RMSF=1.32
8e-05\Dipole=0.2445528,0.2656117,0.0939366\PG=C01 [X(C3H8N1)]\@

r.CHCH3-NHCHO

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H6N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3
-NHCHO.freq\0,2\H,1.3489649247,-0.2207510593,-2.0217325392\C,1.151718
8233,0.1122377708,-0.9860206619\O,1.9642963584,0.7115690944,-0.3012358
927\N,-0.1144391613,-0.2306881077,-0.5666988329\C,-0.6495886825,0.0923
490489,0.6680425337\H,-0.7033486947,-0.7170194081,-1.2328613424\H,0.03
7716194,0.5752366877,1.3483113211\C,-1.9483459264,-0.4970075845,1.0923
495526\H,-1.8616005063,-1.5497299091,1.4159326608\H,-2.6948836438,-0.4
743030356,0.2847388774\H,-2.362850298,0.0633553126,1.9361614479\Versi
on=IA64L-G03RevC.02\State=2-A\HF=-247.8618366\S2=0.756203\S2-1=0.\S2A=
0.750024\RMSD=5.033e-09\RMSF=7.993e-06\Dipole=-1.2926045,-0.7534923,-0
.417654\PG=C01 [X(C3H6N1O1)]\@

r.CHCH3-NHCOCH3

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C4H8N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
NHCOCH3.freq\0,2\H,-0.3258144766,2.679397848,-1.3573296471\C,0.334516
5461,1.8108541797,-1.4541154806\C,0.2933741055,1.0086561467,-0.1646869
763\H,1.3497164502,2.1918626199,-1.603219675\H,0.037105032,1.241847043
3,-2.3413746861\N,-0.1821930629,-0.2855060017,-0.2857836277\O,0.649419
9972,1.4681679441,0.9132939603\C,-0.3421536277,-1.1558509082,0.7783802
946\H,-0.4717648167,-0.5999596595,-1.2030263105\H,0.0220203813,-0.7834
364728,1.7254321693\C,-0.6633424052,-2.5863016688,0.5233629961\H,0.204
4994727,-3.1699856858,0.1664710245\H,-1.4548076504,-2.703836492,-0.232
0144088\H,-1.0153306415,-3.0668372396,1.4415502416\Version=IA64L-G03R
evC.02\State=2-A\HF=-287.1851652\S2=0.755404\S2-1=0.\S2A=0.75002\RMSD=
8.509e-09\RMSF=1.537e-05\Dipole=-0.4388384,-0.8091555,-1.1706116\PG=C0
1 [X(C4H8N1O1)]\@

r.CHCH3-NO2

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C2H4N1O2(2)\CYL509\11-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3
-NO2.freq\0,2\O,-0.6837150332,0.3036094178,-1.1618754294\N,-0.6105485
892,-0.0719011574,0.0193077088\C,0.6678545414,-0.1293660353,0.62006574
35\O,-1.5785227022,-0.4057799219,0.7271401172\C,1.8657646666,0.2503170
301,-0.1531950686\H,0.6526999233,-0.4648431939,1.6485991713\H,2.764335
3194,0.1488070054,0.4594069025\H,1.7869908196,1.2849071961,-0.51464411
52\H,1.9660006979,-0.3739048422,-1.0518574717\Version=IA64L-G03RevC.0
2\State=2-A\HF=-283.6687346\S2=0.757699\S2-1=0.\S2A=0.750037\RMSD=8.20
9e-09\RMSF=6.110e-06\Dipole=1.6079474,0.0080006,0.5079452\PG=C01 [X(C2
H4N1O2)]\@

r.CHCH3-OCF3

1\1\GINC-AC27\FOpt\UB3LYP\Gen\C3H4F3O1(2)\CYL509\11-Apr-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3
-OCF3.freq\0,2\C,1.5128822387,-0.0075939093,0.122494639\O,0.299953297
9,-0.4777317208,-0.3812607337\C,-0.8295314643,0.121048917,0.0717637558
\F,-0.8512640696,1.4414853422,-0.2088715859\F,-0.9734636232,-0.0009563
911,1.4038861331\F,-1.8687794644,-0.4575191293,-0.5276887928\H,1.51870

84977,1.0385160361,0.4139453424\C,2.6968411077,-0.6890215586,-0.453630
4134\H,3.6015904343,-0.3681409532,0.0717439096\H,2.8319186367,-0.46411
92809,-1.5252794556\H,2.6085691701,-1.7780911262,-0.3600236046\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-491.419808\S2=0.75313\S2-1=0.\S2A=0.7
50007\RMSD=9.934e-09\RMSF=1.412e-05\Dipole=0.7665919,0.0833423,-0.0584
274\PG=C01 [X(C3H4F3O1)]\\@

r.CHCH3-OCH2CH3

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C4H9O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-OC
H2CH3.freq\0,2\H,-0.1224182624,-2.6318825196,1.977485937\C,-0.0329243
16,-2.1732551711,0.9866298745\C,-0.0550964606,-0.6592585243,1.10405052
06\O,0.0657178515,-0.1049052906,-0.2051335658\C,0.01350817,1.260188374
4,-0.2698843051\C,0.0832308814,1.8170014251,-1.6491444544\H,-0.5898161
666,1.7506463543,0.4980284842\H,-0.9954968964,-0.3143665708,1.56215803
66\H,0.7722501909,-0.2989884951,1.7321698616\H,0.904060244,-2.51016090
13,0.5317998204\H,-0.8624206092,-2.5248247069,0.3646385823\H,0.9493580
922,1.4147617434,-2.1893092019\H,0.1770681626,2.9075878334,-1.6133994\
H,-0.8106372162,1.5784129629,-2.252413407\\Version=IA64L-G03RevC.02\St
ate=2-A\HF=-233.0040348\S2=0.75296\S2-1=0.\S2A=0.750006\RMSD=2.551e-09
\RMSF=7.329e-06\Dipole=-0.1713522,-0.0461615,0.3799855\PG=C01 [X(C4H9O
1)]\\@

r.CHCH3-OCH3

1\1\GINC-AC4\FOpt\UB3LYP\Gen\C3H7O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-OC
H3.freq\0,2\C,-0.8768082675,0.3577848194,-1.544950187\O,-0.6492386315
,-0.0531125963,-0.2065010778\C,0.6357170616,0.107141779,0.2350326332\H
,-0.2305547343,-0.1932133169,-2.2440903068\H,-1.9222276942,0.137928865
,-1.7724245104\H,-0.6941737353,1.4338107628,-1.6660937353\C,0.87560444
87,-0.3763305426,1.6225548453\H,1.4146369134,0.0223155143,-0.526996344
1\H,1.8791253143,-0.0902580351,1.9549184605\H,0.7939079687,-1.47396427
44,1.7126685136\H,0.1461155633,0.0567049193,2.3182027963\\Version=IA64
L-G03RevC.02\State=2-A\HF=-193.6847587\S2=0.752942\S2-1=0.\S2A=0.75000
6\RMSD=8.765e-09\RMSF=5.070e-06\Dipole=0.1409126,0.0347715,-0.4128461\
PG=C01 [X(C3H7O1)]\\@

r.CHCH3-OCHO

1\1\GINC-AC4\FOpt\UB3LYP\Gen\C3H5O2(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-OC
HO.freq\0,2\C,-0.3768203032,0.0042360894,-0.8161310541\O,-0.339839860
1,0.1993776579,0.550143888\C,0.8565615146,0.1199369808,1.188289099\H,0
.694622727,0.3232131992,2.2554224864\O,1.9160554779,-0.1313539848,0.67
26368566\H,0.5321611671,-0.3738434193,-1.26613673\C,-1.7358315048,-0.1
259487101,-1.3925301503\H,-1.6827028378,-0.0915183093,-2.48509884\H,-2
.3929573646,0.683984986,-1.0515145632\H,-2.2243068734,-1.0753720022,-1
.1126856775\\Version=IA64L-G03RevC.02\State=2-A\HF=-267.7181698\S2=0.7
53942\S2-1=0.\S2A=0.750011\RMSD=7.624e-09\RMSF=1.263e-05\Dipole=-0.794
6944,-0.0032004,-0.0726245\PG=C01 [X(C3H5O2)]\\@

r.CHCH3-OCOCH3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-O
COCH3.freq\0,2\C,-1.3761457189,-0.0036509583,0.1699385337\O,-0.092088
6025,-0.4695575669,-0.0253239731\C,0.9475412218,0.4212321184,0.0516811
117\C,2.2616579592,-0.29285257,-0.1401555745\O,0.7974801068,1.60392193
17,0.2507040422\H,-1.489374247,1.0728230443,0.1908587786\C,-2.44781779
14,-0.9658668046,-0.1827684728\H,3.0733895189,0.4350691412,-0.12454005
73\H,2.2656894363,-0.8374348397,-1.0900214605\H,2.4100022746,-1.028404

7114,0.6579993406\H,-2.2732255653,-1.9457923037,0.279740179\H,-2.52479
11914,-1.1344725384,-1.2711569112\H,-3.4162362852,-0.5898734236,0.1619
0599\\Version=IA64L-G03RevC.02\State=2-A\HF=-307.0439996\S2=0.75362\S2
-1=0.\S2A=0.750009\RMSE=7.107e-09\RMSF=1.299e-05\Dipole=-0.0398355,-0.
7607323,-0.2252352\PG=C01 [X(C4H7O2)]\\@

r.CHCH3-Si_CH3_3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C5H13Si1(2)\CYL509\11-Apr-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3
-Si_CH3_3.freq\\0,2\H,1.2329922908,-1.6532116763,-1.8250453879\C,1.263
9857616,-1.6601528266,-0.728762902\H,2.318912045,-1.6824617031,-0.4293
811847\H,0.8047045247,-2.5965414872,-0.3899752885\Si,0.3780070963,-0.1
51446905,-0.0020791877\C,-1.3966609343,-0.1568537875,-0.5763438034\C,0
.454420899,-0.2159484355,1.8947022956\C,1.2553742327,1.4339554767,-0.5
75721896\H,-1.7218043361,-0.9005538109,-1.3076316629\C,-2.4687054768,0
.7967769492,-0.1369604453\H,2.2909604113,1.4625842734,-0.2135857087\H,
0.7497016444,2.3316426206,-0.1998189173\H,1.2820146028,1.5030702191,-1
.6695017141\H,1.4930524992,-0.1778491775,2.24661816\H,0.0042264652,-1.
1372890779,2.2823085136\H,-0.0772498018,0.6287680215,2.3493396859\H,-2
.1136943865,1.5325806614,0.5937191377\H,-3.3197021526,0.2663764631,0.3
197666889\H,-2.8867000479,1.3564770853,-0.9891831878\\Version=IA64L-G0
3RevC.02\State=2-A\HF=-487.8395284\S2=0.753683\S2-1=0.\S2A=0.750009\RM
SE=4.838e-09\RMSF=3.425e-05\Dipole=-0.109482,0.0339078,-0.0110673\PG=C
01 [X(C5H13Si1)]\\@

r.CHCH3-P_CH3_2

1\1\GINC-AC25\FOpt\UB3LYP\Gen\C4H10P1(2)\CYL509\11-Apr-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-
P_CH3_2.freq\\0,2\C,-0.8661161086,1.5164215585,1.1108707744\H,-0.13707
60673,2.2965204505,1.3540487597\H,-1.5000515572,1.3669872802,1.9910213
862\H,-1.4872976151,1.8603546495,0.2766650801\P,0.034478697,-0.0699566
5,0.7206151544\C,-1.3749420458,-1.1310326459,0.0991903642\C,0.91288737
68,0.3793099965,-0.7748795671\H,-0.9823154793,-2.0647252916,-0.3155453
18\H,-1.97128985,-0.6249704921,-0.6678677996\H,-2.0210484772,-1.391201
5532,0.9444403323\H,1.328780243,1.3873280921,-0.8014091642\C,1.5228913
728,-0.6190467638,-1.7131850844\H,2.5700874054,-0.8505937942,-1.455197
047\H,1.535348835,-0.2334757682,-2.7418736149\H,0.9793585357,-1.570786
6944,-1.7254888535\\Version=IA64L-G03RevC.02\State=2-A\HF=-499.7498714
\S2=0.755798\S2-1=0.\S2A=0.750023\RMSE=8.162e-09\RMSF=1.879e-06\Dipole
=-0.281388,0.1384433,-0.2700761\PG=C01 [X(C4H10P1)]\\@

r.CHCH3-SC_CH3_2CN

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C6H10N1S1(2)\CYL509\11-Apr-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH
3-SC_CH3_2CN.freq\\0,2\C,1.7930614341,-0.0352366197,-0.0744037386\H,1.
7583749131,-0.1163694344,1.0098697814\C,3.1112596381,0.0094589701,-0.7
780078212\S,0.3703389529,-0.5202902647,-0.953629289\C,-1.025176861,0.2
031658371,0.0769378857\C,-0.9738449564,1.7415665349,0.0522947309\C,-2.
3321322396,-0.3327449064,-0.5384210106\C,-0.8856785199,-0.2785428744,1
.4581469091\H,-0.0162246997,2.1056337896,0.4329155063\H,-1.0979188007,
2.0928815151,-0.9762952696\H,-1.7787844936,2.1568430482,0.6695403303\H
, -2.4096361884,-0.0047198605,-1.5798758788\H,-3.1912264598,0.060503083
3,0.0145671514\H,-2.3679184008,-1.4249467066,-0.5084328487\N,-0.765507
0904,-0.6376028438,2.5566490839\H,3.810832131,0.6491384499,-0.22631041
62\H,3.015662477,0.4061155357,-1.7954611224\H,3.5850349362,-0.98321692
82,-0.8582739288\\Version=IA64L-G03RevC.02\State=2-A\HF=-687.5344669\S
2=0.755014\S2-1=0.\S2A=0.750018\RMSE=3.395e-09\RMSF=2.189e-05\Dipole=-
0.1058004,0.6764413,-1.0046839\PG=C01 [X(C6H10N1S1)]\\@

r.CHCH3-SCH2COOCH3

```
1\1\GINC-AC26\FOpt\UB3LYP\Gen\C5H9O2S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
SCH2COOCH3.freq\0,2\S,1.2866829695,0.8773704283,-0.4080250311\C,1.33
67375255,0.8873707383,1.3394170476\C,2.6683100735,0.9408846502,2.01505
36368\H,0.4632670147,0.5012193881,1.8564196554\C,-0.5255769976,0.99514
75913,-0.7164379901\C,-1.2382034514,-0.2806859704,-0.3196481159\O,-1.6
277725392,-0.5304857152,0.802029966\O,-1.3604330318,-1.1208057385,-1.3
656234301\C,-1.9630215155,-2.3922646074,-1.067072995\H,-0.928734215,1.
8295260592,-0.1391485847\H,-0.6351841004,1.1873721889,-1.7853998404\H,
-2.9739160769,-2.2545309124,-0.6747502617\H,-1.3646006551,-2.933289156
9,-0.3294764776\H,-1.9872356038,-2.9324886869,-2.0135697639\H,2.550632
5765,1.2763518978,3.0521910233\H,3.1720468931,-0.0402969156,2.05012085
69\H,3.3529674144,1.6358265029,1.5128921036\Version=IA64L-G03RevC.02\
State=2-A\HF=-744.5405382\S2=0.754219\S2-1=0.\S2A=0.750014\RMSE=9.831e
-09\RMSF=1.637e-06\Dipole=-0.2474615,-0.2636162,-0.3652591\PG=C01 [X(C
5H9O2S1)]\@
```

r.CHCH3-SCH2Ph

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C9H11S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
SCH2Ph.freq\0,2\C,1.9827675117,0.9397999845,-0.7914642272\S,2.1153942
222,-0.5696798168,0.0686748358\C,0.768387916,-0.4099485197,1.333191108
2\H,0.9897778283,1.3738280261,-0.8783723537\C,3.0462049783,1.308828821
6,-1.7755439016\C,-0.6250167165,-0.2864707366,0.7700865525\H,1.0106024
727,0.4437281912,1.9722345981\H,0.8732017506,-1.3196888141,1.933257210
3\C,-1.3146979297,0.9302774178,0.8424747345\C,-1.2598291279,-1.3842057
389,0.1702540179\C,-2.608688093,1.050656273,0.3293502194\C,-2.55064268
2,-1.2675893488,-0.3400906342\C,-3.2300280812,-0.0480822873,-0.2627541
002\H,-4.2372341386,0.0418126854,-0.6606368716\H,-3.0295909242,-2.1290
85231,-0.7979998181\H,-3.1288502041,2.0026158409,0.3957780387\H,-0.732
1850322,-2.3324153384,0.099366314\H,-0.8371856731,1.7877079248,1.31148
72992\H,4.0477282445,1.0631914696,-1.4018207311\H,3.0175636243,2.38628
94506,-1.9787326458\H,2.9291178419,0.7972976689,-2.7463810285\Version
=IA64L-G03RevC.02\State=2-A\HF=-747.7208868\S2=0.75433\S2-1=0.\S2A=0.7
50014\RMSE=6.501e-09\RMSF=3.248e-06\Dipole=-0.5027361,0.2090676,0.0946
062\PG=C01 [X(C9H11S1)]\@
```

r.CHCH3-SCH3

```
1\1\GINC-AC26\FOpt\UB3LYP\Gen\C3H7S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-S
CH3.freq\0,2\S,0.1169812873,0.0388876941,-0.7848061483\C,0.1437311434
,-0.1046157508,0.9525511272\C,1.4576298836,-0.0811348637,1.6647488504\
H,-0.7210345411,-0.5654442384,1.4249332249\C,-1.6803334143,0.135477300
3,-1.102143028\H,-1.8137593422,0.2008752785,-2.1846350489\H,-2.1079398
106,1.0233546771,-0.629654267\H,-2.1868232749,-0.7618196355,-0.7348869
785\H,1.312889258,0.1703402769,2.7224316052\H,1.9817976704,-1.05188939
24,1.6346536484\H,2.1370037677,0.6640198124,1.2331144918\Version=IA64
L-G03RevC.02\State=2-A\HF=-516.6704115\S2=0.754181\S2-1=0.\S2A=0.75001
3\RMSE=6.629e-09\RMSF=1.008e-05\Dipole=-0.4850504,-0.0874792,0.1667749
\PG=C01 [X(C3H7S1)]\@
```

r.CHCH3-SO2CH3

```
1\1\GINC-AC8\FOpt\UB3LYP\Gen\C3H7O2S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
SO2CH3.freq\0,2\C,0.0037654796,-0.0850277296,-1.3380195253\S,0.049694
3844,-0.1402806068,0.4283570538\C,1.7942456032,0.1266554911,0.81954038
82\O,-0.7122435411,1.010871506,0.9403030496\O,-0.2884588472,-1.5093896
585,0.8602168745\H,2.3970081721,-0.6513540723,0.3459515231\H,1.8783343
```

882,0.0517408242,1.9068914523\H,2.0931846416,1.1211533819,0.4829056966
\H,0.6497295924,-0.8020364295,-1.8386493535\C,-1.0817690197,0.63542087
19,-2.0511994478\H,-0.7003965081,1.0895510753,-2.9747455415\H,-1.51402
49218,1.413792216,-1.4169261769\H,-1.8907787868,-0.0525038675,-2.34522
83441\\Version=IA64L-G03RevC.02\State=2-A\HF=-667.0490374\S2=0.754254\
S2-1=0.\S2A=0.750013\RMSD=9.581e-09\RMSF=2.159e-06\Dipole=1.1757673,0.
3170246,-1.2473742\PG=C01 [X(C3H7O2S1)]\\@

r.CHCH3-SOCH3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C3H7O1S1(2)\CYL509\11-Apr-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT IOP(2/17=4) MAXDISK=1342177280\\r.CHCH
3-SOCH3.freq\\0,2\H,0.7797673414,1.6123129725,-1.3509788052\C,0.892748
5479,1.7264260435,-0.2704461019\H,1.9332308549,1.9463229925,-0.0178462
611\H,0.2382883498,2.5153871691,0.1111004333\S,0.4661329593,0.12646898
23,0.5488105511\O,1.2356540701,-0.9764292797,-0.142733113\C,-1.2325092
019,0.0498606738,0.0468330803\H,-1.8792484136,0.8050683711,0.489961689
1\C,-1.7714190405,-1.1959092633,-0.5607410671\H,-0.9586185598,-1.77288
91059,-1.0134615767\H,-2.5171731791,-0.9591661397,-1.3310026297\H,-2.2
725281359,-1.8413704627,0.1792477687\\Version=AM64L-G03RevC.02\State=2
-A\HF=-591.8383026\S2=0.755477\S2-1=0.\S2A=0.750023\RMSD=6.678e-09\RMS
F=1.055e-05\Dipole=-0.9127452,1.0731556,0.0778401\PG=C01 [X(C3H7O1S1)]
\\@

r.CHCH3-Ph

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C8H9(2)\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-Ph.
freq\\0,2\H,-3.3802621611,-0.4398432256,-0.1580217683\C,-2.3098441934,
-0.2549353417,-0.1455148638\C,-1.464175551,-1.0508363939,0.6380688922\
C,-0.0955058014,-0.8213015489,0.6597554564\C,0.4867026015,0.2263220129
, -0.1112448284\C,-0.3969307965,1.0203734088,-0.899267982\C,-1.76213360
68,0.7826423093,-0.9136594764\H,-1.8820999184,-1.8570378359,1.23599684
65\C,1.8779782669,0.4890491588,-0.1133157608\C,2.8933073894,-0.2791554
021,0.674426511\H,2.2292165749,1.3100657428,-0.733952383\H,0.020947168
,1.8269042745,-1.4976164805\H,0.5436212365,-1.449183546,1.2735734492\H
, -2.4110484093,1.4051446135,-1.5246346605\H,3.900569762,0.1131433765,0
.5079144221\H,2.9058421764,-1.3461087116,0.4048076726\H,2.6968237184,-
0.2360339071,1.7564452118\\Version=IA64L-G03RevC.02\State=2-A\HF=-310.
2333485\S2=0.7799\S2-1=0.\S2A=0.750612\RMSD=3.245e-09\RMSF=3.733e-05\D
ipole=0.1438951,-0.0211913,0.0395936\PG=C01 [X(C8H9)]\\@

r.CHCH3-C6H4CN

1\1\GINC-AC23\FOpt\UB3LYP\Gen\C9H8N1(2)\CYL509\11-Apr-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-C
6H4CN.freq\\0,2\N,-4.0384145562,-0.9086688661,0.1510352346\C,-2.894813
9719,-0.686056843,0.1351892882\C,-1.4937103848,-0.4133376372,0.1158418
294\C,-0.5994799715,-1.2140103126,0.8623170244\C,0.7536599714,-0.94661
87169,0.8406089842\C,1.292237933,0.1319847786,0.0743756934\C,0.3680753
314,0.9261209937,-0.670499399\C,-0.9870955733,0.6599608923,-0.64968244
03\H,-0.9885005749,-2.0388172319,1.4509532573\C,2.6800308021,0.3791773
891,0.0727227752\H,3.3012145531,-0.2757156459,0.6793315634\C,3.3561972
018,1.4767461362,-0.6875811182\H,0.7361148717,1.7566601063,-1.26435951
07\H,1.4338303039,-1.5676222467,1.4177710492\H,-1.6752497714,1.2743513
815,-1.221854811\H,4.4429260054,1.4131650768,-0.5870473353\H,3.0498536
674,2.472087262,-0.3315158365\H,3.1181048085,1.4427732801,-1.760280841
7\\Version=IA64L-G03RevC.02\State=2-A\HF=-402.4795594\S2=0.783113\S2-1
=0.\S2A=0.750736\RMSD=4.947e-09\RMSF=2.030e-05\Dipole=2.130588,0.49212
59,-0.0821996\PG=C01 [X(C9H8N1)]\\@

r.CHCH3-C6H4NO2

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C8H8N1O2(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
C6H4NO2.freq\0,2\O,-2.6055459739,1.5647883046,-1.2985285451\N,-1.381
8020181,1.71747288,-1.35952667\C,-0.5418667446,0.785488555,-0.61783981
31\O,-0.8219782076,2.6070930043,-2.0071859101\C,-1.1461389073,-0.23607
35521,0.1275742584\C,-0.3508604277,-1.1199553904,0.8308616083\C,1.0739
215235,-1.0124690965,0.8126945835\C,1.6420836181,0.0459440048,0.038175
1581\C,0.8520808638,0.931401088,-0.6662123598\H,1.2795763799,1.7342375
533,-1.2540210728\C,1.9098210529,-1.8994013959,1.5201411135\H,2.982265
0765,-1.7344576595,1.4466168289\C,1.4349495555,-3.0412406848,2.3623654
731\H,-0.8195072827,-1.9103448686,1.4080959284\H,2.7234527856,0.149344
0744,0.0080646211\H,-2.2264913399,-0.3122751496,0.1374977781\H,2.27680
17865,-3.5946299444,2.7862467444\H,0.8257997145,-3.751500619,1.7848396
521\H,0.8069672531,-2.6998951852,3.1985017197\Version=IA64L-G03RevC.0
2\State=2-A\HF=-514.7384418\S2=0.779712\S2-1=0.\S2A=0.750565\RMSD=7.85
0e-09\RMSF=2.236e-05\Dipole=1.2992598,-1.5838779,1.257513\PG=C01 [X(C8
H8N1O2)]\@
```

r.CHCH3-C6H4OCH3

```
1\1\GINC-AC27\FOpt\UB3LYP\Gen\C9H11O1(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
C6H4OCH3.freq\0,2\C,-1.3682097888,-0.0487573243,-0.9113602447\C,-1.34
44323124,-0.053110463,0.4977340589\C,-0.1119515932,-0.0086759926,1.165
5834958\C,1.0724556649,0.0391596132,0.4380503755\C,1.0831622942,0.0449
021169,-0.9841969752\C,-0.1913686122,-0.0012581629,-1.6279597151\C,2.2
739854922,0.0931051586,-1.7445851325\O,-2.5642502177,-0.101855022,1.10
93530344\C,-2.6049323047,-0.1085662237,2.526760342\C,3.6535190459,0.14
36511315,-1.1639713381\H,2.1759264268,0.0934922408,-2.8275197628\H,-0.
226970236,0.0014291386,-2.7149376866\H,2.0142648,0.0730076979,0.977675
7276\H,-0.0674492495,-0.0110617636,2.2491710394\H,-2.3320343561,-0.083
5999572,-1.4103081197\H,-2.0907360513,-0.9857685049,2.9417603962\H,-3.
6619295004,-0.1497303939,2.7964462647\H,-2.1586978939,0.8020950829,2.9
482748524\H,4.4117042618,0.1756008195,-1.9518857564\H,3.871946736,-0.7
319092859,-0.5332228145\H,3.8046094888,1.028585979,-0.5266076154\Vers
ion=IA64L-G03RevC.02\State=2-A\HF=-424.7562419\S2=0.778215\S2-1=0.\S2A
=0.750529\RMSD=6.194e-09\RMSF=1.199e-05\Dipole=0.0809319,0.0011205,0.5
535132\PG=C01 [X(C9H11O1)]\@
```

r.CHCH3-C6H4OH

```
1\1\GINC-AC19\FOpt\UB3LYP\Gen\C8H9O1(2)\CYL509\15-May-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CHCH3-C
6H4OH.a2.freq\0,2\C,-1.1746632865,0.3117938899,0.967642326\C,-1.17099
06327,-1.0898236714,0.9556047982\C,-0.2259117654,-1.7759478692,0.17429
61237\C,0.6924790869,-1.0674488231,-0.5761016742\C,0.7207686467,0.3598
901462,-0.59017418\C,-0.2514536628,1.0218593285,0.2132906092\C,1.67389
58909,1.0551371915,-1.3692271496\O,-2.0564371311,-1.8412439177,1.67864
83844\H,2.3750035428,0.4600444568,-1.9493639072\C,1.7833017115,2.54659
09155,-1.4496289563\H,-0.2744103845,2.1070711181,0.2391461732\H,1.4198
321068,-1.6077138526,-1.1774966746\H,-0.2361753558,-2.8616174049,0.175
7473405\H,-1.9067563169,0.8450317345,1.5728883154\H,-2.6466392176,-1.2
468171319,2.1676043456\H,2.5970585625,2.8463050758,-2.1163974918\H,1.9
788212277,3.0033359024,-0.4671073336\H,0.8602069537,3.0120047965,-1.82
84192245\Version=IA64L-G03RevC.02\State=2-A\HF=-385.4496937\S2=0.7786
65\S2-1=0.\S2A=0.750549\RMSD=4.126e-09\RMSF=1.573e-05\Dipole=-0.311360
7,0.0017193,-0.4815388\PG=C01 [X(C8H9O1)]\@
```

r.CHCH3-CF2CF3

```
1\1\GINC-AC12\FOpt\UB3LYP\Gen\C4H4F5(2)\CYL509\11-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C
```

F2CF3.freq\0,2\F,-0.9227140264,0.3439307956,-1.5903331144\C,-0.613032
2914,0.149985705,-0.2724677609\C,0.9329402072,0.1751937948,-0.1825271
527\C,-1.240764601,-1.0996771855,0.2287429026\F,-1.0485018477,1.241439
8547,0.4341258003\F,1.4499726717,-0.8448689252,-0.8898059617\F,1.31872
32842,0.0386297419,1.1006696334\F,1.4349059402,1.3214235604,-0.6574503
519\H,-1.3494689008,-1.8960478866,-0.5000285637\C,-1.4517993499,-1.349
4439572,1.6798074396\H,-0.5696283595,-1.8223927338,2.1429733573\H,-2.2
97649258,-2.0265312721,1.8409817177\H,-1.6387914697,-0.4164506901,2.21
98868661\Version=IA64L-G03RevC.02\State=2-A\HF=-653.9812932\S2=0.7537
09\S2-1=0.\S2A=0.750009\RMSD=5.813e-09\RMSF=4.708e-06\Dipole=-0.368716
5,-0.7291193,0.4258317\PG=C01 [X(C4H4F5)]\@

r.CHCH3-CF2H

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H5F2(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C
F2H.freq\0,2\C,0.1379446229,0.2603650983,-0.5808477415\C,0.2950055903
,0.2931214306,0.8959909423\H,0.3854799908,1.2777308925,1.3448618499\H,
1.088003949,0.2452935172,-1.1385621642\F,-0.5573366272,1.3641277392,-1
.0051018166\F,-0.5583094952,-0.8613430996,-0.970474748\C,0.6309240491,
-0.9315282439,1.672880373\H,1.7171858022,-1.132333928,1.6819247003\H,0
.1448466181,-1.8140502979,1.2445895907\H,0.3220531686,-0.83345165,2.71
92336622\Version=IA64L-G03RevC.02\State=2-A\HF=-316.946275\S2=0.75370
9\S2-1=0.\S2A=0.750009\RMSD=7.175e-09\RMSF=2.209e-05\Dipole=0.6819611,
-0.0841701,0.5633064\PG=C01 [X(C3H5F2)]\@

r.CHCH3-CF3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H4F3(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C
F3.freq\0,2\F,0.6206118705,-0.0411605433,-1.2718112978\C,0.3729942426
,0.2286719023,0.0332956869\F,1.5598578464,0.2843383713,0.6746698245\C,
-0.5315739754,-0.7738219959,0.6464361672\F,-0.1542344059,1.4853981214,
0.0671725037\C,-1.7669995605,-1.2198773332,-0.0511412986\H,-0.37602573
72,-0.9716957118,1.7015558102\H,-1.6050347852,-1.302158699,-1.13095648
85\H,-2.5940238866,-0.5049672116,0.097982647\H,-2.1075576309,-2.188197
3615,0.3295954252\Version=IA64L-G03RevC.02\State=2-A\HF=-416.1995334\
S2=0.753615\S2-1=0.\S2A=0.750009\RMSD=8.722e-09\RMSF=1.222e-05\Dipole=
-0.6600653,-0.5668453,0.2958664\PG=C01 [X(C3H4F3)]\@

r.CHCH3-CCl2H

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H5Cl2(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
CCl2H.freq\0,2\C,0.2267751291,-0.2480716458,-0.1680821527\C,0.3061579
007,-0.3110503899,1.2903301341\H,1.1412309284,-0.5557793353,-0.6716750
735\Cl,-0.0070901538,1.5224676828,-0.7383812136\Cl,-1.1116824135,-1.26
0038004,-0.8231705141\C,1.5877118698,-0.0533903387,2.0062790074\H,-0.6
309458396,-0.3065608815,1.8391704933\H,2.4557248494,-0.3994403834,1.43
27594475\H,1.5971262499,-0.5485986839,2.9835910475\H,1.7321280595,1.02
41489907,2.1913715227\Version=IA64L-G03RevC.02\State=2-A\HF=-1037.666
3942\S2=0.754754\S2-1=0.\S2A=0.750017\RMSD=4.141e-09\RMSF=1.311e-05\Di
pole=0.7198141,-0.3090789,0.8013143\PG=C01 [X(C3H5Cl2)]\@

r.CHCH3-CCl3

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C3H4Cl3(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-
CCl3.freq\0,2\C,-0.0834428581,-0.1392344394,0.0299497395\C,0.04789950
67,-0.0730284501,1.493899339\Cl,1.6025027482,-0.2061426417,-0.74906670
32\Cl,-0.9284501844,1.3119073702,-0.6531187253\Cl,-0.9776752516,-1.623
2890928,-0.4600699717\C,0.5495570847,1.1289926882,2.2143287836\H,-0.00
2057751,-1.0284664247,2.0057339121\H,1.6450869456,1.2128115511,2.12569

57296\H,0.3122092892,1.0579859794,3.2801489197\H,0.1222648102,2.055204
296,1.817696069\\Version=IA64L-G03RevC.02\State=2-A\HF=-1497.2473275\S
2=0.754449\S2-1=0.\S2A=0.750015\RMSD=5.307e-09\RMSF=2.139e-05\Dipole=0
.0910395,0.1613122,0.9919795\PG=C01 [X(C3H4Cl3)]\\@

r.CHCH3-CH2Cl

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C3H6Cl1(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-
CH2Cl.freq\0,2\C,-0.6947622136,0.4667445811,-0.9736334909\C,-0.634743
7651,0.496533852,0.4834473125\Cl,1.0957612285,-0.0121789642,1.10875320
25\H,-0.3460976974,1.3461206976,-1.510623086\C,-0.9014584711,-0.794916
3495,-1.7391494858\H,-1.2919908439,-0.2282562853,0.9655023992\H,-0.770
9544124,1.4885207538,0.9124859549\H,0.0590257496,-1.3003584662,-1.9360
04104\H,-1.3632768343,-0.6022583667,-2.7144379001\H,-1.5288601486,-1.5
068984431,-1.1897137206\\Version=IA64L-G03RevC.02\State=2-A\HF=-578.07
77305\S2=0.755368\S2-1=0.\S2A=0.750021\RMSD=3.557e-09\RMSF=8.971e-06\D
ipole=-0.855187,0.1407988,-0.5917699\PG=C01 [X(C3H6Cl1)]\\@

r.CHCH3-CH2F

1\1\GINC-AC4\FOpt\UB3LYP\Gen\C3H6F1(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH
2F.freq\0,2\C,-0.5869984322,-0.339133857,-0.0941912485\C,0.6758394143
,0.4415707364,-0.1199255841\F,1.7525354111,-0.3758319749,-0.4627773535
\H,-0.6830172947,-1.1341476727,-0.8297788563\C,-1.7944103627,0.1481371
974,0.6325474681\H,0.8796986307,0.8989520925,0.8604216578\H,0.64625593
55,1.2620916597,-0.8606631113\H,-1.5281880385,0.6403908518,1.577402024
3\H,-2.4824033492,-0.6740384015,0.8606315987\H,-2.3717483012,0.8857947
83,0.0463990549\\Version=IA64L-G03RevC.02\State=2-A\HF=-217.70215\S2=0
.753849\S2-1=0.\S2A=0.750011\RMSD=3.104e-09\RMSF=1.294e-05\Dipole=-0.6
587954,0.3966147,0.136868\PG=C01 [X(C3H6F1)]\\@

r.CHCH3-CH2OH

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C3H7O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH
2OH.freq\0,2\C,-0.6012586148,-0.359956231,-0.0554587787\C,0.661258343
3,0.4256349115,-0.0945802947\O,1.7334359048,-0.4366275964,-0.465847697
3\H,-0.6695679125,-1.2079829442,-0.7319293577\C,-1.8302937511,0.175352
6355,0.5972646604\H,0.8414863063,0.8957468822,0.8908362217\H,0.5743800
349,1.2655230881,-0.8179265768\H,2.5153603872,0.115093595,-0.617758848
7\H,-1.5979272674,0.6918663929,1.538749986\H,-2.5481485041,-0.62271179
75,0.818107744\H,-2.3613061469,0.9092976593,-0.0366511125\\Version=IA6
4L-G03RevC.02\State=2-A\HF=-193.6793476\S2=0.753935\S2-1=0.\S2A=0.7500
11\RMSD=3.003e-09\RMSF=3.001e-06\Dipole=-0.0001813,0.6664566,-0.004713
5\PG=C01 [X(C3H7O1)]\\@

r.CHCH3-CH2Ph

1\1\GINC-AC23\FOpt\UB3LYP\Gen\C9H11(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH
2Ph.freq\0,2\C,-1.6891103922,-1.6182206895,0.2996602361\C,-0.30679644
58,-1.5042063686,-0.2687294355\C,0.2815417927,-0.106126766,-0.20476319
04\C,0.7638736806,0.530949297,-1.3537195249\C,0.360291672,0.576665889,
1.017810872\C,1.3139017322,1.8131681913,-1.2878226808\C,0.9084895127,1
.8567659967,1.0891717402\C,1.3883414767,2.4805469246,-0.065218909\H,1.
8152739317,3.4785412195,-0.0108895822\H,1.6815857155,2.2897551726,-2.1
930681927\H,0.9617726497,2.3686192684,2.0468281258\H,0.7079245895,0.01
74437154,-2.3113181491\H,-0.0160454344,0.0966429894,1.9182413553\H,0.3
561627742,-2.2089958921,0.2604701909\H,-0.293093633,-1.8463609788,-1.3
208715305\C,-2.278490714,-2.9457025271,0.6430854829\H,-2.3498318617,-0
.7594576612,0.2034732787\H,-1.5541202439,-3.5882560249,1.162736345\H,-

2.5987567225,-3.5064961802,-0.2546109902\H,-3.1631256555,-2.8444753128
,1.2821616051\\Version=IA64L-G03RevC.02\State=2-A\HF=-349.5277595\S2=0
.754013\S2-1=0.\S2A=0.750012\RMSD=4.353e-09\RMSF=5.776e-06\Dipole=-0.0
752288,-0.1618551,-0.0406573\PG=C01 [X(C9H11)]\\@

r.CHCH3-CH_CH2_2

1\1\GINC-AC9\FOpt\UB3LYP\Gen\C5H9(2)\CYL509\15-May-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\CHCH3-CH_C
H2_2.freq\\0,2\C,-1.5219976092,0.4093661216,-0.6135983159\C,-1.4250480
054,0.5469352947,0.8749202565\C,-0.1404947033,0.4756398766,0.058209863
1\H,-1.8264200243,-0.5497930264,-1.0237307332\H,-1.8398019444,1.268531
3475,-1.1992052616\H,-1.668789827,-0.3175687903,1.4874985941\H,-1.6845
775948,1.4998159871,1.3288618908\H,0.3785829203,1.4240363115,-0.075206
9757\C,0.7314379058,-0.6984469382,0.1238377381\H,0.2692741117,-1.66182
12329,0.3347795142\C,2.1489851117,-0.6758116273,-0.3459907798\H,2.6166
486844,0.3019460953,-0.1707255707\H,2.241419334,-0.8765582265,-1.42928
09966\H,2.756368142,-1.43468483,0.1627369665\\Version=IA64L-G03RevC.02
\State=2-A\HF=-195.8636954\S2=0.754723\S2-1=0.\S2A=0.750017\RMSD=3.429
e-09\RMSF=9.727e-06\Dipole=-0.0409701,0.0623245,-0.0643959\PG=C01 [X(C
5H9)]\\@

r.CHCH3-CH2CH=CH2

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C5H9(2)\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH2
CH=CH2.freq\\0,2\C,0.2866543292,0.2672371038,-0.3752757334\C,0.2764690
321,0.1220425399,1.118029307\H,1.3280369395,0.2058951368,-0.7324882786
\H,-0.0656935468,1.2726305904,-0.674643619\C,-0.5493622696,-0.77121980
51,-1.0815422784\C,1.366251994,0.6844415706,1.9687576292\H,-0.65918814
68,-0.1706597343,1.5900693068\C,-1.5903731648,-0.5101067333,-1.8724099
728\H,-0.2631601634,-1.8079467817,-0.8994377684\H,-2.1594892863,-1.302
3803505,-2.3516117716\H,-1.9129456696,0.5097659389,-2.074209793\H,2.35
78656183,0.4913927282,1.5362755687\H,1.3495047307,0.265001671,2.981223
7176\H,1.287229999,1.7819327457,2.0794689276\\Version=IA64L-G03RevC.02
\State=2-A\HF=-195.8684135\S2=0.75401\S2-1=0.\S2A=0.750011\RMSD=7.871e
-09\RMSF=5.428e-06\Dipole=0.1049887,0.0968865,0.0923183\PG=C01 [X(C5H9
)\\@

r.CHCH3-CH2CH3

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C4H9(2)\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH2
CH3.freq\\0,2\C,0.5555574203,-0.2673402007,-0.6737033302\H,1.629806190
6,-0.4450036786,-0.6476241905\C,-0.3336391712,-1.3956585156,-1.0823078
071\C,0.029625773,0.9479675683,0.0239685956\H,0.6929090055,1.803678869
8,-0.1656454594\C,-0.1143780483,0.774314629,1.5551846956\H,-0.95341405
79,1.2164013216,-0.3900087327\H,0.8522256505,0.5408504761,2.0161030401
\H,-0.8053378312,-0.0413304395,1.7966872712\H,-0.49830542,1.6909704997
,2.019346831\H,0.1312663362,-2.0219705298,-1.8532687856\H,-1.292768999
1,-1.0303379292,-1.4742553932\H,-0.5793767166,-2.068959476,-0.24018750
48\\Version=IA64L-G03RevC.02\State=2-A\HF=-157.7910493\S2=0.753956\S2-
1=0.\S2A=0.750011\RMSD=3.582e-09\RMSF=6.221e-06\Dipole=-0.030311,-0.03
55287,0.0619377\PG=C01 [X(C4H9)]\\@

r.CHCH3-CH_CH3_2

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C5H11(2)\CYL509\11-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CH
_CH3_2.freq\\0,2\C,-0.2491410721,1.6246052114,0.0357645259\H,0.1649475
114,1.8856932821,1.0174406491\H,-1.341776421,1.64174856,0.1164905943\H
,0.0495114182,2.4053773728,-0.6753747197\C,0.261440905,0.235270419,-0.
4223025992\C,1.7919024338,0.2471810189,-0.5725422135\H,-0.1791081014,0

.0440926386,-1.4142319275\C,-0.1927577505,-0.854515704,0.5047575615\H,
0.4133585575,-1.0487883729,1.3896862285\C,-1.5755519532,-1.4165110905,
0.4603383327\H,2.1611318907,-0.7140371143,-0.9468532879\H,2.2756679319
,0.4375167398,0.3943451315\H,2.1166692593,1.0316726152,-1.2663534763\H
, -1.6299836752,-2.3994812349,0.9435964112\H,-1.9337475192,-1.526005346
7,-0.5724044836\H,-2.3120262304,-0.7739682681,0.9775652355\Version=IA
64L-G03RevC.02\State=2-A\HF=-197.1053575\S2=0.753924\S2-1=0.\S2A=0.750
011\RMSD=3.781e-09\RMSF=2.354e-06\Dipole=-0.076072,0.037325,0.0095666\
PG=C01 [X(C5H11)]\@

r.CHCH3-C_CH3_3

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C6H13(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C_
CH3_3.freq\0,2\C,-0.3121428909,-0.1464928126,1.642561641\C,-0.0262796
808,0.3642588476,0.2037809595\C,-0.6695015613,1.7568235317,0.034220061
5\C,-0.6394847478,-0.588430164,-0.7965432474\H,0.1139191176,0.53577555
97,2.3901600876\H,0.1255110482,-1.1383344884,1.8053380142\H,-1.3902535
527,-0.2191452909,1.8274080104\C,1.5002143903,0.4850562919,0.011622386
6\C,0.0040723168,-1.864141563,-1.2357325684\H,-1.7029792481,-0.4628648
585,-0.9962700935\H,1.9204557051,1.2045208726,0.7246770299\H,1.7454478
02,0.8306385985,-0.9996872961\H,2.0069948888,-0.4731000777,0.172962307
3\H,-0.2762884236,2.4648667669,0.7741209885\H,-1.7575748928,1.70631152
22,0.164808853\H,-0.4706185108,2.1629707283,-0.9643666552\H,1.0007882,
-1.7030556689,-1.6700110084\H,-0.605252438,-2.3767796123,-1.9874139515
\H,0.1485833464,-2.5742488408,-0.4011816833\Version=IA64L-G03RevC.02\
State=2-A\HF=-236.4174759\S2=0.753966\S2-1=0.\S2A=0.750011\RMSD=6.624e
-09\RMSF=1.248e-06\Dipole=0.0138315,-0.0673235,0.0411514\PG=C01 [X(C6H
13)]\@

r.CHCH3-CCH

1\1\GINC-AC12\FOpt\UB3LYP\Gen\C4H5(2)\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CCH
.freq\0,2\C,0.754806387,0.0012705646,0.0177818613\C,0.7977621923,0.00
22896274,1.5176688499\H,1.702254515,0.0022269535,-0.5187781118\C,-0.40
75326596,-0.000220238,-0.7153186292\C,-1.4473138902,-0.004013538,-1.36
8582327\H,-2.3508708295,-0.0058143329,-1.9337819083\H,-0.2076772448,0.
001528222,1.9468468545\H,1.335857662,-0.8777627141,1.8987310334\H,1.33
41037206,0.8838633754,1.8976836014\Version=IA64L-G03RevC.02\State=2-A
\HF=-155.3210186\S2=0.771277\S2-1=0.\S2A=0.750199\RMSD=3.870e-09\RMSF=
3.813e-05\Dipole=0.088612,0.0004148,0.1579355\PG=C01 [X(C4H5)]\@

r.CHCH3-CH=C_CH3_2

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C6H11(2)\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CH
=C_CH3_2.freq\0,2\H,2.9618917405,-0.2947215532,-0.6924514761\C,2.2968
968338,-0.5552098296,0.1456999605\C,0.9922924703,0.1871255667,0.063865
9435\C,1.0939894891,1.6866556354,0.073164689\C,-0.2148961458,-0.509937
8715,-0.0146304126\C,-1.5025011435,-0.0015049288,-0.0963484938\H,-1.65
91671104,1.0754598532,-0.1049410458\C,-2.7311899866,-0.8537704428,-0.1
76048444\H,-0.132046905,-1.5991835488,-0.0110578769\H,2.1539736663,-1.
6407183539,0.134868335\H,2.8503096005,-0.2974825105,1.0621418281\H,1.7
054754861,2.0447173789,-0.7687945821\H,1.5952498445,2.0411581218,0.986
4406438\H,0.1237492576,2.1854465742,0.0132734688\H,-2.4838952541,-1.92
11672325,-0.1618443546\H,-3.3055928108,-0.6555063197,-1.093544594\H,-3
.4174966197,-0.6581511859,0.6616901988\Version=IA64L-G03RevC.02\State
=2-A\HF=-235.2183589\S2=0.777519\S2-1=0.\S2A=0.750169\RMSD=5.593e-09\R
MSF=1.395e-05\Dipole=0.0545812,0.0604591,0.0035682\PG=C01 [X(C6H11)]\@
@

r.CHCH3-CH=CH2

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1\1\GINC-AC8\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\11-Apr-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CH=C
H2.freq\0,2\H,-1.0778165593,-1.9173803931,1.1218665213\C,-0.021826403
4,-1.6781385312,1.0272810443\H,0.684516436,-2.364132028,1.4825249304\C
,0.4006659054,-0.5440544023,0.3530585612\C,-0.4315288989,0.3852619587,
-0.2575265135\H,1.4755696475,-0.3621840889,0.2946591709\C,0.0425708102
,1.6051455319,-0.9813835083\H,-1.508475937,0.2218488146,-0.2105528576\
H,1.1355196425,1.680412312,-0.9737421288\H,-0.3610982313,2.5249213616,
-0.5324306575\H,-0.2875034778,1.607226679,-2.0309024806\Version=IA64L
-G03RevC.02\State=2-A\HF=-156.5806348\S2=0.780027\S2-1=0.\S2A=0.750184
\RMSD=5.353e-09\RMSF=1.496e-05\Dipole=-0.0046281,0.1559514,-0.0956951\
PG=C01 [X(C4H7)]\@
```

r.CHCH3-CH=CHCH3

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1\1\GINC-AC30\FOpt\UB3LYP\Gen\C5H9(2)\CYL509\11-Apr-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CH=
CHCH3.freq\0,2\C,0.0787622394,0.3312600129,2.5439201125\H,1.141240877
7,0.5870675881,2.4644918689\H,-0.0102089091,-0.5192488023,3.2364394548
\H,-0.4337051816,1.1752583344,3.0295867445\C,-0.5141601445,0.019751832
4,1.2060764251\C,0.1866380951,0.0476033993,0.0082653729\H,-1.571078866
2,-0.2467026156,1.1813135544\H,1.2447808378,0.317075745,0.055116554\C,
-0.3402812454,-0.2372057699,-1.2439314943\C,0.4381833921,-0.1997357209
,-2.5210226819\H,-1.3940607752,-0.5083529873,-1.3125419987\H,1.4827184
586,0.0827412687,-2.3485066216\H,0.0108169647,0.5181756909,-3.23712235
13\H,0.4346425733,-1.1760567449,-3.028623612\Version=IA64L-G03RevC.02
\State=2-A\HF=-195.9004704\S2=0.778752\S2-1=0.\S2A=0.750178\RMSD=5.536
e-09\RMSF=5.964e-06\Dipole=0.0126781,0.003099,0.00058\PG=C01 [X(C5H9)]
\@
```

r.CHCH3-CHO

```
1\1\GINC-AC8\FOpt\UB3LYP\Gen\C3H5O1(2)\CYL509\11-Apr-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CH
O.freq\0,2\O,1.1011309936,0.,-1.1109639546\C,1.0036181284,0.,0.124941
6933\H,1.9148279191,0.,0.7549005934\C,-0.2460256839,0.,0.821450026\C,-
1.5552793069,0.,0.1180773428\H,-0.2240028968,0.,1.9101615113\H,-1.4071
890197,0.,-0.9640446269\H,-2.1532813887,0.8788033622,0.3999398932\H,-2
.1532813887,-0.8788033622,0.3999398932\Version=IA64L-G03RevC.02\State
=2-A\HF=-192.4968911\S2=0.76597\S2-1=0.\S2A=0.750074\RMSD=1.902e-09\R
MSF=7.072e-05\Dipole=-0.5985097,0.,1.0093389\PG=CS [SG(C3H3O1),X(H2)]\
\@
```

r.CHCH3-CN

```
1\1\GINC-SC30\FOpt\UB3LYP\6-31G(d)\C3H4N1(2)\MLC501\29-Oct-2004\0\B
3LYP/6-31G* OPT FREQ MAXDISK=134217728\ANuni_rad-cl-6dub3\0,2\C,0.75
43429042,-0.2983335115,0.3122792987\N,1.8737632074,-0.1694924694,0.651
2865892\C,-0.5657744262,-0.4432506421,-0.0889032139\C,-1.3947270475,0.
6895274827,-0.6074519143\H,-1.0042180897,-1.435250357,-0.0169189576\H,
-2.2901219682,0.8309596994,0.0139675375\H,-0.8347741583,1.6274002584,-
0.6264006175\H,-1.7502768181,0.4756777102,-1.6251991097\Version=DEC-A
XP-OSF/1-G03RevB.03\State=2-A\HF=-171.416282\S2=0.766962\S2-1=0.\S2A=0
.750126\RMSD=9.889e-09\RMSF=1.080e-05\Dipole=-1.4561102,-0.0162055,-0.
4740771\PG=C01 [X(C3H4N1)]\@
```

r.CHCH3-COCH3

```
1\1\GINC-AC4\FOpt\UB3LYP\Gen\C4H7O1(2)\CYL509\11-Apr-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CO
CH3.freq\0,2\C,-0.3313160136,0.0626280645,-1.9106954823\C,-0.34313829
31,-0.0645291373,-0.3929383381\C,0.8832622219,0.2152034274,0.318082932
```

\O,-1.3735227252,-0.3948079113,0.2120283397\H,-1.3098587421,-0.2182266735,-2.3048963642\H,0.4369363796,-0.5819278821,-2.3552877668\H,-0.1045695582,1.0924447118,-2.2142387634\H,1.7642131852,0.5020873692,-0.2542931474\C,0.9819270129,0.1270798951,1.7979488183\H,1.75123814,-0.5983078137,2.1012776596\H,0.0214331594,-0.1711316953,2.2239870184\H,1.284379669,1.0912317761,2.232837067\\Version=IA64L-G03RevC.02\State=2-A\HF=-231.8198862\S2=0.763581\S2-1=0.\S2A=0.750066\RMSD=7.181e-09\RMSF=2.009e-05\Dipole=1.0643299,0.3182341,-0.2705753\PG=C01 [X(C4H7O1)]\\@

r.CHCH3-CON_CH2CH3_2

1\1\GINC-AC14\FOpt\UB3LYP\Gen\C7H14N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CON_CH2CH3_2.freq\\0,2\H,0.9316553889,-2.6531404872,2.3677618182\C,0.6268264318,-2.2718383871,1.3859626899\C,0.876409748,-0.7617782372,1.2919068001\N,0.5450657287,-0.1897739025,-0.0117517811\C,1.6090836608,-0.1344408113,-1.0176695287\C,2.4170714222,1.1663569707,-0.9687459163\C,-0.6798905951,0.3588884533,-0.3492045295\O,-0.8409036264,0.9196476945,-1.4449604606\C,-1.7878937716,0.2415387569,0.5988411666\C,-3.1046728065,0.8607455839,0.2948156187\H,-1.6842284142,-0.3309993548,1.5146944157\H,1.935412246,-0.550433601,1.4821821052\H,0.3246897684,-0.2329935521,2.0746859337\H,1.1429183671,-0.240161047,-1.999443049\H,2.2636726829,-0.999718348,-0.858628585\H,-0.4335059563,-2.5045405237,1.2400534586\H,1.1956093175,-2.8111891863,0.6205549285\H,1.7630866581,2.0180402899,-1.1754728615\H,3.2132664299,1.1500027131,-1.7224485861\H,2.8839132616,1.3136905953,0.0125745653\H,-3.0608957288,1.3876329024,-0.6604548216\H,-3.4051748185,1.5665097272,1.0839703941\H,-3.9002548309,0.1017016594,0.2464786312\\Version=IA64L-G03RevC.02\State=2-A\HF=-405.1202825\S2=0.755884\S2-1=0.\S2A=0.750024\RMSD=6.239e-09\RMSF=5.606e-06\Dipole=0.3731055,-0.6445936,1.1321325\PG=C01 [X(C7H14N1O1)]\\@

r.CHCH3-CON_CH3_2

1\1\GINC-AC25\FOpt\UB3LYP\Gen\C5H10N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CON_CH3_2.freq\\0,2\C,1.455649718,-0.1259050189,-0.2547411723\C,0.0959585216,0.3953786061,-0.1188803223\N,-0.9154025199,-0.4870738872,0.2304168788\O,-0.1365281923,1.5991466217,-0.3051631481\H,1.6974963152,-1.1438604411,0.0318950217\C,2.5573628445,0.7611611816,-0.7118210375\C,-0.7165310804,-1.902343819,0.4950169754\C,-2.2290216475,0.0522612043,0.5458704238\H,-1.6695653394,-2.4214487415,0.352657057\H,-0.0015306904,-2.3410094698,-0.2046476822\H,-0.3750895869,-2.1019919083,1.5225115884\H,-3.0052802199,-0.4739880072,-0.0241972397\H,-2.4562220998,-0.0547491941,1.6167751842\H,-2.2357172682,1.1088660934,0.2826712671\H,3.3188006039,0.8864713485,0.0735359309\H,2.1650910836,1.7445950103,-0.9778663708\H,3.0815502427,0.3301466216,-1.5776169265\\Version=IA64L-G03RevC.02\State=2-A\HF=-326.4877792\S2=0.756084\S2-1=0.\S2A=0.750025\RMSD=9.270e-09\RMSF=2.959e-06\Dipole=0.0915462,-1.3288043,0.2938787\PG=C01 [X(C5H10N1O1)]\\@

r.CHCH3-CONH2

1\1\GINC-AC15\FOpt\UB3LYP\Gen\C3H6N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CHCH3-CONH2.freq\\0,2\C,0.7751835723,-0.5119521949,-0.2560404886\C,-0.547214192,0.0037653109,0.0877108252\N,-1.5876307596,-0.9071132211,0.0125808441\O,-0.7460845613,1.1829128558,0.390283775\H,0.8826194985,-1.5563085831,-0.5440991466\C,1.9703193152,0.368430001,-0.2367714734\H,-1.3978235942,-1.8986271069,0.0517799434\H,-2.4627383984,-0.6030792029,0.4178381846\H,2.736713336,-0.0092208715,0.456688299\H,1.6843182594,1.3788371093,0.0645266974\H,2.4492705328,0.4134296542,-1.2264632666\\Version=IA64L-G03RevC.02\State=2-A\HF=-247.8713928\S2=0.756503\S2-1=0.\S2A=0.7500

28\RMSD=6.652e-09\RMSF=4.064e-06\Dipole=0.198599,-1.3577038,-0.0341869
\PG=C01 [X(C3H6N1O1)]\@

r.CHCH3-CONHCH3

1\1\GINC-AC25\FOpt\UB3LYP\Gen\C4H8N1O1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-CONHCH3.a2.freq\0,2\H,-1.7834289348,1.0801815145,-2.4255169846\C,-1.8562859097,0.9570148099,-1.3374166815\N,-0.5495188524,0.9778510883,-0.7131674801\C,-0.0558469545,-0.0861178494,0.0119090492\C,1.2804489795,0.1109638605,0.5711044481\O,-0.6984835061,-1.129202537,0.1752126713\H,1.802094535,1.0506650685,0.3952833178\C,1.9391304695,-0.949409738,1.3750398281\H,0.0218566427,1.8042804286,-0.8108226308\H,-2.3024511806,-0.0140788804,-1.1181902897\H,-2.5052084498,1.7470916691,-0.9383141657\H,2.8929095261,-1.2618999078,0.9236984011\H,1.2820683941,-1.8187208098,1.4528096815\H,2.181979975,-0.5935629025,2.3877037973\Version=IA64L-G03RevC.02\State=2-A\HF=-287.1824199\S2=0.755484\S2-1=0.\S2A=0.750022\RMSD=6.289e-09\RMSF=6.086e-06\Dipole=0.5786193,1.2261726,-0.2769755\PG=C01 [X(C4H8N1O1)]\@

r.CHCH3-COOC_CH3_3

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C7H13O2(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-COOC_CH3_3.freq\0,2\H,-1.1788776446,-1.3436342625,-2.6664054472\C,-1.1489956661,-1.0187004997,-1.6201115946\C,0.3069907229,-0.8005992146,-1.191515847\C,0.9796070524,0.3305989429,-1.9783698818\O,0.3733203404,-0.5223646686,0.2502346281\C,-0.2267938597,0.5687205634,0.7933402262\O,-0.8648246961,1.410475976,0.1695912966\C,-0.013077125,0.6117618915,2.2306557778\C,1.1085801463,-2.0990612534,-1.3191939097\C,-0.5677171434,1.7084253794,3.0635138347\H,0.5680125778,-0.1861023579,2.6830888543\H,1.1382216001,-2.4234934541,-2.3647895558\H,0.6523012025,-2.895032754,-0.7216568798\H,2.1366537634,-1.9541166684,-0.9715328944\H,-1.731135829,-0.1012753149,-1.5209270717\H,-1.6120121675,-1.8008759883,-1.0083494494\H,1.0333519955,0.0586186966,-3.0387208935\H,2.0014427173,0.4897043209,-1.6164691253\H,0.4216173529,1.2633366886,-1.8832721968\H,0.2312384068,2.2471405433,3.5948604285\H,-1.2393805874,1.316060199,3.8418001024\H,-1.1209633066,2.4179050354,2.4438550965\Version=IA64L-G03RevC.02\State=2-A\HF=-424.9988277\S2=0.756426\S2-1=0.\S2A=0.750027\RMSD=9.373e-09\RMSF=3.214e-05\Dipole=0.3449374,-0.4687042,0.2877367\PG=C01 [X(C7H13O2)]\@

r.CHCH3-COOCH2CH3

1\1\GINC-AC18\FOpt\UB3LYP\Gen\C5H9O2(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-COOCH2CH3.freq\0,2\C,-1.775422006,0.3171303384,0.\C,-0.4722887923,-0.3195890374,0.\O,-0.2797746375,-1.529589923,0.\O,0.5351091421,0.5961109767,0.\C,1.8702295057,0.0524226093,0.\C,2.8397953639,1.2198412744,0.\H,-1.8111662428,1.4025172323,0.\C,-3.0278565879,-0.4801086602,0.\H,1.9956120165,-0.5848090313,0.8822746186\H,1.9956120165,-0.5848090313,-0.8822746186\H,2.6986017129,1.8452573308,-0.8874427575\H,3.8705619534,0.8487271358,0.\H,2.6986017129,1.8452573308,0.8874427575\H,-2.8025621353,-1.5490702662,0.\H,-3.6473409856,-0.2467091388,-0.8788687451\H,-3.6473409856,-0.2467091388,0.8788687451\Version=IA64L-G03RevC.02\State=2-A\HF=-346.3673835\S2=0.756705\S2-1=0.\S2A=0.750029\RMSD=5.721e-09\RMSF=6.296e-05\Dipole=-0.0856661,0.688165,0.\PG=CS [SG(C5H3O2),X(H6)]\@

r.CHCH3-COOCH3

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-COOCH3.freq\0,2\C,0.0843438887,0.,-1.3810154728\C,0.0617466883,0.,0.06

```
85830642\O,1.0504509824,0.,0.7912911319\O,-1.2122654773,0.,0.551834798
8\C,-1.3175357097,0.,1.9804841023\H,-2.3866109245,0.,2.1971097049\H,-0
.8671300035,0.,-1.9043848432\C,1.3625597819,0.,-2.1360794843\H,-0.8409
601417,-0.8886408644,2.4049303548\H,-0.8409601417,0.8886408644,2.40493
03548\H,2.2136616153,0.,-1.4512203479\H,1.4349138298,0.8788459963,-2.7
941029625\H,1.4349138298,-0.8788459963,-2.7941029625\Version=IA64L-G0
3RevC.02\State=2-A\HF=-307.0484417\S2=0.756694\S2-1=0.\S2A=0.750029\R
MSD=6.778e-09\RMSF=6.993e-05\Dipole=-0.4985987,0.,-0.4129517\PG=CS [SG
(C4H3O2),X(H4)]\@
```

r.CHCH3-COOH

```
1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H5O2(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C
OOH.freq\0,2\C,0.0374549591,-0.4166977759,-0.8643633535\C,-0.19747511
88,-0.0408030846,0.5144384077\O,0.2318410765,0.9693372753,1.0576681418
\O,-0.9695527212,-0.9486178761,1.179787446\C,0.8539592359,0.4306219623
,-1.7687719711\H,-0.4030925478,-1.3428676385,-1.2210480699\H,-1.062398
479,-0.6005927148,2.0853458351\H,1.7166018912,-0.1273726496,-2.1621955
031\H,1.2154168315,1.3175239285,-1.2433192942\H,0.2715310041,0.7488272
701,-2.6462461694\Version=IA64L-G03RevC.02\State=2-A\HF=-267.7416356\
S2=0.75701\S2-1=0.\S2A=0.75003\RMSD=3.982e-09\RMSF=1.209e-04\Dipole=-0
.1088419,-0.4357159,-0.4614308\PG=C01 [X(C3H5O2)]\@
```

r.CHCH3-COPh

```
1\1\GINC-AC11\FOpt\UB3LYP\Gen\C9H9O1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHCH3-C
OPh.freq\0,2\C,-2.6823449689,-0.0475371091,-0.0106570813\C,-2.6978631
538,-0.2084056505,1.3776567387\C,-1.4947304238,-0.2456124814,2.0841729
312\C,-0.2807727104,-0.1322510118,1.406615504\C,-0.2540587573,0.024337
9378,0.0121461361\C,-1.4711143044,0.0727279016,-0.6856207195\C,1.01190
15261,0.1641246101,-0.7863259767\O,0.9561447029,0.5312560444,-1.975393
1593\C,2.2870863566,-0.1532609993,-0.1884847518\H,2.3286555538,-0.5480
053666,0.8224473308\C,3.5608240983,-0.0033775366,-0.93807634\H,-1.4387
415456,0.2070226346,-1.7616805091\H,0.641538858,-0.1463078019,1.979183
1039\H,-1.4999891964,-0.3600594912,3.1648174155\H,-3.6163841851,-0.014
3440491,-0.5652135551\H,-3.642925888,-0.3004839301,1.9063465177\H,4.25
88396272,0.6535171259,-0.3985439129\H,3.3733391286,0.4060273717,-1.932
6054434\H,4.0729440506,-0.9718888131,-1.0401643167\Version=IA64L-G03R
evC.02\State=2-A\HF=-423.5593374\S2=0.764324\S2-1=0.\S2A=0.750069\RMSD
=8.339e-09\RMSF=3.007e-06\Dipole=0.1804628,-0.3547644,1.0270648\PG=C01
[X(C9H9O1)]\@
```

r.C_CH3_2-H

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C3H7(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-H
.freq\0,2\C,-0.0069292949,0.0061238658,0.5342025695\H,-0.1507124013,0
.2664787859,1.5805655268\C,1.1626771975,0.5872164135,-0.1887225809\C,-
1.1427362801,-0.6199916595,-0.2048846605\H,2.0069966244,0.7766900704,0
.4839135631\H,0.9188549359,1.5513110255,-0.6729569834\H,1.5106979438,-
0.0772135321,-0.9924187046\H,-0.7860922738,-1.2754711412,-1.0120643615
\H,-1.7943113328,0.1325878496,-0.687035295\H,-1.7835032312,-1.21447477
69,0.4564242862\Version=IA64L-G03RevC.02\State=2-A\HF=-118.4781563\S2
=0.754001\S2-1=0.\S2A=0.750011\RMSD=3.418e-09\RMSF=9.131e-06\Dipole=-0
.0307482,0.0591747,-0.0446532\PG=C01 [X(C3H7)]\@
```

r.C_CH3_2-BH2

```
1\1\GINC-AC27\FOpt\UB3LYP\Gen\C3H8B1(2)\CYL509\19-May-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-BH2.a3.freq\0,2\H,-1.4197923486,-0.0048230969,-2.0410707974\B,-1.426
```

5589994,-0.0027233268,-0.8423084678\C,-0.1106795293,-0.0002100938,-0.0
653475164\H,-2.4729665922,0.0003624231,-0.2573890108\C,1.2260872878,-0
.0027908743,-0.7469594329\C,-0.0618449068,0.0046253547,1.434367851\H,1
.13999917,-0.0055359683,-1.836584704\H,1.8225678406,0.8742876652,-0.44
87249745\H,1.8213064179,-0.8792242744,-0.4443035245\H,0.4922340161,-0.
8686741233,1.8141612446\H,-1.0576315445,0.0027220915,1.8851018054\H,0.
4857009272,0.8847555976,1.8079868901\\Version=IA64L-G03RevC.02\State=2
-A\HF=-143.934591\S2=0.752527\S2-1=0.\S2A=0.750005\RMSD=4.084e-09\RMSF
=4.328e-05\Dipole=0.6853414,0.0007948,0.4046452\PG=C01 [X(C3H8B1)]\\@

r.C_CH3_2-CH3

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C4H9(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CH
3.freq\0,2\H,0.2007477047,-0.863139384,-1.9968647676\C,0.2634299248,-
1.1297574188,-0.9339591821\H,1.3068119858,-1.453420627,-0.7552440096\H
, -0.3670997203,-2.0121821124,-0.7656775476\C,-0.133637046,0.0127758348
, -0.0508665654\C,0.3082545913,1.3965015974,-0.4155170687\C,-0.53093002
43,-0.2706488122,1.3650506161\H,1.3585753,1.5903123038,-0.124602748\H,
-0.2975051592,2.1622673845,0.0857774746\H,0.2504768248,1.5699704292,-1
.4977469674\H,0.3461131403,-0.423650002,2.0228649621\H,-1.1377960942,-
1.1819118489,1.4425555949\H,-1.1030286564,0.5585266496,1.8006912097\\V
ersion=IA64L-G03RevC.02\State=2-A\HF=-157.7983171\S2=0.75402\S2-1=0.\S
2A=0.750012\RMSD=5.521e-09\RMSF=9.546e-06\Dipole=0.0705059,-0.0067671,
0.0268622\PG=C01 [X(C4H9)]\\@

r.C_CH3_2-NH2

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H8N1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-NH2.freq\0,2\H,-1.7103069848,0.2864284252,-1.1325896944\N,-0.7097962
137,0.465829674,-1.1147865753\C,-0.0418114041,-0.1957449218,-0.0605591
29\H,-0.3145275864,0.2658892614,-2.0298378567\C,-0.723318425,-0.134276
1644,1.2719771913\C,1.4543575281,-0.1659888866,-0.1279396471\H,-0.2559
244852,-0.826713501,1.9811237528\H,-1.7862466873,-0.4050994528,1.19652
41363\H,-0.6849050959,0.8737945808,1.726713533\H,1.8727910088,0.836700
9711,0.0818416933\H,1.8211475488,-0.458203152,-1.1223930308\H,1.891179
584,-0.8575450144,0.6012530032\\Version=IA64L-G03RevC.02\State=2-A\HF=
-173.8363629\S2=0.753194\S2-1=0.\S2A=0.750008\RMSD=7.879e-09\RMSF=1.02
8e-05\Dipole=-0.1959921,-0.2247167,-0.2996602\PG=C01 [X(C3H8N1)]\\@

r.C_CH3_2-OH

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H7O1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-OH.freq\0,2\C,0.0551994718,0.2150689131,-0.0226852277\O,-0.202583415
9,0.3066639885,1.3351619228\C,1.2728479544,-0.5525455673,-0.4339175821
\C,-1.1995677229,0.1777223811,-0.8300843263\H,0.641894064,0.2785343136
,1.8115731926\H,-0.9833249816,0.3457450142,-1.8906886804\H,-1.89895938
91,0.9503756276,-0.4913236188\H,-1.7245266202,-0.7921720439,-0.7496379
133\H,2.1667341833,-0.2189755457,0.1138157864\H,1.475873085,-0.4185054
208,-1.5017270173\H,1.172098766,-1.6397882139,-0.2531843154\\Version=I
A64L-G03RevC.02\State=2-A\HF=-193.697974\S2=0.753182\S2-1=0.\S2A=0.750
008\RMSD=9.139e-09\RMSF=1.588e-05\Dipole=0.5366151,-0.1738331,-0.05558
76\PG=C01 [X(C3H7O1)]\\@

r.C_CH3_2-F

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H6F1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-F.freq\0,2\C,-0.5301976837,-0.1244029458,-1.3537544834\C,-0.18060332
17,-0.0966825995,0.0932998821\C,0.9334076166,-0.8741844763,0.702696013
6\F,-0.3511367897,1.1334384225,0.6631683487\H,0.1990186475,0.433290248

4,-1.9687740012\H,-1.512428189,0.3307957591,-1.5246637296\H,-0.5547081
223,-1.1543950534,-1.7241309564\H,1.9225358591,-0.4496393696,0.4528662
204\H,0.9195361237,-1.9095951945,0.3471939926\H,0.8506371212,-0.879782
0625,1.7955448625\\Version=IA64L-G03RevC.02\State=2-A\HF=-217.7163798\
S2=0.753217\S2-1=0.\S2A=0.750008\RMSD=4.133e-09\RMSF=2.085e-05\Dipole=
0.211618,-0.4484107,-0.3141125\PG=C01 [X(C3H6F1)]\\@

r.C_CH3_2-SiH3

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H9Si1(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_
2-SiH3.freq\0,2\H,-1.3875247509,0.0000005584,-1.9947891269\Si,-1.3404
090537,0.0000005137,-0.4983199658\C,0.3873254869,-0.000000186,0.181853
038\H,-2.0749548893,1.2162980954,-0.0474070725\H,-2.0749559525,-1.2162
964792,-0.0474071868\C,1.1467098437,-1.2750259652,0.4206751148\C,1.146
7103586,1.2750250981,0.4206761639\H,1.991638634,1.3739305913,-0.281750
531\H,1.5898821138,1.2897111851,1.4292533241\H,0.5278243319,2.17226859
21,0.3159277128\H,1.9916379734,-1.3739313014,-0.281751779\H,0.52782342
3,-2.1722691212,0.3159260811\H,1.5898817329,-1.2897129941,1.4292521992
\\Version=IA64L-G03RevC.02\State=2-A\HF=-409.1774311\S2=0.753997\S2-1=
0.\S2A=0.750012\RMSD=8.317e-09\RMSF=2.781e-05\Dipole=0.4493821,-0.0000
002,0.137664\PG=C01 [X(C3H9Si1)]\\@

r.C_CH3_2-PH2

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H8P1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-PH2.freq\0,2\H,-1.9590269019,-0.959276461,0.194169438\P,-1.313437845
,0.2959501974,0.3981740835\H,-1.2142803402,0.1663166019,1.8150217536\C
,0.3796395928,-0.1704265722,-0.0559945606\C,1.5316548878,0.5399847512,
0.594327897\C,0.6238158875,-0.835505241,-1.3798935194\H,1.5336021398,-
1.451033739,-1.3405265655\H,0.778899042,-0.1046346106,-2.1931900403\H,
-0.2057498147,-1.483938009,-1.6846955205\H,2.4262248688,-0.098632574,0
.5983517414\H,1.3193857584,0.824789424,1.6313459134\H,1.8118507135,1.4
628387795,0.0562731254\\Version=IA64L-G03RevC.02\State=2-A\HF=-460.427
1495\S2=0.754732\S2-1=0.\S2A=0.750018\RMSD=4.261e-09\RMSF=5.025e-06\Di
pole=0.3437218,-0.2334412,0.0039664\PG=C01 [X(C3H8P1)]\\@

r.C_CH3_2-SH

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C3H7S1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-SH.freq\0,2\H,-0.8855065907,0.7287362723,-1.7103640028\S,-0.06869306
82,1.1584923531,-0.7234199597\C,-0.1249439392,-0.2971740858,0.27930267
62\C,-0.3373269024,-1.6336934903,-0.3613850921\C,0.5956386581,-0.19358
86847,1.5888005584\H,1.6812103752,-0.3720531158,1.4912277615\H,0.21308
21851,-0.9448070113,2.2913998511\H,0.469582666,0.7933247934,2.04851948
16\H,0.5653461138,-2.0000173493,-0.8817015729\H,-1.1465989868,-1.61282
72262,-1.1024502429\H,-0.5982335709,-2.3814964478,0.3977792243\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-516.6733311\S2=0.754181\S2-1=0.\S2A=0
.750014\RMSD=5.760e-09\RMSF=7.609e-06\Dipole=-0.1031524,-0.5173884,-0.
0225666\PG=C01 [X(C3H7S1)]\\@

r.C_CH3_2-Cl

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C3H6Cl1(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-Cl.freq\0,2\Cl,-0.0576213085,0.1868421635,-1.3327798979\C,-0.109208,
-0.1867836999,0.3849213837\C,1.0186519707,-1.0154386727,0.9017186926\C
, -0.8704595686,0.7749220468,1.2343250185\H,1.9594811584,-0.4422842628,
0.9699946535\H,1.2120938817,-1.8789835931,0.2564542046\H,0.7828173189,
-1.3793072713,1.9087076106\H,-0.3296387837,1.7271352071,1.372566253\H,
-1.0350973792,0.344172372,2.2290062717\H,-1.8440003643,1.0167527238,0.

7947387029\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-578.0829001\\S2=0.753925\\S2-1=0.\\S2A=0.750012\\RMSD=6.556e-09\\RMSF=5.940e-06\\Dipole=0.091988,-0.0378438,0.7259761\\PG=C01 [X(C3H6C11)]\\@

r.C_CH3_2-Br

1\\1\\GINC-AC4\\FOpt\\UB3LYP\\Gen\\C3H6Br1(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-Br.freq\\0,2\\Br,-0.1112211217,0.5002945451,-0.8617626182\\C,0.1571396953,-0.6077676675,0.6850250421\\C,1.406305223,-0.3490037435,1.4585119692\\C,-1.0798881918,-1.1632245044,1.3068937528\\H,2.2807021566,-0.2668480208,0.8049610197\\H,1.5777465011,-1.169384682,2.166857624\\H,1.3481457763,0.5838965045,2.044971236\\H,-0.8110661289,-1.9514275723,2.0214884172\\H,-1.7561442233,-1.5893691475,0.5588646228\\H,-1.6479851832,-0.3972006675,1.8619641317\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-2691.7678948\\S2=0.754234\\S2-1=0.\\S2A=0.750014\\RMSD=9.212e-09\\RMSF=2.041e-05\\Dipole=0.0573272,-0.3059922,0.70219\\PG=C01 [X(C3H6Br1)]\\@

r.C_CH3_2-N_CH3_2

1\\1\\GINC-AC23\\FOpt\\UB3LYP\\Gen\\C5H12N1(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-N_CH3_2.freq\\0,2\\C,1.1445975808,0.4816632728,1.4082703403\\H,2.2154160888,0.7056095386,1.367264787\\H,1.0132673881,-0.3959692264,2.0441502452\\H,0.6342514692,1.3366556729,1.8883457804\\N,0.6625728378,0.21720896,0.0588178098\\C,-0.6490719977,-0.2879919525,-0.0818437667\\C,1.1022827759,1.2318270219,-0.8900848503\\C,-1.1370149584,-1.2487324945,0.9671527241\\C,-1.1837958998,-0.446988515,-1.4783264592\\H,2.1761315731,1.4004615894,-0.7601171395\\H,0.585267971,2.199728253,-0.7566206995\\H,0.9408904595,0.8964935407,-1.9164154391\\H,-0.5828481172,-1.1406023338,-2.0975780309\\H,-1.2397535431,0.4993737313,-2.03147803\\H,-2.199131427,-0.8536815503,-1.4406186304\\H,-0.5218766882,-2.1666508745,1.0355274378\\H,-2.157008774,-1.5669396555,0.7303560263\\H,-1.1646012694,-0.8136054015,1.9744510948\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-252.4490303\\S2=0.753319\\S2-1=0.\\S2A=0.750008\\RMSD=5.751e-09\\RMSF=7.283e-06\\Dipole=0.2060285,0.1913328,0.0584235\\PG=C01 [X(C5H12N1)]\\@

r.C_CH3_2-NHCH3

1\\1\\GINC-AC23\\FOpt\\UB3LYP\\Gen\\C4H10N1(2)\\CYL509\\19-May-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-NHCH3.a2.freq\\0,2\\C,0.7554590612,-0.9191269075,1.6110683328\\H,0.6939316401,-0.7953988779,2.6965384331\\H,1.7934685657,-0.7343074903,1.3173146662\\H,0.5138420866,-1.967373184,1.3648730389\\N,-0.127465787,0.0501512869,0.9766080513\\C,-0.2863300195,0.0565540287,-0.4225318306\\C,0.9462225054,-0.0962218955,-1.2633588111\\C,-1.3894722725,0.9415769142,-0.9225513746\\H,-1.0210277924,0.1109166359,1.4544835476\\H,-2.3145507378,0.8034701079,-0.3443256544\\H,-1.621900258,0.7197238707,-1.9702253908\\H,-1.1391873259,2.0182852531,-0.8672863844\\H,1.6321931802,0.769297469,-1.1798975604\\H,1.5297621823,-0.9881062444,-1.003630622\\H,0.6704533203,-0.184259388,-2.3198583324\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-213.1433423\\S2=0.753214\\S2-1=0.\\S2A=0.750008\\RMSD=3.981e-09\\RMSF=3.025e-05\\Dipole=-0.1023895,-0.1914352,0.2963191\\PG=C01 [X(C4H10N1)]\\@

r.C_CH3_2-NHCHO

1\\1\\GINC-AC29\\FOpt\\UB3LYP\\Gen\\C4H8N1O1(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-NHCHO.freq\\0,2\\H,0.8807807774,0.1095764133,-2.5298109728\\C,0.9565927654,0.1727436348,-1.4269009141\\O,1.98153764,0.5106098843,-0.8549632775\\N,-0.2390433311,-0.172846532,-0.8390650388\\C,-0.5878196635,-0.2757459098,0.5099702668\\H,-0.9528305931,-0.4667071134,-1.4959514979\\C,0.275781662,0.3291943836,1.5695368823\\C,-2.030811886,-0.5695874041,0.779746

178\H,-2.1492426771,-1.0389463233,1.7626005111\H,-2.4608320897,-1.2529
772888,0.0348032079\H,-2.6589336501,0.3401415187,0.7848942852\H,1.3364
682808,0.1709472284,1.3719438188\H,0.0149021571,-0.0982653775,2.544347
3996\H,0.128232725,1.4216493654,1.6462202615\\Version=IA64L-G03RevC.02
\State=2-A\HF=-287.1791462\S2=0.756785\S2-1=0.\S2A=0.750028\RMSD=4.670
e-09\RMSF=1.226e-05\Dipole=-1.4231539,-0.3915674,-0.2177672\PG=C01 [X(
C4H8N1O1)]\@

r.C_CH3_2-NHCOCH3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C5H10N1O1(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH
3_2-NHCOCH3.freq\0,2\H,-0.4154557735,2.6614216204,-1.9180862787\C,0.2
662590428,1.8047875903,-1.8992984894\C,0.2091496113,1.1602103176,-0.52
00599891\H,1.2764520483,2.1928839658,-2.0653081715\H,0.0098322872,1.13
22644663,-2.7247879165\N,-0.1586066026,-0.1725892187,-0.5258963594\O,0
.4765427394,1.7952100313,0.494051288\C,-0.3487465806,-1.0552799209,0.5
42647335\H,-0.4114357007,-0.5433930347,-1.4325929685\C,0.2316224013,-0
.7720620397,1.8911411\C,-0.6898867577,-2.4596385251,0.14933609\H,0.202
1120292,-3.0647235408,-0.0982646985\H,-1.3549102352,-2.4955174368,-0.7
246233439\H,-1.2003116292,-2.9746610469,0.9705729824\H,1.3177042491,-0
.9756162983,1.9223653898\H,-0.2377436882,-1.4249813526,2.6357926078\H,
0.1012744126,0.2706624053,2.1812003301\\Version=IA64L-G03RevC.02\State
=2-A\HF=-326.5014207\S2=0.755878\S2-1=0.\S2A=0.750023\RMSD=8.790e-09\R
MSF=6.890e-06\Dipole=-0.3058954,-0.9469616,-1.0176399\PG=C01 [X(C5H10N
1O1)]\@

r.C_CH3_2-NO2

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C3H6N1O2(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3
_2-NO2.freq\0,2\O,-0.7460695012,0.3605448996,-1.5652422367\N,-0.71953
04688,0.0328059714,-0.36423878\C,0.5475774399,-0.025002958,0.277194158
7\O,-1.7252448013,-0.2478474399,0.3142082109\C,1.7353254222,0.31291216
78,-0.5481532233\C,0.5590993333,-0.417528565,1.7096430941\H,2.64972906
45,0.2359184285,0.0440652994\H,1.6539635867,1.3284776184,-0.9573303406
\H,1.8113647918,-0.3517383688,-1.4187194186\H,1.580152132,-0.429010918
3,2.097084036\H,0.1081190929,-1.4087140909,1.8495267085\H,-0.048114138
6,0.2715619849,2.3112132044\\Version=IA64L-G03RevC.02\State=2-A\HF=-32
2.9941353\S2=0.755509\S2-1=0.\S2A=0.750022\RMSD=8.794e-09\RMSF=5.717e-
06\Dipole=1.5938704,-0.0726717,0.8068647\PG=C01 [X(C3H6N1O2)]\@

r.C_CH3_2-OCF3

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H6F3O1(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3
_2-OCF3.freq\0,2\C,1.3540877678,-0.0928153377,0.0447745051\O,0.137387
8104,-0.5099177051,-0.5340674202\C,-1.0418933621,-0.1179501996,-0.0042
707138\F,-1.3190023848,1.1812407624,-0.2586634763\F,-1.0917836328,-0.2
759212163,1.3338866257\F,-2.0060924692,-0.8573372018,-0.5565899939\C,1
.4814904008,1.320349778,0.5158782494\C,2.489275429,-0.8343383463,-0.57
34019262\H,3.4026100026,-0.6825557582,0.0103158168\H,2.6946400103,-0.4
975670895,-1.6047987886\H,2.2765823292,-1.9077792416,-0.6189498194\H,2
.4728183453,1.4614971474,0.9566585728\H,0.7347068654,1.5783722587,1.27
32578735\H,1.3736849318,2.0440578595,-0.3095233799\\Version=IA64L-G03R
evC.02\State=2-A\HF=-530.7408543\S2=0.753321\S2-1=0.\S2A=0.750008\RMSD
=7.103e-09\RMSF=3.245e-05\Dipole=0.8342178,0.2062915,0.0377923\PG=C01
[X(C4H6F3O1)]\@

r.C_CH3_2-OCH2CH3

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C5H11O1(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_

2-OCH2CH3.freq\0,2\H,0.2917470556,-3.0498458875,1.7510064536\C,0.2315
216212,-2.5423592881,0.7818459504\C,0.1343668152,-1.0383393466,0.97848
322\O,0.0426728524,-0.4371559108,-0.311318794\C,0.1174937468,0.9375401
52,-0.3997874838\C,0.1352366636,1.3845106139,-1.82682122\C,-0.55119576
87,1.7815973612,0.6448443013\H,-0.7489469951,-0.7863195699,1.582620517
4\H,1.0206373078,-0.654925548,1.5050848398\H,1.121512799,-2.7978716746
,0.198068076\H,-0.6476699539,-2.9171362102,0.2477511989\H,0.822024495,
0.7665071248,-2.4156675381\H,0.4546126567,2.4297782674,-1.902662093\H,
-0.8588401635,1.3100448554,-2.3051510309\H,-0.2258881262,1.5403772976,
1.6635882832\H,-1.6533546275,1.6814012683,0.6263274539\H,-0.3217557354
,2.8375404084,0.4681955839\\Version=IA64L-G03RevC.02\State=2-A\HF=-272
.3227187\S2=0.753191\S2-1=0.\S2A=0.750008\RMSD=4.883e-09\RMSF=5.878e-0
6\Dipole=-0.0690229,0.0253128,0.418171\PG=C01 [X(C5H11O1)]\@

r.C_CH3_2-OCH3

1\1\GINC-AC21\FOpt\UB3LYP\Gen\C4H9O1(2)\CYL509\16-May-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\C_CH3_2
-OCH3.a2.freq\0,2\C,-0.8879820501,-0.4692017126,-1.6481082272\O,-0.69
70766528,0.4230020907,-0.5626888484\C,0.371422683,0.1928845762,0.28001
24472\H,-1.1798745368,-1.4733727447,-1.3129371885\H,-1.6972375584,-0.0
500021885,-2.2508079774\H,0.0170865865,-0.5487574261,-2.265996195\C,0.
4980033262,1.2840151151,1.294671178\C,0.7381089155,-1.2167024072,0.639
0920547\H,1.4774735068,1.2473786673,1.7840713772\H,-0.2682491895,1.213
1812116,2.0884867786\H,0.3811110436,2.2651855914,0.8215313836\H,1.6511
740133,-1.2169701373,1.243238045\H,0.9245924588,-1.8485695054,-0.23725
70873\H,-0.0467803498,-1.7180636231,1.2371769347\\Version=IA64L-G03Rev
C.02\State=2-A\HF=-233.003536\S2=0.75318\S2-1=0.\S2A=0.750008\RMSD=3.0
36e-09\RMSF=9.224e-06\Dipole=0.0774912,-0.4298342,-0.1423484\PG=C01 [X
(C4H9O1)]\@

r.C_CH3_2-OCHO

1\1\GINC-AC7\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\16-May-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-
OCHO.a3.freq\0,2\C,-0.2384861519,0.3179164807,-0.6483119653\O,-0.2307
927925,0.4939491175,0.7438379754\C,0.5661958614,-0.2445012305,1.550000
0128\H,0.3615433142,0.0519526342,2.5896081249\O,1.3696100431,-1.077868
3457,1.2160492331\C,-0.4473709174,-1.0601244669,-1.185635168\C,-0.7553
918597,1.5362706778,-1.3353317785\H,-0.5658574539,1.4744886974,-2.4117
446271\H,-0.2758388655,2.4416261958,-0.9470435868\H,-1.844358408,1.661
1903678,-1.1988186858\H,0.3110481502,-1.757032592,-0.820843669\H,-0.41
17593195,-1.0377007913,-2.2793693274\H,-1.4349970177,-1.4605394531,-0.
8952125033\\Version=IA64L-G03RevC.02\State=2-A\HF=-307.0365492\S2=0.75
3708\S2-1=0.\S2A=0.75001\RMSD=5.854e-09\RMSF=1.253e-05\Dipole=-0.66587
02,0.4349999,-0.2653244\PG=C01 [X(C4H7O2)]\@

r.C_CH3_2-OCOCH3

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C5H9O2(2)\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2
-OCOCH3.freq\0,2\C,-1.1684367793,-0.0664284646,0.058945353\O,0.110083
8689,-0.5633123758,-0.2261687078\C,1.2337489611,0.0940147703,0.1882734
442\C,2.463497623,-0.6153682059,-0.3285078087\O,1.2310650988,1.0945050
862,0.8662723208\C,-1.4970024716,1.323102038,-0.38150681\C,-2.18003821
29,-1.1627356554,0.0624102807\H,3.3528702474,-0.1601779281,0.108591938
1\H,2.5106589392,-0.5343826418,-1.420289129\H,2.423787457,-1.680799819
3,-0.0818204185\H,-1.8380281302,-2.0129888228,0.6631659102\H,-2.385020
6725,-1.5452414755,-0.9536593824\H,-3.1293051436,-0.8042398089,0.47363
53698\H,-0.7962395214,2.052505977,0.0317650494\H,-2.5095850642,1.58452
47009,-0.0577371255\H,-1.4689445757,1.4157512404,-1.4821678705\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-346.3618799\S2=0.753562\S2-1=0.\S2A=0

.750009\RMSD=6.047e-09\RMSF=8.870e-06\Dipole=-0.1988564,-0.5638313,-0.5603393\PG=C01 [X(C5H9O2)]\@

r.C_CH3_2-Si_CH3_3

1\1\GINC-AC7\FOpt\UB3LYP\Gen\C6H15Si1(2)\CYL509\16-May-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-Si_CH3_3.a2.freq\0,2\H,1.4653253845,-1.7957775043,-1.375779291\C,1.4652984977,-1.6387176596,-0.2905111306\H,2.5112942939,-1.6366115409,0.0398951259\H,0.9780634907,-2.5057112598,0.1714420218\Si,0.6164300125,-0.0130472517,0.1880240409\C,-1.1682676617,-0.0138419445,-0.3741537288\C,0.7060767339,0.2042832194,2.0745073324\C,1.5516657351,1.4363086072,-0.6111906366\C,-1.8269038004,-1.1516851534,-1.1029051112\C,-2.0592103343,1.1712906871,-0.1113273259\H,2.5846582981,1.4869555117,-0.2441863169\H,1.0751668009,2.397939851,-0.3853217554\H,1.5899222529,1.3351630457,-1.7022441718\H,1.7479431022,0.2672396965,2.4134464951\H,0.2355702899,-0.6368843821,2.597156562\H,0.1987120245,1.1205230507,2.3999185658\H,-1.5553916183,1.985985787,0.4211927425\H,-2.9410082611,0.8856718004,0.4864425021\H,-2.4564167871,1.5908545288,-1.0508359706\H,-1.157023168,-1.9986383631,-1.280896767\H,-2.2181694505,-0.8277505449,-2.082465313\H,-2.7006218501,-1.5321246903,-0.546617398\Version=IA64L-G03RevC.02\State=2-A\HF=-527.1576574\S2=0.753866\S2-1=0.\S2A=0.750011\RMSD=5.125e-09\RMSF=2.602e-06\Dipole=-0.1018965,-0.0038862,-0.0338194\PG=C01 [X(C6H15Si1)]\@

r.C_CH3_2-P_CH3_2

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C5H12P1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-P_CH3_2.freq\0,2\C,-1.0823135698,1.1976028786,1.3518626333\H,-0.3724390112,1.8987142588,1.8006346264\H,-1.8151158256,0.9348197419,2.1222498941\H,-1.6025959743,1.6951114789,0.5253976263\P,-0.2089561594,-0.3650891751,0.8231947129\C,-1.6604293596,-1.299423111,0.0982129835\C,0.7153119285,0.1419325404,-0.6463901397\H,-1.3159759179,-2.2210822673,-0.380122075\H,-2.2159750308,-0.7055921624,-0.6359566271\H,-2.3341608611,-1.5838009959,0.9138030849\C,1.4046010171,1.4756897637,-0.7254593603\C,1.2498311817,-0.9222794863,-1.5671485012\H,2.3122500501,-1.1433107783,-1.3648339093\H,1.1998645561,-0.5901498794,-2.6149551103\H,0.7060769208,-1.8700648146,-1.4961707307\H,2.4401460896,1.4309024218,-0.3434221079\H,0.8886103773,2.264128084,-0.1690286426\H,1.4816498306,1.8055270263,-1.7719824158\Version=IA64L-G03RevC.02\State=2-A\HF=-539.0666098\S2=0.755495\S2-1=0.\S2A=0.750022\RMSD=3.198e-09\RMSF=1.438e-06\Dipole=-0.2536363,0.2238288,-0.2767691\PG=C01 [X(C5H12P1)]\@

r.C_CH3_2-SC_CH3_2CN

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C7H12N1S1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-SC_CH3_2CN.freq\0,2\C,1.6958121985,0.0523582902,-0.1627693995\C,1.9737231636,0.1545917216,1.3091751362\C,2.8391582671,0.2567511285,-1.1153232815\S,0.2922119873,-0.7887966441,-0.797853277\C,-1.2294355755,0.1240755755,-0.1359083374\C,-1.1041305535,1.638833769,-0.3637365802\C,-2.4137088493,-0.4714425964,-0.9245491815\C,-1.4137107753,-0.1620884768,1.2934501658\H,-0.2322897722,2.0476207746,0.1533019501\H,-0.9987066047,1.8375557388,-1.434290486\H,-2.0001216191,2.1502934734,0.0063660219\H,-2.2897844094,-0.2589045648,-1.9904806869\H,-3.3513406572,-0.0216848228,-0.5813031609\H,-2.4798542471,-1.5542840227,-0.785340697\N,-1.5828065287,-0.3731692396,2.4238464401\H,3.5871341137,-0.5506286831,-1.0397871263\H,3.3698471964,1.1897550758,-0.8771697022\H,2.5071431622,0.3052373159,-2.1563161109\H,2.5837106862,-0.6988971383,1.65217345\H,1.0700569629,0.1660673507,1.9220612282\H,2.552211838,1.0623240161,1.5274815392\Version=IA64L-G03RevC.02\State=2-A\HF=-726.8507065\S2=0.755974\S2-1=

=0.\S2A=0.750025\RMSD=7.184e-09\RMSF=2.584e-06\Dipole=0.3165931,0.681279,-1.1013221\PG=C01 [X(C7H12N1S1)]\@

r.C_CH3_2-SCH2COOCH3

1\1\GINC-AC2\FOpt\UB3LYP\Gen\C6H11O2S1(2)\CYL509\19-May-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-SCH2COOCH3.a2.freq\0,2\S,0.925384106,-0.414790574,-1.3026855987\C,1.980852019,-0.1555205038,0.0706911069\C,2.3807249428,-1.3502610114,0.8835394907\C,2.2947583102,1.2266454865,0.5548559053\C,-0.4426237329,0.8294105405,-1.0896186265\C,-1.3139338287,0.4743747113,0.0906465766\O,-1.0457355425,0.7287601518,1.2473038723\O,-2.4172783292,-0.1995971263,-0.2948004235\C,-3.2695836422,-0.6450045445,0.7735020145\H,-0.0138616575,1.8223609714,-0.9435276085\H,-1.0046678048,0.8005357705,-2.0249104957\H,-3.6289026328,0.2057289397,1.3585092329\H,-2.7285304076,-1.3278472008,1.4339615956\H,-4.1010601679,-1.1574529242,0.2891131635\H,3.4163415348,-1.255919013,1.2363964502\H,1.7441137767,-1.4515263502,1.7797994391\H,2.2933278997,-2.2842286473,0.3192872973\H,3.2204671029,1.2240031161,1.1435302789\H,2.4247170678,1.9328377145,-0.2744567224\H,1.4948561558,1.6169845331,1.2035405534\Version=IA64L-G03RevC.02\State=2-A\HF=-783.8584295\S2=0.755871\S2-1=0.\S2A=0.750025\RMSD=3.832e-09\RMSF=6.444e-06\Dipole=-0.394287,0.054442,0.0559188\PG=C01 [X(C6H11O2S1)]\@

r.C_CH3_2-SCH2Ph

r.C_CH3_2-SCH3

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C4H9S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-SCH3.freq\0,2\S,0.2840299735,0.0374450867,-1.0606677702\C,0.3032724705,0.0471893323,0.6995757457\C,1.6768222979,0.0657382351,1.3047713732\C,-0.8297648841,-0.5163839328,1.503614093\C,-1.4621578744,0.3782577491,-1.4856017055\H,-1.4906171922,0.5005928757,-2.5713616096\H,-1.8038816382,1.3035012263,-1.013893643\H,-2.1200728145,-0.4489420607,-1.2079943872\H,1.643526011,0.5090158379,2.3090846442\H,2.1015856376,-0.9470000066,1.4212770585\H,2.3825137212,0.6480009426,0.7021870887\H,-0.761322516,-0.1704658269,2.5428131228\H,-1.8134900293,-0.2215951301,1.1232012509\H,-0.8117528143,-1.6210375478,1.5312137587\Version=IA64L-G03RevC.02\State=2-A\HF=-555.9879237\S2=0.75446\S2-1=0.\S2A=0.750015\RMSD=2.829e-09\RMSF=6.500e-06\Dipole=-0.5065901,0.0015902,0.2316193\PG=C01 [X(C4H9S1)]\@

r.C_CH3_2-SO2CH3

1\1\GINC-AC18\FOpt\UB3LYP\Gen\C4H9O2S1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-SO2CH3.freq\0,2\C,-0.2401116458,-0.0235191257,-1.0713966743\S,-0.0161514881,-0.1200245737,0.6974399853\C,1.409575344,0.9455895913,1.0469966542\O,-1.1862358807,0.5041713555,1.339144391\O,0.3856969298,-1.4976645621,1.0308457799\H,2.2872266414,0.5610214332,0.5228740827\H,1.568906127,0.9028288556,2.1278929654\H,1.1812167185,1.9689696521,0.7413912739\C,0.5073865265,-0.9760450266,-1.9430800779\C,-1.095942169,1.0638643926,-1.6290429277\H,-0.4878441986,1.8446420606,-2.1156310458\H,-1.7060029742,1.5320337256,-0.8532693664\H,-1.7630316855,0.6623636334,-2.4041563618\H,0.9191682041,-1.8082860412,-1.3677686594\H,1.3339205026,-0.4729650605,-2.4721487733\H,-0.1562722527,-1.3816084173,-2.7190070929\Version=IA64L-G03RevC.02\State=2-A\HF=-706.3712105\S2=0.754263\S2-1=0.\S2A=0.750013\RMSD=6.963e-09\RMSF=1.617e-05\Dipole=0.9291497,0.9459003,-1.4050599\PG=C01 [X(C4H9O2S1)]\@

r.C_CH3_2-SOCH3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C4H9O1S1(2)\CYL509\11-Apr-2008\0\#\B3LYP

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/GEN 6D INT(GRID=ULTRAFINE) OPT IOP(2/17=4) MAXDISK=1342177280\\r.C_CH
3_2-SOCH3.freq\\0,2\\H,1.144521855,1.1066864565,-1.6474113931\\C,1.25919
76411,1.4306890109,-0.6099862153\\H,2.3085609017,1.6558136168,-0.400715
0076\\H,0.6380479239,2.3061912173,-0.4010384159\\S,0.7750784029,0.032312
0999,0.5029357403\\O,1.5224697538,-1.1891881637,0.013371395\\C,-0.938306
3101,-0.1037291813,0.0032430955\\C,-1.3497494559,-1.2838351707,-0.80655
36251\\H,-0.4717684245,-1.8696137121,-1.096839141\\H,-1.8900043165,-0.97
29782201,-1.7140682758\\H,-2.0317627559,-1.9428644374,-0.2459974891\\C,-
1.9198428831,0.8546268112,0.595767973\\H,-1.4347368207,1.6344161376,1.1
948608189\\H,-2.64115131,0.3397794326,1.2503328946\\H,-2.5105134819,1.35
25723987,-0.1878943639\\Version=AM64L-G03RevC.02\\State=2-A\\HF=-631.159
0778\\S2=0.755545\\S2-1=0.\\S2A=0.750024\\RMSD=9.405e-09\\RMSF=2.569e-06\\Di
pole=-1.0083125,1.1552991,-0.1490519\\PG=C01 [X(C4H9O1S1)]\\@
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r.C_CH3_2-Ph

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1\\1\\GINC-AC27\\FOpt\\UB3LYP\\Gen\\C9H11(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-
Ph.freq\\0,2\\H,-3.6820256896,-0.6947084974,0.0075852294\\C,-2.61448914,
-0.4932813758,0.0053818269\\C,-1.7426439555,-1.2787409358,0.7688619518\\
C,-0.3779420257,-1.0253914942,0.7693460688\\C,0.1832950785,0.0346289462
,-0.0003643159\\C,-0.7286786833,0.8166597846,-0.7670723125\\C,-2.0918555
198,0.5552930221,-0.7609760851\\H,-2.1346642472,-2.0964198637,1.3688635
426\\C,1.5885111581,0.299746631,-0.003223541\\C,2.5289531971,-0.54409830
35,0.8147394971\\C,2.1537165294,1.4275025562,-0.8243871223\\H,-0.3531719
459,1.6361353484,-1.3711991318\\H,0.2727820049,-1.6512658815,1.37131593
48\\H,-2.7572644551,1.1734326392,-1.3588186479\\H,3.5642856864,-0.2211754
2498,0.6976165576\\H,2.4905576166,-1.6057008834,0.5278837375\\H,2.292185
5496,-0.5075960529,1.8887731352\\H,3.2393046401,1.4958921802,-0.7107895
553\\H,1.7315927274,2.4022794061,-0.537433995\\H,1.94321828,1.3057928706
,-1.8976326132\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-349.549293\\S2=0
.775881\\S2-1=0.\\S2A=0.750465\\RMSD=9.882e-09\\RMSF=4.490e-06\\Dipole=0.24
95303,0.0470364,-0.0005681\\PG=C01 [X(C9H11)]\\@
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r.C_CH3_2-C6H4CN

```
1\\1\\GINC-AC8\\FOpt\\UB3LYP\\Gen\\C10H10N1(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_
2-C6H4CN.freq\\0,2\\N,-4.436358223,-0.7883644639,0.0230158764\\C,-3.2892
346758,-0.58446767,0.0171090732\\C,-1.8834007557,-0.3346384302,0.009813
8484\\C,-1.0083109619,-1.1447281737,0.7640833373\\C,0.3517470522,-0.9019
877791,0.7560815256\\C,0.9212554848,0.1637777055,-0.004724336\\C,0.01181
37495,0.9666797009,-0.7579170795\\C,-1.3486173516,0.7259783025,-0.75179
30458\\H,-1.4141243182,-1.9621152603,1.352006676\\C,2.3233313475,0.41288
83383,-0.0120153065\\C,3.2601910583,-0.4514523668,0.7886720376\\C,2.8970
842335,1.5454133843,-0.8207836298\\H,0.3911936253,1.7893860091,-1.35388
06768\\H,0.9973380726,-1.5426106782,1.3466492247\\H,-2.017086369,1.35243
76374,-1.3341660119\\H,3.9829104105,1.6020079504,-0.709080812\\H,2.48366
81507,2.5187346291,-0.5192354904\\H,2.6818574406,1.4363807578,-1.893822
6984\\H,4.2978256342,-0.1304071322,0.6664295386\\H,3.2047278422,-1.50800
20302,0.4888885895\\H,3.0310419872,-0.4220387064,1.8639419786\\Version=
IA64L-G03RevC.02\\State=2-A\\HF=-441.7959561\\S2=0.778425\\S2-1=0.\\S2A=0.7
50547\\RMSD=6.032e-09\\RMSF=9.107e-06\\Dipole=2.3288664,0.4138013,-0.0121
516\\PG=C01 [X(C10H10N1)]\\@
```

r.C_CH3_2-C6H4NO2

```
1\\1\\GINC-AC25\\FOpt\\UB3LYP\\Gen\\C9H10N1O2(2)\\CYL509\\11-Apr-2008\\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH
3_2-C6H4NO2.freq\\0,2\\O,-2.9460508456,1.7940405859,-1.3450692765\\N,-1.
7210747572,1.9238139455,-1.4390643238\\C,-0.8801984176,0.973200505,-0.7
279955305\\O,-1.1634314352,2.8080942353,-2.0974333787\\C,-1.4765327225,-
```

0.0435667019,0.0291154986\C,-0.6773592269,-0.9451353501,0.7034982902\C,
0.7509667761,-0.8743557377,0.6539767073\C,1.3074223367,0.1840992308,-
0.1343152488\C,0.5132074353,1.088444944,-0.8107547396\H,0.9432070192,1
.8857441551,-1.4045196073\C,1.5940063398,-1.790104853,1.3389907472\C,3
.0940721462,-1.66994028,1.2527733023\C,1.0882112487,-2.9229993237,2.18
29969301\H,-1.1611399368,-1.722698485,1.282442421\H,2.3839769416,0.286
1862609,-0.2079856871\H,-2.5570365862,-0.1046664044,0.0722082603\H,1.4
673828914,-2.8319000587,3.2116923805\H,1.4710189765,-3.882223629,1.804
0557029\H,0.0015647705,-2.9985920314,2.2366121287\H,3.5835191099,-2.45
34644745,1.838337694\H,3.4524291351,-0.7029122793,1.6321031627\H,3.455
6837318,-1.7571038412,0.2188093115\\Version=IA64L-G03RevC.02\State=2-A
\HF=-554.0551628\S2=0.777016\S2-1=0.\S2A=0.75047\RMSD=5.655e-09\RMSF=1
.886e-06\Dipole=1.5679449,-1.7381961,1.3002783\PG=C01 [X(C9H10N1O2)]\\
@

r.C_CH3_2-C6H4OCH3

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C10H13O1(2)\CYL509\11-Apr-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3
_2-C6H4OCH3.freq\0,2\C,-1.6004024515,-0.0548907127,-0.5639298022\C,-1
.5610197645,-0.0618728777,0.8418374903\C,-0.3187756775,-0.0205020428,1
.4900755059\C,0.8539837902,0.0266986725,0.7440672742\C,0.8525053236,0.
0352391726,-0.6779341956\C,-0.4322998341,-0.0078883538,-1.2996871656\C
,2.0601141693,0.0838013604,-1.4381681594\O,-2.7726301334,-0.109803098,
1.4714612996\C,-2.7905757037,-0.1191022287,2.8889317037\C,3.3969001453
,0.1272494177,-0.7474742691\C,2.0175750169,0.0919624674,-2.9429605033\H,
-0.5024915618,-0.0040973066,-2.3824826434\H,1.798424024,0.0579473076
,1.2774571675\H,-0.255757335,-0.0246908323,2.5727815763\H,-2.569737681
, -0.0873533796,-1.0525458378\H,-2.2710419031,-0.9976967269,3.294516779
9\H,-3.8431499896,-0.1592558516,3.175830159\H,-2.3362726271,0.79001198
5,3.3054218295\H,4.2165009633,0.1603451555,-1.4711162621\H,3.563313853
4,-0.751118659,-0.105153318\H,3.501050958,1.007963011,-0.0952931143\H,
3.0247527019,0.1340027443,-3.3676553212\H,1.459373072,0.9534537379,-3.
3402478742\H,1.5280465085,-0.8052556502,-3.35175081\\Version=IA64L-G03
RevC.02\State=2-A\HF=-464.0719665\S2=0.774955\S2-1=0.\S2A=0.750422\RMS
D=4.452e-09\RMSF=1.173e-05\Dipole=0.1686785,0.0032696,0.4472401\PG=C01
[X(C10H13O1)]\\@

r.C_CH3_2-C6H4OH

1\1\GINC-AC26\FOpt\UB3LYP\Gen\C9H11O1(2)\CYL509\11-Apr-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_
2-C6H4OH.freq\0,2\C,-1.9025447822,-0.0810601872,-0.3265622383\C,-1.92
63129906,-0.1013930871,1.075328506\C,-0.7187011341,-0.0568285977,1.784
2634036\C,0.4902270199,0.0068641796,1.106258806\C,0.5560386125,0.02947
52802,-0.3162421324\C,-0.6952505277,-0.0174394009,-1.0005943007\C,1.79
93791345,0.0950298088,-1.0152320242\O,-3.1479154588,-0.1648142901,1.68
94269407\C,3.1000369273,0.1412837332,-0.2588689406\C,1.8308081687,0.11
8478551,-2.5200474602\H,-0.7101529236,-0.0034063833,-2.0853932807\H,1.
406529578,0.0401931918,1.6862078028\H,-0.7291564564,-0.0722580036,2.87
34575745\H,-2.844314543,-0.1161119851,-0.8659387559\H,-3.0149557857,-0
.1720822251,2.650091695\H,2.8571503662,0.1740683363,-2.8942069683\H,1.
2845027977,0.9789633738,-2.9355743428\H,1.3705437251,-0.7789170563,-2.
9612087663\H,3.9539825043,0.1868378043,-0.9408685495\H,3.2413830952,-0
.7419391682,0.3828069768\H,3.1657287437,1.0167047561,0.4053893734\\Ver
sion=IA64L-G03RevC.02\State=2-A\HF=-424.7654568\S2=0.775363\S2-1=0.\S2
A=0.750437\RMSD=9.898e-09\RMSF=8.077e-06\Dipole=0.3439074,0.0096009,0.
4136865\PG=C01 [X(C9H11O1)]\\@

r.C_CH3_2-CF2CF3

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C5H6F5(2)\CYL509\11-Apr-2008\0\#\B3LYP/G

```
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|C_CH3_2
-CF2CF3.freq\|0,2\F,-0.7116833774,0.9390026278,-1.3721196583\C,-0.3649
589824,0.5214893158,-0.1135076392\C,1.1215960755,0.0945486342,-0.20456
20832\C,-1.2886822151,-0.5443781154,0.3771586516\F,-0.3891987259,1.617
5796511,0.7091354547\F,1.2481948813,-0.9519771673,-1.0426478859\F,1.56
59948848,-0.2830021004,1.0093164179\F,1.8980268249,1.0902759503,-0.649
4501504\C,-1.7898869071,-1.5679870349,-0.5902028888\C,-1.4112759568,-0
.7731351439,1.8493559296\H,-0.7098911835,-1.550004363,2.1977360831\H,-
2.4194151737,-1.1245846852,2.1012807123\H,-1.2052471027,0.1345755156,2
.4215412895\H,-1.8319237589,-1.1788045034,-1.6102831838\H,-2.792357922
4,-1.9092413313,-0.3040308847\H,-1.1439273338,-2.4620772206,-0.6038034
382\|Version=IA64L-G03RevC.02\State=2-A\HF=-693.3034547\S2=0.753804\S2
-1=0.\S2A=0.750011\RMSD=3.659e-09\RMSF=6.290e-06\Dipole=-0.5625501,-0.
6919624,0.3126917\PG=C01 [X(C5H6F5)]\|@
```

r.C_CH3_2-CF2H

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C4H7F2(2)\CYL509\11-Apr-2008\0\|#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|C_CH3_2
-CF2H.freq\|0,2\C,0.0471250576,-0.0389671266,-0.8370900399\C,0.1962530
414,0.0360043402,0.6464633399\C,0.4470710149,1.3702171257,1.2730108101
\H,1.0026159129,-0.0409015545,-1.3872892529\F,-0.6740173489,1.03147948
62,-1.3112251119\F,-0.6172496653,-1.1852959626,-1.2048956629\C,0.51425
54593,-1.2174503858,1.3970114366\H,1.6031659862,-1.3973677769,1.456308
0288\H,0.0637751658,-2.0946768772,0.9252310172\H,0.1557599513,-1.15393
69543,2.4317833926\H,1.5249622935,1.6117629416,1.3108132781\H,0.091051
5795,1.3869601657,2.3104340706\H,-0.0481552004,2.1736846222,0.72143315
82\|Version=IA64L-G03RevC.02\State=2-A\HF=-356.2679173\S2=0.753779\S2-
1=0.\S2A=0.75001\RMSD=4.157e-09\RMSF=1.689e-06\Dipole=0.6653189,0.0450
608,0.5825406\PG=C01 [X(C4H7F2)]\|@
```

r.C_CH3_2-CF3

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H6F3(2)\CYL509\11-Apr-2008\0\|#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|C_CH3_2
-CF3.freq\|0,2\F,0.4566322897,0.2713530021,-1.6423491511\C,0.412966210
7,0.3806361874,-0.293592795\F,1.6884255548,0.322691084,0.1568041086\C,
-0.4545836551,-0.657165975,0.3299879985\F,-0.0305821545,1.6449243084,-
0.0260215366\C,-1.725484262,-1.0285547076,-0.3629006141\C,-0.259379803
2,-0.9672256427,1.7787748435\H,-1.6260846103,-0.9766396064,-1.45039026
14\H,-2.5517849867,-0.3550301459,-0.0765913944\H,-2.0361392139,-2.0429
764359,-0.0863655333\H,0.7884115799,-0.8752365584,2.0768916539\H,-0.60
21194908,-1.9831374466,2.0078696604\H,-0.8436754307,-0.2838345298,2.41
90684892\|Version=IA64L-G03RevC.02\State=2-A\HF=-455.521504\S2=0.75369
\S2-1=0.\S2A=0.75001\RMSD=8.641e-09\RMSF=1.374e-05\Dipole=-0.595704,-0
.5950115,0.4248107\PG=C01 [X(C4H6F3)]\|@
```

r.C_CH3_2-CCl2H

```
1\1\GINC-AC14\FOpt\UB3LYP\Gen\C4H7Cl2(2)\CYL509\11-Apr-2008\0\|#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|C_CH3_
2-CCl2H.freq\|0,2\C,0.3776947737,-0.2221278222,-0.3822706182\C,0.39285
67488,-0.1464322056,1.0826588932\H,1.3431254316,-0.484794369,-0.807227
4168\Cl,0.0146790891,1.4618638056,-1.1359299178\Cl,-0.8114845809,-1.41
32618387,-1.0471205993\C,1.7054727722,0.1349521682,1.7479379761\C,-0.8
690850334,0.024977228,1.8645129321\H,2.5567192521,-0.2377753818,1.1676
937111\H,1.742273556,-0.31911305,2.7457251313\H,1.8566015636,1.2185887
74,1.8882623112\H,-0.7808502757,-0.4429032521,2.8524670542\H,-1.734639
6043,-0.4020261161,1.3517758569\H,-1.079172131,1.0935737496,2.03612704
42\|Version=IA64L-G03RevC.02\State=2-A\HF=-1076.9872879\S2=0.754591\S2
-1=0.\S2A=0.750016\RMSD=9.302e-09\RMSF=2.096e-06\Dipole=0.5906389,-0.1
763109,0.983807\PG=C01 [X(C4H7Cl2)]\|@
```

r.C_CH3_2-CCl3

1\1\GINC-AC2\FOpt\UB3LYP\Gen\C4H6Cl3(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CCl3.freq\0,2\C,-0.0950087737,0.0245121771,-0.1846947156\C,0.0701339094,0.0257652406,1.2812721346\Cl,1.5130479807,-0.5171896543,-0.9869618267\Cl,-0.5022827207,1.6412728348,-0.8608621851\Cl,-1.3701707868,-1.1504928238,-0.7329950319\C,0.397147616,1.2932965674,2.0107627985\C,0.2485136339,-1.277393505,1.9992965104\H,1.3298346093,1.7450483714,1.6403280503\H,0.5251670593,1.0875187644,3.0773411298\H,-0.3857795294,2.051458924,1.8959921136\H,1.2998714309,-1.4053912319,2.3002439213\H,-0.0372503409,-2.1417587137,1.3981532039\H,-0.3466675877,-1.2849950582,2.9220449561\Version=IA64L-G03RevC.02\State=2-A\HF=-1536.566147\S2=0.754617\S2-1=0.\S2A=0.750016\RMSD=6.799e-09\RMSF=1.573e-06\Dipole=0.0639222,0.1100017,1.1576686\PG=C01 [X(C4H6Cl3)]\@

r.C_CH3_2-CH2Cl

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H8Cl1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CH2Cl.freq\0,2\C,-0.652957969,0.1810818331,-0.7077159942\C,-0.6510919708,0.1932867389,0.7500095882\Cl,1.0771527932,-0.296183511,1.4506848735\C,-0.1285662573,1.3639805869,-1.4600978747\C,-0.8399637705,-1.1116619424,-1.4385897083\H,-1.3063038566,-0.5499397783,1.2035784353\H,-0.8107204109,1.1780033946,1.1885076552\H,0.1311129674,-1.5926120661,-1.6444862227\H,-1.3253261086,-0.9555514432,-2.4100652228\H,-1.4358345512,-1.8279802129,-0.862421012\H,0.9492485515,1.2537771739,-1.6670882254\H,-0.2526880816,2.2967886257,-0.8991650583\H,-0.6256061886,1.4725106932,-2.4321392655\Version=IA64L-G03RevC.02\State=2-A\HF=-617.3992574\S2=0.755365\S2-1=0.\S2A=0.750021\RMSD=6.052e-09\RMSF=1.809e-05\Dipole=-0.8327163,0.2322778,-0.744729\PG=C01 [X(C4H8Cl1)]\@

r.C_CH3_2-CH2F

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H8F1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CH2F.freq\0,2\C,-0.4370106513,-0.074258851,0.1389318767\C,0.8067337255,0.7488048477,0.1218001266\F,1.9284753692,-0.030648937,-0.1768511294\C,-0.6190122179,-1.1227462807,-0.9118992011\C,-1.621552492,0.4402944936,0.8935492542\H,0.9728772247,1.2343595598,1.0937371654\H,0.7679921293,1.546788824,-0.6434677518\H,-1.3274291162,0.9982208451,1.7914308111\H,-2.2814462834,-0.3800150353,1.204399722\H,-2.2441015646,1.121862812,0.2849305235\H,0.3404738673,-1.5647649025,-1.1948779789\H,-1.0738958652,-0.7101270214,-1.831735854\H,-1.285698901,-1.9230499055,-0.5670488109\Version=IA64L-G03RevC.02\State=2-A\HF=-257.0239335\S2=0.753915\S2-1=0.\S2A=0.750012\RMSD=2.829e-09\RMSF=9.903e-06\Dipole=-0.6391382,0.3144496,0.0733778\PG=C01 [X(C4H8F1)]\@

r.C_CH3_2-CH2OH

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C4H9O1(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CH2OH.freq\0,2\C,-0.4547286283,-0.0760345968,0.1351759981\C,0.7908658339,0.7511769599,0.0999043895\O,1.9293967148,-0.0853748271,-0.1114048414\C,-0.6331230947,-1.1680258513,-0.8715657455\C,-1.6527605687,0.4714221375,0.8447919393\H,0.8852975746,1.3187682538,1.0417988842\H,0.7271632024,1.507938163,-0.7122739464\H,2.6740323716,0.4885133707,-0.3454948746\H,-1.3745180411,1.0595060747,1.7283247098\H,-2.3263820726,-0.3323520894,1.1695306162\H,-2.2571859653,1.1355613705,0.1984810699\H,0.3252883354,-1.6258994669,-1.1303410357\H,-1.0822027039,-0.7913228252,-1.8103609201\H,-1.3081876727,-1.9489461299,-0.4982652608\Version=IA64L-G03RevC.02\State=2-A\HF=-233.0001494\S2=0.753991\S2-1=0.\S2A=0.750012\RMS

D=1.857e-09\RMSF=5.713e-06\Dipole=0.0047204,0.6175678,-0.1385966\PG=C01 [X(C4H9O1)]\@

r.C_CH3_2-CH2Ph

1\1\GINC-AC19\FOpt\UB3LYP\Gen\C10H13(2)\CYL509\16-May-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\C_CH3_2-CH2Ph.a2.freq\0,2\C,-1.615605576,-0.0475217463,-1.4505836255\C,-1.5993241707,0.1976176883,0.0386737689\C,-0.1946615505,0.1285748043,0.6347981157\C,0.333671009,-1.0872085038,1.090555161\C,0.6157356148,1.2705389206,0.6989565416\C,1.6342332981,-1.1621649699,1.5910978916\C,1.9168852188,1.2003830129,1.1987106202\C,2.4321476692,-0.0178517905,1.6452770715\H,3.4440047537,-0.0737302162,2.0377745866\H,2.0222755016,-2.1142887094,1.9444709246\H,2.526375501,2.0994941471,1.2446261221\H,-0.2840096756,-1.982329772,1.0602766901\H,0.2194436767,2.2258679482,0.3613394632\H,-2.0268558954,1.186446317,0.2542908365\H,-2.2338673989,-0.5450313595,0.5415580145\C,-1.5506735042,-1.4560694177,-1.95480281\C,-1.2491396466,1.0727097079,-2.3743035647\H,-2.1589200259,-2.1355546225,-1.3433023446\H,-0.5211405871,-1.8584873278,-1.9404239974\H,-1.8989913087,-1.528027331,-2.9928814778\H,-1.6627209994,2.0316013189,-2.0350590297\H,-1.6101402091,0.8876484102,-3.3938774004\H,-0.1550635046,1.2123449623,-2.4490674093\Version=IA64L-G03RevC.02\State=2-A\HF=-388.8473824\S2=0.754054\S2-1=0.\S2A=0.750012\RMSD=3.748e-09\RMSF=2.739e-06\Dipole=0.0039343,-0.016256,-0.0953382\PG=C01 [X(C10H13)]\@

r.C_CH3_2-CH_CH2_2

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C6H11(2)\CYL509\16-May-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CCH32-CH_CH2_2.a1.freq\0,2\C,-1.53617478,0.8624293372,-0.6235714254\C,-1.4275274524,0.9459341863,0.8687408796\C,-0.1523557775,0.8272068461,0.0377205593\H,-1.9042163655,-0.0634289193,-1.0571996582\H,-1.8083617572,1.7548455682,-1.1815533439\H,-1.7324716686,0.0839558919,1.4560128451\H,-1.6190446009,1.8995202964,1.3537675361\H,0.4034034101,1.7588403689,-0.0532270582\C,0.7019109243,-0.3731558713,0.0410762567\C,0.1172311527,-1.7522232852,0.0806755397\C,2.1502992353,-0.2412117922,-0.3211105861\H,2.5323113951,0.7676411004,-0.1251590477\H,2.3379665549,-0.4511931165,-1.390877113\H,2.7732454113,-0.9521906266,0.240141028\H,0.7735445873,-2.4458271028,0.6241102047\H,-0.8664325504,-1.7849423465,0.5631449363\H,-0.0102442304,-2.1810976397,-0.9303476719\Version=IA64L-G03RevC.02\State=2-A\HF=-235.1820093\S2=0.754762\S2-1=0.\S2A=0.750018\RMSD=8.503e-09\RMSF=6.271e-06\Dipole=-0.0356214,0.0345211,-0.0465273\PG=C01 [X(C6H11)]\@

r.C_CH3_2-CH2CH=CH2

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C6H11(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CH2CH=CH2.freq\0,2\C,0.4138749086,0.3818169641,-0.6748555203\C,0.4165899257,0.1792628665,0.8213229418\H,1.4528183455,0.4810238665,-1.0226898068\H,-0.0852206153,1.3332935109,-0.9384621002\C,-0.2548452865,-0.735618062,-1.4413512713\C,1.6141825772,0.5982004878,1.6166299572\C,-0.8883718329,-0.0035693666,1.5332393557\C,-1.3174240659,-0.5963830078,-2.2351970502\H,0.1849281585,-1.7248649585,-1.3064282297\H,-1.7534541518,-1.4401590872,-2.7636940082\H,-1.7895937918,0.3718025841,-2.3921108076\H,2.5513186099,0.4078508514,1.0787960521\H,1.6621606316,0.0760756926,2.5811950743\H,1.6009015149,1.6796600137,1.8520239105\H,-0.7644953801,-0.5666001261,2.4677734941\H,-1.6222263383,-0.5266404505,0.9104973718\H,-1.3411743412,0.9662988115,1.8143685729\Version=IA64L-G03RevC.02\State=2-A\HF=-235.1881713\S2=0.75408\S2-1=0.\S2A=0.750013\RMSD=9.764e-09\RMSF=3.014e-06\Dipole=0.0737311,0.0813634,0.0837851\PG=C01 [X(C6H11)]\@

r.C_CH3_2-CH2CH3

```
1\1\GINC-AC2\FOpt\UB3LYP\Gen\C5H11(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-C
H2CH3.freq\0,2\C,0.0676160483,-0.2873033795,-0.3966107964\C,1.5478505
557,-0.3098833118,-0.6277800383\C,-0.7890777894,-1.2771282958,-1.12312
17891\C,-0.5522782267,0.9066641434,0.2774284336\H,-0.1540157039,1.8389
971593,-0.1591477132\C,-0.3147270108,0.9544923739,1.8021444399\H,-1.63
37096006,0.9219105155,0.0889143461\H,0.7556144599,0.9599120562,2.03803
52202\H,-0.7588198547,0.0825559081,2.2952754063\H,-0.7576909282,1.8571
232418,2.2400418137\H,-0.3241242615,-2.2717282727,-1.1569302435\H,-0.9
661449,-0.9858108461,-2.1762950837\H,-1.7776837636,-1.3807697802,-0.65
88814274\H,2.0923021925,0.2745901395,0.1237148498\H,1.8186937446,0.114
4558953,-1.6130992575\H,1.9492771528,-1.3322851986,-0.6139894093\Vers
ion=IA64L-G03RevC.02\State=2-A\HF=-197.1101675\S2=0.75411\S2-1=0.\S2A=
0.750013\RMSD=6.148e-09\RMSF=4.628e-06\Dipole=-0.0030817,0.0234161,-0.
0560703\PG=C01 [X(C5H11)]\@
```

r.C_CH3_2-CH_CH3_2

```
1\1\GINC-AC29\FOpt\UB3LYP\Gen\C6H13(2)\CYL509\11-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-
CH_CH3_2.freq\0,2\C,0.2681249464,1.8401999888,0.6910772831\H,1.110749
2196,1.5613506535,1.3349255533\H,-0.6037229007,2.0058343329,1.33355572
8\H,0.5245009462,2.7926989205,0.2114772702\C,-0.0187123092,0.757636286
1,-0.3695258225\C,1.2067086595,0.5797752718,-1.2984438736\H,-0.8446116
614,1.1283559675,-0.9937402487\C,-0.4660979177,-0.5547326848,0.2350454
082\C,0.4362566871,-1.3126747785,1.1631436438\C,-1.6030124557,-1.30314
92207,-0.3918800707\H,1.0039709212,-0.1492989321,-2.0913924156\H,2.079
9020005,0.2290868167,-0.7348670171\H,1.4781607504,1.5301126386,-1.7750
898818\H,-2.0850168495,-1.9820399592,0.3244564628\H,-1.2750478357,-1.9
358651458,-1.2389467052\H,-2.3706688851,-0.6263841269,-0.787580259\H,1
.1260459124,-0.659790021,1.7091059535\H,1.0575887346,-2.0540942362,0.6
273158671\H,-0.1414560152,-1.8822960844,1.9042802819\Version=IA64L-G0
3RevC.02\State=2-A\HF=-236.4231242\S2=0.754042\S2-1=0.\S2A=0.750012\RM
SD=9.635e-09\RMSF=9.552e-07\Dipole=0.019065,-0.0345889,-0.0528044\PG=C
01 [X(C6H13)]\@
```

r.C_CH3_2-C_CH3_3

```
1\1\GINC-AC30\FOpt\UB3LYP\Gen\C7H15(2)\CYL509\11-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-
C_CH3_3.freq\0,2\C,-0.1147216881,-0.0066426273,1.7961897488\C,0.28364
70903,0.4331529323,0.361039189\C,-0.1888166341,1.8916170689,0.13945110
89\C,-0.3654966778,-0.4987630818,-0.6587524231\H,0.3375118016,0.656356
1754,2.5451772375\H,0.224948228,-1.028465385,2.0039877093\H,-1.2008024
815,0.0225364713,1.9380334286\C,1.8227199285,0.4176944368,0.2611656389
\C,0.4057513822,-1.6014019973,-1.3246686611\C,-1.8621858823,-0.6261587
01,-0.7052313979\H,2.2536031231,1.1071439479,0.9967129053\H,2.16516260
67,0.7354529829,-0.7307259698\H,2.2364633977,-0.5771375301,0.459897421
9\H,0.2749937886,2.5598496885,0.8758633923\H,-1.2740315839,1.994807747
9,0.24236381\H,0.0884304914,2.244419969,-0.8605962708\H,1.3896554613,-
1.2820180237,-1.6849273227\H,-0.1492369448,-2.0007968884,-2.1826094385
\H,0.5855709418,-2.458512466,-0.6479602592\H,-2.2133172392,-0.78689197
82,-1.7342683494\H,-2.3833883297,0.2519939587,-0.3117684092\H,-2.22094
83737,-1.4957268542,-0.1243391055\Version=IA64L-G03RevC.02\State=2-A\
HF=-275.7334783\S2=0.754088\S2-1=0.\S2A=0.750012\RMSD=7.423e-09\RMSF=4
.277e-06\Dipole=-0.0058699,-0.056529,0.0349307\PG=C01 [X(C7H15)]\@
```

r.C_CH3_2-CCH

```
1\1\GINC-AC27\FOpt\UB3LYP\Gen\C5H7(2)\CYL509\11-Apr-2008\0\#\B3LYP/GEN
```

```
6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-C
CH.freq\\0,2\\C,0.2848620674,0.0006935245,0.172742207\\C,0.2804253488,0.
0016713382,1.6776228483\\C,1.6156468228,0.0016787272,-0.5299728121\\C,-0
.8948854974,-0.0006544085,-0.5410002553\\C,-1.9442592902,-0.0043162806,
-1.1776952946\\H,-2.8562565563,-0.0059505505,-1.7289820044\\H,-0.7350754
364,0.0011437203,2.0814877271\\H,0.809071692,-0.8786470249,2.0735694557
\\H,0.8077668279,0.8832460999,2.0725101766\\H,1.5017520355,0.0011542324,
-1.6168766026\\H,2.2102272367,0.883260642,-0.2462734333\\H,2.2117774921,
-0.8786445234,-0.245615479\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-194
.6407445\\S2=0.769993\\S2-1=0.\\S2A=0.75018\\RMSD=5.219e-09\\RMSF=3.517e-05
\\Dipole=0.2003462,0.000469,0.1216234\\PG=C01 [X(C5H7)]\\@
```

r.C_CH3_2-CH=C_CH3_2

```
1\\1\\GINC-AC11\\FOpt\\UB3LYP\\Gen\\C7H13(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GE
N 6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-
CH=C_CH3_2.freq\\0,2\\H,3.2169426568,-0.7429565571,-0.6535642629\\C,2.52
63280713,-0.8720511088,0.1940180764\\C,1.2823816999,-0.0399277889,0.023
8700573\\C,1.5242085593,1.4418505464,-0.1108004502\\C,0.0373926751,-0.67
13495219,0.0061373179\\C,-1.2699944278,-0.1826540981,-0.0217484737\\C,-1
.6750897908,1.2652905101,0.0865598555\\C,-2.4135893918,-1.1507528504,-0
.176044725\\H,0.0982199583,-1.7614697258,0.0159493188\\H,2.3017434155,-1
.939390961,0.2881228578\\H,3.0896074145,-0.5704912923,1.0912847341\\H,2.
4903633948,1.6253599303,-0.5985965531\\H,1.5742870185,1.94497317,0.8682
563244\\H,0.756310012,1.9481101949,-0.70002056\\H,-2.0717008603,-2.18813
11281,-0.249954037\\H,-3.0049486148,-0.9305189892,-1.0788719601\\H,-3.11
59848001,-1.0831446847,0.6689527819\\H,-0.9690213218,1.8640429621,0.666
2936649\\H,-2.6563667155,1.3489736302,0.5714888668\\H,-1.779275929,1.742
2093198,-0.9012911252\\Version=IA64L-G03RevC.02\\State=2-A\\HF=-274.5306
002\\S2=0.777562\\S2-1=0.\\S2A=0.750172\\RMSD=4.109e-09\\RMSF=8.348e-06\\Dip
ole=-0.0070344,0.1267177,-0.0012437\\PG=C01 [X(C7H13)]\\@
```

r.C_CH3_2-CH=CH2

```
1\\1\\GINC-AC29\\FOpt\\UB3LYP\\Gen\\C5H9(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GEN
6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-C
H=CH2.freq\\0,2\\H,-0.5242368702,-2.1075238886,1.1577096524\\C,0.4980157
798,-1.7664551814,1.0293703403\\H,1.2769789659,-2.4018048675,1.43736812
75\\C,0.8192868923,-0.5858978905,0.382597458\\C,-0.046840741,0.344345614
8,-0.1975278263\\H,1.8817411316,-0.3465382692,0.3142311944\\C,0.49252321
32,1.5797897237,-0.861603848\\C,-1.5416282122,0.1939221752,-0.206553710
6\\H,1.5855304707,1.6263101096,-0.8191629581\\H,0.0971818862,2.493456292
3,-0.3915281414\\H,0.1932588024,1.6299917232,-1.9198859086\\H,-1.8848721
169,-0.7182864292,0.2869438531\\H,-1.928813229,0.1833461787,-1.23635106
64\\H,-2.0249106332,1.0468224995,0.292980767\\Version=IA64L-G03RevC.02\\
State=2-A\\HF=-195.8989799\\S2=0.778444\\S2-1=0.\\S2A=0.750172\\RMSD=3.226e
-09\\RMSF=4.760e-06\\Dipole=-0.1006167,0.1860046,-0.1113998\\PG=C01 [X(C5
H9)]\\@
```

r.C_CH3_2-CH=CHCH3

```
1\\1\\GINC-AC30\\FOpt\\UB3LYP\\Gen\\C6H11(2)\\CYL509\\11-Apr-2008\\0\\#B3LYP/GE
N 6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\C_CH3_2-
CH=CHCH3.freq\\0,2\\C,0.4919724998,0.5239204359,2.7752400008\\H,1.538151
2692,0.8103289922,2.6197914915\\H,0.4759609261,-0.3062957443,3.49737039
91\\H,-0.0160339207,1.3666288924,3.2679923407\\C,-0.1753012768,0.1511234
012,1.4875823252\\C,0.4605107162,0.1706187941,0.2553905618\\H,-1.2196643
836,-0.1481619509,1.55276043\\H,1.5079066983,0.4808451522,0.2645998929\\
C,-0.0614430283,-0.1544162892,-0.9981045679\\C,0.7991409163,-0.06829839
27,-2.2275578407\\C,-1.4780581532,-0.6028775372,-1.2239481746\\H,1.81643
90009,0.2634631028,-1.9953324982\\H,0.3773964892,0.6308465166,-2.966431
7674\\H,0.8705409069,-1.0412081179,-2.7383478894\\H,-1.505704841,-1.5989
```

526878,-1.6909448966\H,-1.9989502481,0.0737680405,-1.9181273891\H,-2.0669719414,-0.6516846692,-0.3049439411\\Version=IA64L-G03RevC.02\State=2-A\HF=-235.2183589\S2=0.777513\S2-1=0.\S2A=0.750169\RMSE=9.544e-09\RMSE=6.812e-06\Dipole=-0.0511965,-0.023022,-0.0590574\PG=C01 [X(C6H11)]\@

r.C_CH3_2-CHO

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C4H7O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CHO.freq\0,2\O,1.1216985821,0.,-1.6422264818\C,1.0450634696,0.,-0.4056567715\H,1.9688772751,0.,0.209276573\C,-0.188413493,0.,0.3277164153\C,-1.4880682328,0.,-0.4062342642\C,-0.1795420476,0.,1.8211353721\H,-1.3170145957,0.,-1.4847930557\H,-2.0914254005,0.8796214155,-0.1379940306\H,-2.0914254005,-0.8796214155,-0.1379940306\H,0.8379897939,0.,2.2263686584\H,-0.7074142533,-0.8787245686,2.2205916151\H,-0.7074142533,0.8787245686,2.2205916151\\Version=IA64L-G03RevC.02\State=2-A\HF=-231.820201\S2=0.76414\S2-1=0.\S2A=0.750064\RMSE=7.700e-09\RMSE=4.731e-05\Dipole=-0.6094473,0.,1.1876377\PG=CS [SG(C4H3O1),X(H4)]\@

r.C_CH3_2-CN

1\1\GINC-AC19\FOpt\UB3LYP\Gen\C4H6N1(2)\CYL509\19-May-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CN.a2.freq\0,2\N,-0.0256544417,0.0000387717,-2.2592572065\C,-0.0133602702,0.0000168635,-1.0826767809\C,0.0032040475,-0.0000059809,0.3090642162\C,1.3096409556,-0.0026208039,1.0491995915\C,-1.28456568,0.0025852455,1.0809733475\H,2.1668743843,-0.0043454997,0.372182979\H,1.3824779154,-0.8840162734,1.703002251\H,1.386013258,0.8784855081,1.7029885852\H,-2.1580569479,0.0043209762,0.4249071873\H,-1.3453842525,-0.8786115839,1.7361953679\H,-1.3418575824,0.8840435257,1.7361618295\\Version=IA64L-G03RevC.02\State=2-A\HF=-210.7373236\S2=0.765663\S2-1=0.\S2A=0.750113\RMSE=8.081e-09\RMSE=4.955e-05\Dipole=0.0183844,-0.0000273,1.623592\PG=C01 [X(C4H6N1)]\@

r.C_CH3_2-COCH3

1\1\GINC-AC8\FOpt\UB3LYP\Gen\C5H9O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-COCH3.freq\0,2\C,-0.779338778,-0.1816904847,-1.827350592\C,-0.7328199319,-0.1303632268,-0.3033956757\C,0.5290833561,0.0983654113,0.3757054708\O,-1.779971832,-0.285542307,0.3457070126\H,-1.8117353214,-0.3629525747,-2.1317724464\H,-0.1453169066,-0.9829071245,-2.2262270243\H,-0.4366602083,0.7588237621,-2.2757894863\C,1.8277572145,0.2943402327,-0.3425976572\C,0.548341118,0.1438196248,1.8697818174\H,1.2228936373,-0.6242392591,2.2768528975\H,-0.4536282115,-0.011180795,2.2724621217\H,0.9347402216,1.1098471559,2.2278058735\H,2.5620089888,-0.4637279311,-0.0303741346\H,2.272285548,1.266839823,-0.0818158208\H,1.7372518452,0.2470060554,-1.4296582611\\Version=IA64L-G03RevC.02\State=2-A\HF=-271.1400138\S2=0.762838\S2-1=0.\S2A=0.750062\RMSE=4.922e-09\RMSE=8.363e-06\Dipole=1.2090509,0.1905069,-0.364083\PG=C01 [X(C5H9O1)]\@

r.C_CH3_2-CON_CH2CH3_2

1\1\GINC-AC15\FOpt\UB3LYP\Gen\C8H16N1O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-CON_CH2CH3_2.freq\0,2\H,1.8190566777,-2.0406268859,2.5007457118\C,1.4610490808,-1.9622749037,1.4675700763\C,1.1076608471,-0.5062717003,1.146421566\N,0.6280922593,-0.2890486658,-0.2206609765\C,1.6490229292,-0.2938337798,-1.2772592994\C,2.4524907178,1.0079179286,-1.3825083397\C,-0.5525175041,0.3806687928,-0.5158212578\O,-0.6879325641,0.9725140121,-1.5970269514\C,-1.6898207956,0.3360059034,0.4215181337\C,-2.707862444,1.427561234,0.3129088145\C,-2.0374084649,-0.8476997071,1.2743766589

\H,1.9950155412,0.1223344176,1.313221356\H,0.3485961589,-0.1407918085,
1.8408811277\H,1.1369671048,-0.4821404167,-2.2229627841\H,2.3182847332
, -1.1401333153, -1.0867366859\H,0.5944097396, -2.6212363723, 1.3535564089
\H,2.2548883937, -2.339303635, 0.8142135559\H,1.7867859893, 1.8381047487,
-1.6305609855\H,3.2075360817, 0.9200012599, -2.1726090428\H,2.9766042324
, 1.2422686908, -0.448401228\H, -2.3320406737, 2.2676821543, -0.2733926263\H,
-3.0108367863, 1.7805105806, 1.3095739012\H, -3.625849285, 1.0649618736,
-0.1772084172\H, -1.3869471122, -1.7061397786, 1.094258665\H, -3.071822956
2, -1.1638019328, 1.0730273852\H, -1.9995193401, -0.6109036243, 2.349997988
6\Version=IA64L-G03RevC.02\State=2-A\HF=-444.4336084\S2=0.756385\S2-1
=0.\S2A=0.750028\RMSD=6.295e-09\RMSF=2.603e-06\Dipole=0.3038746,-0.588
3139,1.1307535\PG=C01 [X(C8H16N1O1)]\@

r.C_CH3_2-CON_CH3_2

1\1\GINC-AC23\FOpt\UB3LYP\Gen\C6H12N1O1(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH
3_2-CON_CH3_2.freq\0,2\C,1.2506748701,0.0659412733,-0.2137551976\C,-0
.1439073759,0.5354276011,-0.1629345922\N,-1.1185207633,-0.2953569869,0
.3805043201\O,-0.4197255318,1.6867257994,-0.524846031\C,1.8511935147,-
0.8672992169,0.7954915712\C,2.1771742968,0.7521617451,-1.1663627266\C,
-1.1159134644,-1.7391246244,0.1939482515\C,-2.4378244375,0.2836562239,
0.5893727324\H,-1.890486946,-2.0333116741,-0.5307821653\H,-0.155601241
6,-2.0783990604,-0.1935784886\H,-1.3199003174,-2.2625690868,1.13720070
82\H,-3.0657902174,0.2119899911,-0.3119027395\H,-2.9390847746,-0.25045
92965,1.4047116234\H,-2.3323798725,1.336770909,0.847616035\H,2.7858810
95,0.0207682951,-1.7184040219\H,2.8883912261,1.3998403576,-0.629147878
4\H,1.6283195864,1.376828035,-1.8731256637\H,2.7309955973,-0.399270526
9,1.261899066\H,2.2165019988,-1.7989910754,0.3341286504\H,1.1522190399
, -1.1340823666, 1.5920626496\Version=IA64L-G03RevC.02\State=2-A\HF=-36
5.8031\S2=0.756672\S2-1=0.\S2A=0.75003\RMSD=5.820e-09\RMSF=8.680e-06\D
ipole=0.1613267,-1.2586908,0.3221632\PG=C01 [X(C6H12N1O1)]\@

r.C_CH3_2-CONH2

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C4H8N1O1(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3
_2-CONH2.freq\0,2\C,0.6216411416,-0.1794965236,-0.0763941037\C,-0.727
7444659,0.3717209131,0.0756927309\N,-1.7781628305,-0.5374090773,0.1080
114792\O,-0.947314199,1.5860837434,0.1266949087\C,0.8668642104,-1.6514
516956,-0.2252235955\C,1.7771154134,0.7640169637,-0.0518737986\H,-1.61
67157498,-1.4795758826,0.4352043808\H,-2.6628435766,-0.1310561978,0.38
35141437\H,2.4687846864,0.5246736815,0.7710184796\H,1.429573422,1.7918
573882,0.0641425647\H,2.3676492847,0.6887243611,-0.9775503197\H,1.8662
309272,-1.8458386444,-0.6283084014\H,0.1360273051,-2.124812832,-0.8929
92809\H,0.8096893094,-2.1795162259,0.7421249389\Version=IA64L-G03RevC
.02\State=2-A\HF=-287.1910909\S2=0.756992\S2-1=0.\S2A=0.750032\RMSD=5.
468e-09\RMSF=1.488e-05\Dipole=0.2608186,-1.4039826,0.284358\PG=C01 [X(
C4H8N1O1)]\@

r.C_CH3_2-CONHCH3

1\1\GINC-AC11\FOpt\UB3LYP\Gen\C5H10N1O1(2)\CYL509\11-Apr-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH
3_2-CONHCH3.freq\0,2\H,-2.3161582847,1.312881894,-2.2044415586\C,-2.2
221025814,0.705684584,-1.2992240469\N,-0.8431322338,0.7228410335,-0.84
67343545\C,-0.3604523484,-0.2752485448,-0.0229256473\C,1.0093259802,-0
.1095921802,0.4805276456\O,-1.0487108938,-1.2681979794,0.2462176721\C,
1.8651622177,1.064596442,0.1044692526\C,1.542617871,-1.1407528509,1.41
8144532\H,-0.3533358556,1.6044112334,-0.8768779959\H,-2.5007363248,-0.
3253319582,-1.5225525878\H,-2.9208245499,1.0871955096,-0.5406577164\H,
2.9039698137,0.9092856723,0.4123277752\H,1.5274241298,1.9973967371,0.5

868046524\H,1.8642390018,1.2475338035,-0.979032557\H,2.4644984018,-1.5
952603308,1.0243142645\H,0.8023762831,-1.9253150437,1.5830497599\H,1.8
128533367,-0.6952256171,2.3885146514\\Version=IA64L-G03RevC.02\State=2
-A\HF=-326.5012984\S2=0.756063\S2-1=0.\S2A=0.750026\RMSD=8.135e-09\RMS
F=6.417e-06\Dipole=0.6592195,1.2842822,-0.2639723\PG=C01 [X(C5H10N1O1)
J\\@

r.C_CH3_2-COOC_CH3_3

1\1\GINC-AC27\FOpt\UB3LYP\Gen\C8H15O2(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_
2-COOC_CH3_3.freq\0,2\H,-1.3337586457,-1.2388666183,-2.9665850469\C,-
1.2783305246,-0.9309688304,-1.9161423329\C,0.1889302985,-0.7403654312,
-1.5136361742\C,0.8628573394,0.3928877601,-2.2964202105\O,0.2897935235
\O,-0.4887601156,-0.0695923068\C,-0.2824734905,0.6023197049,0.5056802773
\O,-0.9188941134,1.4554193791,-0.107411924\C,-0.0569797165,0.652345796
8,1.9480341096\C,0.9679893959,-2.0483295246,-1.6805292599\C,-0.6323619
001,1.8008832189,2.7096833403\C,0.7182881721,-0.3898924282,2.687181314
5\H,0.9708141936,-2.3549925595,-2.7318810622\H,0.512110611,-2.84812699
07,-1.0876380431\H,2.0055131226,-1.924765338,-1.3529611091\H,-1.844716
8565,-0.0072152917,-1.7902044997\H,-1.7400360492,-1.7164141434,-1.3074
931961\H,0.8913154389,0.1367311767,-3.3617262161\H,1.8941465024,0.5306
162704,-1.9528716312\H,0.321345065,1.3320337806,-2.1750069135\H,0.1583
595114,2.3611421122,3.2314775798\H,-1.3210844564,1.4472061099,3.492031
622\H,-1.1695863333,2.4813386179,2.0472943372\H,1.5742769892,0.0623899
713,3.2112032431\H,1.0891981331,-1.1745441087,2.0278643349\H,0.0973900
474,-0.8530886946,3.469424062\\Version=IA64L-G03RevC.02\State=2-A\HF=-
464.3198105\S2=0.756399\S2-1=0.\S2A=0.750027\RMSD=6.390e-09\RMSF=1.116
e-05\Dipole=0.4008958,-0.555223,0.3259871\PG=C01 [X(C8H15O2)]\\@

r.C_CH3_2-COOCH2CH3

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C6H11O2(2)\CYL509\11-Apr-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_
2-COOCH2CH3.freq\0,2\C,-1.5400221706,0.1071482863,0.\C,-0.2340821132,
-0.5379043503,0.\O,-0.0593996346,-1.7521784223,0.\O,0.801839433,0.3490
073083,0.\C,2.118648803,-0.2352199487,0.\C,3.1232944,0.9023447351,0.\C
, -1.707953842,1.592223149,0.\C,-2.7538815224,-0.7625056099,0.\H,2.2248
598628,-0.8759724323,0.8820792433\H,2.2248598628,-0.8759724323,-0.8820
792433\H,3.0018048231,1.5318706238,-0.8875867027\H,4.1422714245,0.4999
710153,0.\H,3.0018048231,1.5318706238,0.8875867027\H,-2.4795426149,-1.
818668258,0.\H,-3.3833484682,-0.5578318656,-0.879314011\H,-3.383348468
2,-0.5578318656,0.879314011\H,-0.7523641404,2.1170253502,0.\H,-2.28626
84102,1.9171952917,0.8784646606\H,-2.2862684102,1.9171952917,-0.878464
6606\\Version=IA64L-G03RevC.02\State=2-A\HF=-385.6885843\S2=0.756657\
S2-1=0.\S2A=0.750029\RMSD=7.454e-09\RMSF=2.570e-05\Dipole=-0.0772429,0
.8083657,0.\PG=CS [SG(C6H3O2),X(H8)]\\@

r.C_CH3_2-COOCH3

1\1\GINC-AC15\FOpt\UB3LYP\Gen\C5H9O2(2)\CYL509\19-May-2008\0\#B3LYP/
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_
2-COOCH3.a2.freq\0,2\C,0.2364311817,0.,-1.0713139102\C,0.2401478577,0.
,0.3848653615\O,1.2501699551,0.,1.0801251961\O,-1.013828625,0.,0.92363
9912\C,-1.0548713004,0.,2.3546740036\H,-2.1134837531,0.,2.6186325106\C
, -1.0229762156,0.,-1.8757704522\C,1.5522384036,0.,-1.777216862\H,-0.55
98654564,-0.888389424,2.7578087949\H,-0.5598654564,0.888389424,2.75780
87949\H,2.3794215128,0.,-1.0656177357\H,1.6460286258,0.8792068624,-2.4
325793326\H,1.6460286258,-0.8792068624,-2.4325793326\H,-1.9151205623,0
, -1.2490870479\H,-1.0598468699,0.8784931386,-2.5379681806\H,-1.059846
8699,-0.8784931386,-2.5379681806\\Version=IA64L-G03RevC.02\State=2-A\
HF=-346.3696454\S2=0.756637\S2-1=0.\S2A=0.750029\RMSD=5.645e-09\RMSF=4

.272e-05\Dipole=-0.624193,0.,-0.4576646\PG=CS [SG(C5H3O2),X(H6)]\@

r.C_CH3_2-COOH

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-COOH.freq\0,2\C,0.063276268,-0.0975236991,-0.6330536298\C,0.0048717302,0.2099040179,0.7859215658\O,0.6749641157,1.0695448413,1.3478024081\O,-0.8873457011,-0.5582803347,1.48332666\C,1.0064757313,0.6846665556,-1.4856480601\C,-0.7812258204,-1.1596525407,-1.2587237767\H,-0.8213250854,-0.2481678483,2.4044162307\H,1.7285167912,0.0194056471,-1.9826805035\H,1.5532120343,1.4208282452,-0.8942077192\H,0.4666560197,1.2045341074,-2.2914276041\H,-0.1504764039,-1.917964446,-1.747103083\H,-1.4118929989,-0.734170409,-2.0541130399\H,-1.4260251285,-1.6589473516,-0.5348934213\Version=IA64L-G03RevC.02\State=2-A\HF=-307.0632409\S2=0.756889\S2-1=0.\S2A=0.75003\RMSD=2.794e-09\RMSF=3.096e-06\Dipole=-0.3177447,-0.4758267,-0.5283438\PG=C01 [X(C4H7O2)]\@

r.C_CH3_2-COPh

1\1\GINC-AC28\FOpt\UB3LYP\Gen\C10H11O1(2)\CYL509\11-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_2-COPh.freq\0,2\C,-2.8760246314,-0.4401011579,-0.1844697547\C,-2.9903952034,-0.1782439223,1.1837725665\C,-1.8693244921,0.2304928999,1.9072732138\C,-0.6335211825,0.3567355085,1.2708566259\C,-0.5064314906,0.0853624204,-0.0991870634\C,-1.6469338992,-0.2956787959,-0.8226204744\C,0.7780178929,0.2777877135,-0.8587189359\O,0.7183671178,0.7064359291,-2.0276303043\C,2.0691733018,-0.054953603,-0.2827890366\C,2.2628908549,-0.8885173324,0.9473687709\C,3.2998723009,0.3540863057,-1.0284403726\H,-1.5497652837,-0.4687010825,-1.889701132\H,0.2267820176,0.6974476604,1.8396294948\H,-1.9561664473,0.4565808908,2.9667412819\H,-3.7484305504,-0.7489846475,-0.754233163\H,-3.9509479585,-0.2839708206,1.6810846066\H,4.0235365006,0.8292084797,-0.3508673835\H,3.0579029354,1.0332621289,-1.8467211285\H,3.8086891575,-0.5261368281,-1.4510927946\H,3.0243653203,-1.6588800784,0.7622431186\H,1.3477189836,-1.3807825188,1.2815137792\H,2.6454376746,-0.2823508355,1.7841725161\Version=IA64L-G03RevC.02\State=2-A\HF=-462.8757295\S2=0.764038\S2-1=0.\S2A=0.750068\RMSD=8.521e-09\RMSF=8.007e-06\Dipole=0.2593689,-0.4744326,1.0796591\PG=C01 [X(C10H11O1)]\@

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,1.0308592622,0.0000000327,-0.3644634647\H,-0.5154293956,-0.8927503326,-0.3644637392\H,-0.5154295624,0.8927501093,-0.3644640506\Version=IA64L-G03RevC.02\State=1-A\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.freq\0,1\C,0.2216494897,0.1824344811,0.621922372\H,1.2946348031,0.3896091838,0.6972815937\H,0.0463360637,-0.7259478453,1.2298603591\H,-0.3471256936,0.9819929249,1.1088775997\B,-0.2737110652,-0.1973697855,-0.8080761046\H,0.4624531936,-0.7164042343,-1.5989565713\H,-1.4176399787,-0.0370079881,-1.12821669\Version=IA64L-G03RevC.02\State=1-A\HF=-65.946661\RMSD=4.422e-09\RMSF=5.097e-06\Dipole=0.0739019,0.0207136,0.2648932\PG=C01 [X(C1H5B1)]\@

n.CH3-CH3

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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\Version
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.freq\
\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\PG
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.freq\
\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
8076097\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,-0.1560742\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.freq\\0,1\C,0.329828014,0.2947706031,1.0779089523\H,1.4148829366,0.4124292451,1.123814636\H,0.0021478487,-0.461294262,1.7950251174\H,-0.1369681059,1.2481048785,1.3363958321\S,-0.2309060771,-0.1058464119,-0.6236566073\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=0.3672239,-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.freq\\0,1\H,0.4032782554,-0.5921458858,-1.6616300541\C,0.4111697868,-0.8712830258,-0.6078476021\H,1.4298376382,-1.07392363,-0.2766529778\H,-0.22376772,-1.7412944652,-0.4398672834\Cl,-0.239786288,0.5079448316,0.3544256427\\Version=IA64L-G03RevC.02\State=1-A'\HF=-500.1085334\RMSD=2.241e-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.freq\\0,1\H,0.5450881132,-0.8872049211,-1.8725336704\C,0.5582973233,-1.1785786011,-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=C01 [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,-0.1083733824\C,-1.2919848181,-0.4947347766,-0.1367614288\C,0.58603581,0.7011509797,-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,0.1858883136,1.7091671296,-0.8146768634\H,0.2616488454,0.4352522752,-2.0599931153\\Version=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 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-NHCH3.freq\\0,1\C,0.8373621362,0.2405194459,0.8735800623\H,1.9278042334,0.3401230919,0.850710369\H,0.5907306021,-0.5543118724,1.5882632911\H,0.4109866805,1.1835296623,1.2677945497\N,0.3518696027,-0.1341564229,-0.4481741069\C,-1.1017347834,-0.2107035977,-0.513764155\H,-1.4502181784,-1.029131709,0.1281755775\H,-1.412599271,-0.43733262,-1.5391929074\H,-1.6240643687,0.7100291033,-0.1883205148\H,0.6805089665,0.5472942152,-1.1291070604\\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(C2H7N1)]\@

n.CH3-NHCHO

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H5N1O1\CYL509\07-Apr-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH3-NHCHO.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,-0.2253938874,0.1734899204\H,-1.7345023037,-0.437983103,0.0907050695\C,-0.1003693936,0.2263407607,-0.9355531248\O,1.0805208288,0.5234890044,-0.9932370006\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=-1.2842945,-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/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH3-NHCOCH3.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,-1.8859292358,0.1643002554,-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/GEN 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,-0.0707606588,0.1200632386,0.1045618431\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/GEN 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\State=1-A\HF=-452.7654984\RMSD=2.148e-09\RMSF=8.623e-05\Dipole=-0.3933215,-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-OCH2CH3.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,-0.3461971544,0.2757549969\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, 1.9938081748, -0.9022076558, 0.7175984626\Version=IA64L-G03RevC.02\State=1-A\HF=-194.3442992\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, 0.8814136485\H, -1.204943786, -1.0063521312, -0.8993099362\H, -2.3740882143, 0.0212881877, -0.0042778274\H, 1.4116044481, 1.3668047864, 0.0109883989\Version=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.f req\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, -0.4822665314, -0.8919040107, -2.0212820545\H, -1.9246950009, 0.1744455643, -1.9515394513\H, 1.2236854855, -0.0737014734, 2.3008031958\H, -0.4131363964, -0.7901040633, 2.2174504168\H, -0.2286222068, 0.9636534554, 2.1732376134\Version=IA64L-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/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH3-Si_CH3_3.f req\0,1\H, 0.9123922966, -1.5813407482, -1.7282637361\C, 0.89349911, -1.5476843555, -0.6319087206\H, 1.9337240459, -1.5808878418, -0.2850529517\H, 0.4026938003, -2.465152341, -0.2842811424\Si, -0.0000139699, 0.0000252714, 0.0000161\C, -1.7871729994, 0.0000405237, -0.6317975903\C, 0.0000388678, -0.0000546186, 1.8955732663\C, 0.893642085, 1.5476752889, -0.6318875812\H, -1.8257813505, 0.0004613189, -1.7281484588\H, -2.3362833972, 0.8838570577, -0.2841919891\H, -2.3360500585, -0.884194417, -0.2848915348\H, 1.933443552, 1.5815185025, -0.2838240163\H, 0.402075982, 2.4651974619, -0.2854903476\H, 0.9138204216, 1.5805630668, -1.7282404022\H, 1.0208259185, -0.0000982052, 2.2974160325\H, -0.5103842448, -0.8840877459, 2.2973623876\H, -0.5103237666, 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,-0.6172245734,1.3106163547,0.8253616504\H,0.0732110323,2
.1046517271,1.1300297944\H,-1.2939826874,1.1206613013,1.6655694387\H,-
1.2083381592,1.6677666107,-0.027371338\H,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-clb2-6dub3\0,1\C,2.0004608618,0.9668672623,0.3091125322\H,1.999
9993174,0.9636095319,1.402206942\H,3.036058107,0.9668243234,-0.0412801
942\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-clp-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 clcy)//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,-1.118376907,-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,-0.3482525121,0.\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\St
ate=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\PG
=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,-2.4138084342,-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\RMSE=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\RMSE=4.310e-09\RMSF=2.055e-06\
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\RMSE=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\RMSE=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,-
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\\Version=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\C1,1.6718716277,-0.1726983197,-0.4315163779\C1,-0.
7133263944,1.5426734429,-0.3523841561\C1,-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\C1,0.2261145327,1.1178256213,-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-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-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-CH₂CH₃_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-CH2CH3_
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 6D 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,-0.5734015878,-2.0631518804\\H,-1.7124155395,-1.0300706297,-0.8962253071\\H,1.9949532099,0.7608965147,0.4873892977\\H,1.7355089002,0.4865177741,-1.2440752508\\H,1.9950346124,-0.8895779284,-0.157984684\\H,-0.1997954786,2.0952547737,0.6051832325\\H,-1.7124115163,1.3646650729,0.0405791793\\H,-0.4592531559,1.8212588254,-1.1263346518\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-197.7729779\\RMSD=3.533e-09\\RMSF=1.210e-05\\Dipole=-0.0000044,-0.0000037,0.0000067\\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,1.5288718374,0.3918758605,1.1119682126\\H,0.2562425832,-0.622343289,1.8098143395\\H,-0.0201646545,1.1114055542,1.5788489484\\C,-0.0788363392,-0.0392700264,-0.2004234436\\C,-0.5119842433,-0.2556345702,-1.3062159844\\H,-0.8945575624,-0.4466870126,-2.282681499\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-116.6532693\\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 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH3-CH=C_CH3_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,-1.6133530797,-0.6385583501,-1.7502999777\\H,1.8233886782,0.8744388098,-1.1415984635\\H,2.0464863825,-0.8208107435,-0.7285322611\\H,1.9158568229,0.3881082421,0.5579474133\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-196.5435771\\RMSD=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.freq\\0,1\\C,0.041981285,0.2345551139,1.2227682436\\H,1.1336755235,0.3128042826,1.2625753495\\H,-0.2693715704,-0.5507246578,1.9250050389\\H,-0.3814858116,1.1759665191,1.5982544835\\C,-0.4392576508,-0.0604143514,-0.1690868163\\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\\State=1-A\\HF=-117.9075585\\RMSD=7.366e-09\\RMSF=3.818e-05\\Dipole=-0.0467448,0.0216798,0.1299055\\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
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.fr
eq\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,-1.8674337051\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,0.8143477937,-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,-0.7882110642,-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,-1.3937209281\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.CH2_CH3_-H

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H6\CYL509\10-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-H.f
req\\0,1\C,0.,0.,-0.7648814214\C,0.,0.,0.7648914238\H,1.0208500203,0.,
-1.164349905\H,-0.5104250102,-0.884082051,-1.164349905\H,-0.5104250102
,0.884082051,-1.164349905\H,-1.0208645548,0.,1.1643299002\H,0.51043227
74,-0.8840946383,1.1643299002\H,0.5104322774,0.8840946383,1.1643299002
\\Version=IA64L-G03RevC.02\State=1-A1\HF=-79.8304204\RMSD=8.910e-09\RM
SF=1.283e-04\Dipole=0.,0.,-0.0000032\PG=C03V [C3(C1C1),3SGV(H2)]\\@
```

n.CH2_CH3_-BH2

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H7B1\CYL509\09-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-B
H2.freq\\0,1\C,0.1403785305,-0.3600500086,-0.3663335104\C,0.1950362304
,-0.3963270979,1.1680708524\H,1.1675922315,-0.4237166169,-0.7811932662
\H,-0.3424965158,-1.2639413151,-0.7685503585\B,-0.4351441167,0.9164724
246,-1.0560561761\H,-0.6074589142,1.9395807054,-0.4537426962\H,-0.6685
192994,0.9070884672,-2.2320583118\H,-0.8130610074,-0.3870371791,1.5985
476706\H,0.7029491572,-1.2934318821,1.5415151179\H,0.7242263662,0.4773
583363,1.5653386731\\Version=IA64L-G03RevC.02\State=1-A\HF=-105.257753
1\RMSD=6.807e-09\RMSF=1.158e-05\Dipole=0.1206813,-0.2203488,0.0738634\
PG=C01 [X(C2H7B1)]\\@
```

n.CH2_CH3_-CH3

```
1\1\GINC-AC3\FOpt\RB3LYP\Gen\C3H8\CYL509\09-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH3.
freq\\0,1\H,-0.2908457531,-0.4131248595,-1.4386795741\C,-0.2413222665,
-0.411015837,-0.3412747033\C,1.2252106642,-0.4332866664,0.1019755561\H
,-0.7356874607,-1.3355241845,-0.0131796783\C,-1.0112628215,0.797625273
4,0.2005493259\H,-0.5601876205,1.7383856702,-0.1390784259\H,-1.0087503
428,0.8085542596,1.2976897621\H,-2.0562926848,0.7905545452,-0.13028741
71\H,1.3071723257,-0.46640394,1.1955800756\H,1.7533521927,-1.306294270
8,-0.2985613086\H,1.7554858864,0.4639161598,-0.2409845057\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-119.1442429\RMSD=7.033e-09\RMSF=1.947e-05\
Dipole=-0.0089864,-0.0153216,-0.0127118\PG=C01 [X(C3H8)]\\@
```

n.CH2_CH3_-NH2

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H7N1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-N
H2.freq\\0,1\C,0.4554820147,0.0711040741,0.342527842\H,0.4540777386,0.
1144932982,1.4390678258\H,1.5088504279,0.1092880096,0.0371892796\C,-0.
1682179394,-1.2523561568,-0.1218363005\N,-0.1898830896,1.2939141225,-0.
1477271448\H,-0.1933943375,1.2897851917,-1.1677662752\H,-1.1713687864
,1.2940088724,0.1301210514\H,-1.215148276,-1.3273821495,0.1990677757\H
,-0.1476464494,-1.3340468949,-1.2161649095\H,0.3702268583,-2.116032688
8,0.2884260167\\Version=IA64L-G03RevC.02\State=1-A\HF=-135.1707254\RMS
D=2.554e-09\RMSF=8.562e-05\Dipole=-0.2931979,-0.4313332,-0.2196197\PG=
C01 [X(C2H7N1)]\\@
```

n.CH2_CH3_-OH

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H6O1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-O
H.freq\0,1\C,0.2251207905,0.4053499564,-0.3063064615\O,0.2240711381,0
.4266750048,1.1184487915\H,1.2541959314,0.4294524386,-0.7015418078\H,-
0.3021758219,1.2829986367,-0.715507177\C,-0.4704478237,-0.8703114373,-
0.7520555818\H,0.6653500498,1.2407110061,1.404214306\H,0.0563411048,-1
.7475052426,-0.3623021527\H,-1.4987568213,-0.8945830602,-0.3767392437\
H,-0.4955613483,-0.9347049315,-1.845541997\Version=IA64L-G03RevC.02\S
tate=1-A\HF=-155.0337993\RMSD=5.086e-09\RMSF=1.483e-05\Dipole=0.249492
2,0.4526603,-0.3327718\PG=C01 [X(C2H6O1)]\@
```

n.CH2_CH3_-F

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H5F1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-F
H.freq\0,1\H,-0.3174546323,-0.351465271,-1.4181390028\C,-0.2825488336,
-0.3608015814,-0.321216856\C,1.1467274785,-0.3532967055,0.1850871288\H
,-0.8270759442,-1.2450579669,0.0339239345\F,-0.9518145439,0.7707940565
,0.1402293543\H,1.1665348732,-0.3525276606,1.2797159951\H,1.6834831196
,-1.240403862,-0.1705400817\H,1.675771609,0.536897974,-0.170246671\Ve
rsion=IA64L-G03RevC.02\State=1-A\HF=-179.0564228\RMSD=3.266e-09\RMSF=2
.096e-05\Dipole=0.3844398,-0.5231815,-0.1869932\PG=C01 [X(C2H5F1)]\@
```

n.CH2_CH3_-SiH3

```
1\1\GINC-AC3\FOpt\RB3LYP\Gen\C2H8Si1\CYL509\09-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-S
iH3.freq\0,1\H,0.6310477971,-0.3567901459,-1.5534328871\C,0.619591449
1,-0.4173902229,-0.4567646085\H,1.670330377,-0.3585288771,-0.142180915
3\C,0.0098050491,-1.7573785795,-0.0093633445\Si,-0.2862824637,1.106667
1703,0.2121666625\H,-1.7068888094,1.1161757084,-0.2389088014\H,-0.2786
363622,1.112935622,1.702665107\H,0.3611465952,2.3623177403,-0.26200247
07\H,-1.0306124064,-1.8558694406,-0.3405547227\H,0.567388609,-2.607091
3646,-0.4214307581\H,0.0177997014,-1.8578768127,1.0822798903\Version=
IA64L-G03RevC.02\State=1-A\HF=-370.5207469\RMSD=3.885e-09\RMSF=2.699e-
05\Dipole=0.1687513,-0.2723503,-0.1245916\PG=C01 [X(C2H8Si1)]\@
```

n.CH2_CH3_-PH2

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C2H7P1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-P
H2.freq\0,1\C,0.5936245805,-0.4050412691,0.4400833821\H,0.604441643,-
0.3554658454,1.5363102287\H,1.6452371712,-0.3581248225,0.1299257223\C,
-0.0482994706,-1.7118428941,-0.032508993\P,-0.2005159864,1.192711402,-
0.1506484467\H,-0.3192034421,0.8355647349,-1.5271969156\H,-1.552293667
3,0.8387251111,0.139032685\H,-1.0914510442,-1.7824699266,0.2957107353\
H,-0.0391370091,-1.7852796738,-1.125855212\H,0.488195485,-2.5823156287
,0.3663531217\Version=IA64L-G03RevC.02\State=1-A\HF=-421.7709351\RMSD
=2.374e-09\RMSF=2.416e-05\Dipole=0.0048471,-0.5437202,0.0046162\PG=C01
[X(C2H7P1)]\@
```

n.CH2_CH3_-SH

```
1\1\GINC-AC4\FOpt\RB3LYP\Gen\C2H6S1\CYL509\17-Jun-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CH2_CH3_-SH
H.freq\0,1\C,0.1588396352,0.2767813146,-0.7729872043\S,0.1735487898,0.
3342942995,1.075347548\H,1.1898073245,0.3046989213,-1.1376911995\H,-0.
3668329821,1.1581589252,-1.1518276252\C,-0.5378691554,-1.0016087163,-1
.233829457\H,0.8180167206,1.5151251594,1.1984111469\H,-0.0180159012,-1
.8922521486,-0.8652464449\H,-1.5734600745,-1.0393568436,-0.8796257419\
H,-0.5521186031,-1.046118396,-2.328680936\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-478.0128885\RMSD=4.154e-09\RMSF=4.700e-05\Dipole=0.1406046
,0.2466095,-0.6495396\PG=C01 [X(C2H6S1)]\@
```

n.CH2_CH3_-Cl

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C2H5Cl1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
Cl.freq\0,1\H,0.0284232991,-0.6997839554,-1.4941192292\C,0.0619950684
,-0.7129770764,-0.4030621219\C,1.4870640339,-0.722390668,0.1225299666\
H,-0.5129275568,-1.5677880089,-0.041858156\Cl,-0.844487902,0.769429751
8,0.145121124\H,1.504559043,-0.7206284526,1.2163015885\H,1.9966272984,
-1.62800154,-0.2299176976\H,2.0452576374,0.1481026428,-0.2342726824\Version=IA64L-G03RevC.02\State=1-A\HF=-539.4262586\RMSD=7.014e-09\RMSF=
4.792e-05\Dipole=0.5056968,-0.6993423,-0.2295376\PG=C01 [X(C2H5Cl1)]\@
```

n.CH2_CH3_-Br

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C2H5Br1\CYL509\09-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
Br.freq\0,1\H,0.3760418001,-1.0577817842,-1.5631504363\C,0.409306564,
-1.0772500485,-0.4736120549\C,1.827180978,-1.0949041378,0.066192401\H,
-0.1886928861,-1.9121881237,-0.1077509737\Br,-0.5764123215,0.552427190
2,0.1006580586\H,1.8378363776,-1.0871054156,1.1598234937\H,2.329318442
3,-2.0096597112,-0.2758509053\H,2.4010022649,-0.2352915054,-0.29158530
68\Version=IA64L-G03RevC.02\State=1-A\HF=-2653.1127397\RMSD=7.686e-09
\RMSF=4.360e-05\Dipole=0.5221034,-0.726478,-0.2239082\PG=C01 [X(C2H5Br
1)]\@
```

n.CH2_CH3_-N_CH3_2

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C4H11N1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
N_CH3_2.freq\0,1\C,0.9750415765,-0.720988897,1.0820164648\H,1.0405107
613,-0.6251209423,2.1724732579\H,1.9960776274,-0.7436606717,0.68395417
16\H,0.5021558813,-1.6979876246,0.8634612209\N,0.2652452844,0.42566814
48,0.5395353711\C,0.3297301965,0.5323504744,-0.9180769416\C,-1.0761656
576,0.5539476928,1.0845843845\H,1.3918016469,0.5751437941,-1.194257774
2\H,-0.1025580645,1.5039378363,-1.1923896256\C,-0.3582460066,-0.572897
5197,-1.7410643213\H,-1.0172126978,0.6538361038,2.1750519379\H,-1.7433
076892,-0.3023035052,0.8662508067\H,-1.549172715,1.4599264135,0.688416
257\H,-0.2356635253,-0.3734406139,-2.8121642649\H,0.0717281944,-1.5599
095736,-1.5371203258\H,-1.4332370629,-0.6245687331,-1.5351807779\Version=IA64L-G03RevC.02\State=1-A\HF=-213.7871978\RMSD=1.630e-09\RMSF=2.3
67e-05\Dipole=-0.111934,-0.1798821,-0.1027637\PG=C01 [X(C4H11N1)]\@
```

n.CH2_CH3_-NHCH3

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H9N1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-N
HCH3.a4.freq\0,1\H,-1.1716878595,0.4130677,-2.4183032075\C,-1.1615870
032,0.6109990192,-1.3412115643\N,-0.0088501916,-0.0430454117,-0.734479
4927\C,0.0349590877,0.1029461987,0.7181380603\C,1.2339080429,-0.634768
6941,1.3095063056\H,0.1163471019,1.1758606947,0.9404025663\H,-0.896422
7368,-0.2431950245,1.2107657183\H,-2.1381460997,0.2991882123,-0.922949
7652\H,-1.077345149,1.6958625956,-1.2034400393\H,-0.0314769527,-1.0362
452085,-0.9626022665\H,2.1656271226,-0.2738542247,0.8620732981\H,1.286
1285564,-0.4900702988,2.3941905231\H,1.1652465939,-1.7143557075,1.1226
22812\Version=IA64L-G03RevC.02\State=1-A\HF=-174.479525\RMSD=2.139e-0
9\RMSF=1.613e-05\Dipole=-0.2804104,-0.2233336,0.1168695\PG=C01 [X(C3H9
N1)]\@
```

n.CH2_CH3_-NHCHO

```
1\1\GINC-AC21\FOpt\RB3LYP\Gen\C3H7N1O1\CYL509\20-May-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CH2_CH3_
```

-NHCHO.freq\0,1\O,-1.3999620029,0.6668592827,-1.1638108594\C,-1.43985
26014,-0.0284747133,-0.1628605587\N,-0.370737992,-0.6492158374,0.41038
99577\C,0.9952825374,-0.4870404241,-0.0754034199\C,1.8159671002,0.5047
770686,0.7532835812\H,1.3562546409,1.4979235641,0.7294597317\H,0.91020
95554,-0.142776735,-1.1085465678\H,1.480408836,-1.470625428,-0.0888928
871\H,-0.5232182613,-1.1441770448,1.2790039769\H,-2.3816296076,-0.2387
945205,0.3829151744\H,1.8910662803,0.1863882813,1.8001028415\H,2.83338
83056,0.5861268962,0.3535972859\Version=IA64L-G03RevC.02\State=1-A\HF
=-248.5171089\RMSE=9.571e-09\RMSE=1.411e-06\Dipole=0.5508165,-0.781790
3,1.1350159\PG=C01 [X(C3H7N1O1)]\@

n.CH2_CH3_-NHCOCH3

1\1\GINC-AC14\FOpt\RB3LYP\Gen\C4H9N1O1\CYL509\10-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_
-NHCOCH3.freq\0,1\C,0.8311079311,-1.3119745205,-0.1668278941\C,0.4128
843708,-2.1353499559,1.0549442329\H,1.7214550621,-0.7222063336,0.06289
14634\H,1.0703845079,-1.9696951592,-1.011222224\N,-0.1869165415,-0.36
26443606,-0.5990838632\H,-0.9911428843,-0.7163183884,-1.0971846579\C,-
0.1936881507,0.9415671215,-0.1823074035\O,0.6930789678,1.4194834193,0.
514833859\C,-1.3784370281,1.7733351985,-0.655814643\H,-0.9995200026,2.
6656237986,-1.1626854433\H,-1.9453027067,2.111466786,0.2176482966\H,-2
.0545665685,1.2401747263,-1.3321181393\H,-0.4935778774,-2.7190393556,0
.8536618383\H,1.2084870297,-2.8351672421,1.3363272316\H,0.2163647492,-
1.4776627236,1.9075320496\Version=IA64L-G03RevC.02\State=1-A\HF=-287.
8402368\RMSE=3.423e-09\RMSE=4.966e-06\Dipole=-0.8664862,-0.872709,-0.6
796991\PG=C01 [X(C4H9N1O1)]\@

n.CH2_CH3_-NO2

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C2H5N1O2\CYL509\10-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_
-NO2.a2.freq\0,1\O,-0.7289453532,0.25745488,-1.1649245504\N,-0.637538
0669,-0.1547779038,-0.013551421\C,0.7108732318,-0.077228364,0.67638972
4\O,-1.5521983921,-0.6345812838,0.6486255582\C,1.7957318751,0.52425740
3,-0.195529522\H,0.5197250719,0.5004029728,1.5846092542\H,0.9227317297
, -1.1064679417,0.9777524392\H,1.9509474098,-0.0664504692,-1.1015901224
\H,1.5464551068,1.5458406956,-0.4925313084\H,2.7324264712,0.5449570659
,0.3718504098\Version=IA64L-G03RevC.02\State=1-A\HF=-284.3280903\RMSE
=3.938e-09\RMSE=1.750e-05\Dipole=1.3030358,0.1259265,0.5319331\PG=C01
[X(C2H5N1O2)]\@

n.CH2_CH3_-OCF3

1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H5F3O1\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_
-OCF3.freq\0,1\C,-0.6859800307,-0.0000203066,-1.3649764784\O,-0.66319
02554,-0.0000303064,0.0835506401\C,0.5527972494,-0.0000479456,0.655490
8791\F,1.28994831,1.0837967016,0.3155915182\F,1.289987973,-1.083818822
8,0.3154443447\F,0.3957953762,-0.0001371639,1.9803297063\H,-0.15975224
57,0.8900246457,-1.7260095683\H,-0.1600611683,-0.8902468206,-1.7260115
402\C,-2.1402174671,0.0002351938,-1.7916014343\H,-2.2039962,0.00024239
08,-2.8849758892\H,-2.656082614,-0.8877213993,-1.4135856735\H,-2.65576
91714,0.8883755506,-1.41359037\Version=IA64L-G03RevC.02\State=1-A\HF=
-492.0851411\RMSE=7.769e-09\RMSE=1.413e-04\Dipole=-0.4161467,0.0000235
, -0.8993599\PG=C01 [X(C3H5F3O1)]\@

n.CH2_CH3_-OCH2CH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10O1\CYL509\10-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_
-OCH2CH3.freq\0,1\C,0.5117747779,-1.1266690513,0.3743638045\H,0.518141
0528,-1.0865295112,1.4778164428\H,1.5650695764,-1.0863872321,0.0454274

```
361\C,-0.1489069459,-2.4079389811,-0.1086507333\O,-0.2066715447,-0.024
8784424,-0.1506255621\C,0.3273257281,1.2277307966,0.2385275319\C,-0.52
05732459,2.327241867,-0.3805857634\H,1.3767097378,1.3144954432,-0.0939
454733\H,0.3309457897,1.3150852077,1.3392684294\H,-0.1350531194,3.3136
205393,-0.0998078168\H,-1.5580274605,2.2490311427,-0.0396394413\H,-0.5
12635337,2.2483341386,-1.4725496781\H,-1.1892384156,-2.4534460892,0.22
94037572\H,-0.1425198108,-2.4533854094,-1.2025102049\H,0.3822584589,-3
.2839784777,0.2796120072\\Version=IA64L-G03RevC.02\State=1-A\HF=-233.6
634487\RMSD=8.175e-09\RMSF=1.494e-05\Dipole=0.3242636,0.0390389,0.2366
238\PG=C01 [X(C4H10O1)]\\@
```

n.CH2_CH3_-OCH3

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H8O1\CYL509\10-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-O
CH3.freq\\0,1\C,-0.6505791902,-0.0000541244,-1.6918847014\O,-0.6518280
894,0.0000492538,-0.2822194961\C,0.6537814366,-0.0000744145,0.26695928
84\H,-0.1496632087,-0.8928850976,-2.1018478172\H,-1.6944125192,0.00012
84158,-2.017490702\H,-0.1493114264,0.8925199931,-2.1019764034\H,1.2121
455317,-0.8875058025,-0.0798140541\C,0.5393736748,0.0000953538,1.78246
5551\H,1.2123866409,0.8871334849,-0.0799965965\H,1.5338447159,0.000002
9681,2.2422397795\H,-0.002786977,0.8871687286,2.1256104262\H,-0.003033
5689,-0.8867576098,2.1257905085\\Version=IA64L-G03RevC.02\State=1-A\HF
=-194.3442993\RMSD=2.367e-09\RMSF=1.845e-05\Dipole=0.3841409,-0.000059
3,-0.2353884\PG=C01 [X(C3H8O1)]\\@
```

n.CH2_CH3_-OCHO

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C3H6O2\CYL509\10-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-O
CHO.freq\\0,1\C,-0.3519369906,0.0000958212,-0.8318158649\O,-0.32586472
2,0.0000327032,0.6185226413\C,0.8914858366,0.000328134,1.1812726524\O,
1.9466692194,0.0006553945,0.5951745693\H,0.1859882252,-0.883045563,-1.
1907760554\H,0.1846707379,0.8840940483,-1.1906539464\C,-1.8058492742,-
0.0009405896,-1.2620077074\H,0.7796158895,0.0001624907,2.2768532357\H,
-1.8686060488,-0.0009672461,-2.3556894823\H,-2.3245063649,-0.889009708
2,-0.8870183634\H,-2.3257958487,0.8863610027,-0.8869875541\\Version=IA
64L-G03RevC.02\State=1-A\HF=-268.3820972\RMSD=2.833e-09\RMSF=6.248e-05
\Dipole=-0.7976964,-0.0002676,-0.197997\PG=C01 [X(C3H6O2)]\\@
```

n.CH2_CH3_-OCOCH3

```
1\1\GINC-AC15\FOpt\RB3LYP\Gen\C4H8O2\CYL509\15-May-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\CH2_CH3_-O
COCH3.freq\\0,1\C,-0.4742065331,0.0003334293,-1.3059655881\O,-0.456880
6649,0.0003608371,0.1397908195\C,0.767977913,0.0005177393,0.7151675163
\C,0.6532462076,-0.001638721,2.2224780092\O,1.8042341189,0.0006810695,
0.0874749007\H,0.0644723705,0.8829548251,-1.6659994162\H,0.0643274901,
-0.8823924326,-1.6659843294\C,-1.9261124037,0.0004413264,-1.7451646036
\H,1.650903855,0.0076769885,2.6626467375\H,0.1073605736,-0.8898816986,
2.557384793\H,0.0888016905,0.8739697476,2.5595036\H,-1.9839471816,0.00
04234896,-2.8391988427\H,-2.4481680515,-0.8869363373,-1.3727664643\H,-
2.448009481,0.8879275216,-1.3728038425\\Version=IA64L-G03RevC.02\State
=1-A\HF=-307.7074378\RMSD=9.470e-09\RMSF=6.710e-05\Dipole=-0.7641218,-
0.001467,0.1062498\PG=C01 [X(C4H8O2)]\\@
```

n.CH2_CH3_-Si_CH3_3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H14Si1\CYL509\10-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
Si_CH3_3.freq\\0,1\H,1.0479759596,-1.2544932404,-2.1718040491\C,1.041
4391492,-1.280579916,-1.0752017853\H,2.086025752,-1.2844492379,-0.7401
65663\H,0.5943696286,-2.2352944927,-0.7731059623\Si,0.0908702594,0.197
```

```
350099,-0.3603793265\C,-1.7010940671,0.1532385594,-0.9814475672\C,0.12
33927479,0.1351607313,1.5422714027\C,0.9132565703,1.8077345301,-0.9327
675049\H,-1.7422642982,0.2047885865,-2.0763944856\H,-2.2810895109,0.99
83164475,-0.5904582097\H,-2.2134707291,-0.7674906093,-0.67756931\H,1.9
548791546,1.8685390981,-0.5943348925\H,0.3876863313,2.6875658552,-0.54
17620069\H,0.917633097,1.8863431521,-2.0268861971\H,1.1694848809,0.225
2527114,1.8700513795\C,-0.5086412952,-1.1152741793,2.1805619785\H,-0.3
804832648,1.0357208563,1.9230206081\H,-0.4540300967,-1.0824031344,3.27
58312605\H,-1.5668947577,-1.2143816392,1.9109255823\H,-0.0021244087,-2
.0325940925,1.8574633742\\Version=IA64L-G03RevC.02\State=1-A\HF=-488.5
008035\RMSD=8.138e-09\RMSF=3.435e-05\Dipole=0.0106189,0.0208539,-0.007
9157\PG=C01 [X(C5H14Si1)]\@
```

n.CH2_CH3_-P_CH3_2

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C4H11P1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
P_CH3_2.freq\\0,1\C,1.4727884529,-0.7528663262,0.7581301159\H,1.426986
2561,-0.7856187738,1.8523286551\H,2.5274128323,-0.6614955332,0.4762935
959\H,1.0905239306,-1.7002544635,0.3613180715\P,0.5512357323,0.7494616
87,0.1380260296\C,0.5486013462,0.3782407041,-1.6930825884\C,-1.2195925
89,0.3257518876,0.6102476489\H,-0.1048991265,1.089217111,-2.2106649002
\H,0.2241020983,-0.6398275779,-1.9367344291\H,1.562255682,0.5197803333
,-2.0835747931\H,-1.2701369215,0.4434087701,1.7010683014\C,-1.80236343
68,-1.0325202329,0.2029031115\H,-1.8363919536,1.1365557723,0.199837060
9\H,-2.8387433234,-1.127699508,0.5500949787\H,-1.8099070522,-1.1628729
714,-0.8846279501\H,-1.2363410467,-1.8647546607,0.6350812374\\Version=
IA64L-G03RevC.02\State=1-A\HF=-500.408548\RMSD=3.079e-09\RMSF=1.034e-0
5\Dipole=-0.2080022,-0.4771914,-0.1417801\PG=C01 [X(C4H11P1)]\@
```

n.CH2_CH3_-SC_CH3_2CN

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C6H11N1S1\CYL509\10-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3
_-SC_CH3_2CN.freq\\0,1\C,1.6073267627,0.844078274,0.3200946185\H,1.557
8110219,0.8287300058,1.4134382096\C,3.063135231,0.8995202899,-0.145874
5048\S,0.8175119694,-0.6751292884,-0.3556293637\C,-0.9717179751,-0.466
7811415,0.1380039711\C,-1.1589708766,-0.5305700089,1.6662521479\C,-1.7
360527775,-1.6126274314,-0.557016719\C,-1.4507106665,0.8288115149,-0.3
669602702\H,-0.7925119683,-1.4926067654,2.0357555387\H,-0.6152614157,0
.2702585489,2.1742345386\H,-2.220723419,-0.4328064449,1.9209397589\H,-
1.6269013562,-1.5602403057,-1.6433118095\H,-2.8007520041,-1.555178272,
-0.308144505\H,-1.3484588546,-2.5752643369,-0.2088114098\N,-1.81533740
52,1.8663448129,-0.7426928329\H,1.0524412458,1.7150115812,-0.042454912
4\H,3.1290055914,0.9384583759,-1.2377869693\H,3.5444990563,1.797635776
7,0.2566562335\H,3.6299642399,0.0290677776,0.2014095147\\Version=IA64L
-G03RevC.02\State=1-A\HF=-688.1924681\RMSD=3.822e-09\RMSF=3.655e-06\Di
pole=0.3896559,-0.7869528,0.808011\PG=C01 [X(C6H11N1S1)]\@
```

n.CH2_CH3_-SCH2COOCH3

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H10O2S1\CYL509\10-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3
_-SCH2COOCH3.a2.freq\\0,1\S,1.3485961674,0.9385343894,-0.405166914\C,1
.3539445157,0.9359404741,1.4374339479\H,2.4088112607,0.7881122747,1.69
29294786\H,0.8028191549,0.0555920319,1.7793907871\C,-0.449518739,0.756
0574338,-0.7644497765\C,-0.9409788935,-0.6226779764,-0.3849436727\O,-1
.2587612212,-0.9540716832,0.7396986576\O,-0.9504699892,-1.4551604829,-
1.4448068934\C,-1.3287872107,-2.8122735871,-1.158493782\H,-1.021453873
1,1.5070656936,-0.2148203615\H,-0.555858096,0.928347118,-1.8372181553\
H,-2.336860821,-2.849352736,-0.7373407685\H,-0.6292705368,-3.261219176
1,-0.448395859\H,-1.2917205291,-3.3333790112,-2.1153435061\C,0.8144905
```

148,2.2125278948,2.0786631234\H,0.8953781202,2.1451894135,3.1707530604
\H,1.3726829981,3.0927418196,1.744606135\H,-0.2431177966,2.3667642342,
1.8397166596\\Version=IA64L-G03RevC.02\State=1-A\HF=-745.1994757\RMSD=
8.458e-09\RMSF=1.651e-06\Dipole=-0.2536828,-0.1568157,-0.1074456\PG=C0
1 [X(C5H10O2S1)]\\@

n.CH2_CH3_-SCH2Ph

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C9H12S1\CYL509\10-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
SCH2Ph.freq\\0,1\C,-1.7083555566,-1.2038191673,-1.0666919318\S,-1.6604
797424,-1.1800363065,0.7705645106\C,0.1638518451,-1.1864856042,1.06305
498\H,-1.1447721995,-0.3447507155,-1.444359002\C,-3.1572108362,-1.1545
161966,-1.5508538017\C,0.9018721645,0.0269330091,0.5494280506\H,0.5849
343555,-2.1031824261,0.6364618318\H,0.2506158263,-1.2652491495,2.15218
48865\C,1.7969504165,-0.0853013202,-0.5214451817\C,0.7128829735,1.2873
211461,1.135667082\C,2.4912119973,1.030747554,-0.9957503414\C,1.405439
2254,2.4015120629,0.667160631\C,2.298042203,2.2772104439,-0.4018420442
\H,2.8378257635,3.1469382064,-0.7667635638\H,1.2502930352,3.3695795297
,1.1364205262\H,3.1826275202,0.9227688069,-1.8274434264\H,0.0107675466
,1.3911509821,1.9593251658\H,1.9576440193,-1.0569605237,-0.983840272\H
, -1.2155345177,-2.1166990101,-1.421387211\H,-3.1873728281,-1.172165789
2,-2.6462940224\H,-3.7307836023,-2.0119531299,-1.1828926631\H,-3.65667
56373,-0.2405074433,-1.2128090758\\Version=IA64L-G03RevC.02\State=1-A\
HF=-748.3788149\RMSD=5.631e-09\RMSF=1.401e-06\Dipole=0.4308924,0.05429
96,-0.456767\PG=C01 [X(C9H12S1)]\\@

n.CH2_CH3_-SCH3

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H8S1\CYL509\09-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-S
CH3.freq\\0,1\S,-0.0878663814,0.,-0.8137546424\C,-0.1245108877,0.,1.02
36516462\C,1.7180231359,0.,-1.0850452313\C,-1.5689616479,0.,1.52234865
69\H,1.8812224068,0.,-2.1659811397\H,0.4077434661,0.8865490189,1.38770
04904\H,2.1845619743,0.8942851,-0.6596858819\H,0.4077434661,-0.8865490
189,1.3877004904\H,2.1845619743,-0.8942851,-0.6596858819\H,-1.58968918
,0.,2.6180305215\H,-2.1087928038,0.8865314047,1.1731326242\H,-2.108792
8038,-0.8865314047,1.1731326242\\Version=IA64L-G03RevC.02\State=1-A'\H
F=-517.3282192\RMSD=3.864e-09\RMSF=1.063e-05\Dipole=0.46509,0.,0.48786
14\PG=CS [SG(C3H2S1),X(H6)]\\@

n.CH2_CH3_-SO2CH3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C3H8O2S1\CYL509\10-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
-SO2CH3.freq\\0,1\C,-0.3627089168,-0.0000016825,-2.0075177651\S,-0.399
8031297,0.0000005541,-0.1972817084\C,1.3641463798,-0.0000024262,0.2658
767233\O,-0.9863819351,1.2781224332,0.2389347554\O,-0.9863870623,-1.27
81178733,0.2389379305\H,1.8078456581,-0.8926409949,-0.1864296125\C,1.5
069163458,-0.0000008985,1.7869199667\H,1.807849161,0.8926333241,-0.186
4317398\H,0.138739452,-0.9021525072,-2.3641080485\H,0.1387434171,0.902
1461421,-2.3641100635\H,-1.4066038512,0.0000002629,-2.3302245322\H,2.5
678441167,-0.0000025847,2.0561291214\H,1.0372323293,0.8881065625,2.218
5125308\H,1.0372289199,-0.8881055271,2.2185146427\\Version=IA64L-G03Re
vC.02\State=1-A\HF=-667.7167677\RMSD=8.363e-09\RMSF=3.337e-05\Dipole=1
.4903824,-0.0000043,-0.9615186\PG=C01 [X(C3H8O2S1)]\\@

n.CH2_CH3_-SOCH3

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C3H8O1S1\CYL509\10-Apr-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
-SOCH3.a2.freq\\0,1\C,-0.7698868443,-0.0856881417,-1.2222989379\S,-0.8
170866772,0.0222647548,0.6038206166\O,0.838180507,-0.0033581591,0.9705

```
667741\C,1.4475635837,1.2900801687,1.0140158714\H,-0.285477646,0.81130
37186,-1.6248283328\C,-0.1080260706,-1.3573243418,-1.7481420962\H,2.49
20944266,1.1152092483,1.2896315982\H,0.9729336442,1.9333320535,1.76438
60742\H,1.412162494,1.7916153163,0.0380596727\H,-1.8285133277,-0.03304
84714,-1.5098084358\H,-0.0815132669,-1.3498772667,-2.8447652365\H,0.91
97864144,-1.4317600959,-1.3808897336\H,-0.6514339718,-2.2485514188,-1.
4188986883\\Version=IA64L-G03RevC.02\State=1-A\HF=-592.5138276\RMSD=4.
323e-09\RMSF=1.094e-05\Dipole=0.1315996,0.4839913,-0.6083684\PG=C01 [X
(C3H8O1S1)]\\@
```

n.CH2_CH3_-Ph

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C8H10\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-Ph
.freq\0,1\C,1.0366684014,-1.6544540992,0.5002142181\C,1.0571423135,-1
.6866646117,2.0392821042\H,2.0687945953,-1.6461211791,0.1272662006\H,0
.5788495786,-2.5796527033,0.1275567166\C,0.2880484811,-0.4597662964,-0
.0534788314\C,-1.1195919774,1.7866789386,-1.0103820498\C,-1.0905855627
,-0.5245860732,-0.2971827194\C,0.9483525126,0.7513928671,-0.3009956783
\C,0.2540582831,1.8655542369,-0.7743477212\C,-1.7903961314,0.586104413
2,-0.7705196529\H,-1.6200682389,-1.458312279,-0.1176678897\H,2.0200715
394,0.8197228134,-0.1244544054\H,0.7871466544,2.7939559079,-0.96341656
96\H,-2.8589329171,0.5121970449,-0.9566034344\H,-1.66179203,2.65195421
19,-1.3824537452\H,0.0397436693,-1.7281641641,2.4442646225\H,1.6057495
532,-2.5620229734,2.4060158654\H,1.5382596746,-0.7891129313,2.44395462
31\\Version=IA64L-G03RevC.02\State=1-A\HF=-310.8802273\RMSD=9.779e-09\
RMSF=1.460e-05\Dipole=0.051142,-0.0816902,0.053388\PG=C01 [X(C8H10)]\\@
```

n.CH2_CH3_-C6H4CN

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C9H9N1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-C
6H4CN.freq\0,1\C,1.4078652696,-2.258715084,0.784541374\C,1.4301308562
,-2.2924826985,2.3243299785\H,2.4384139548,-2.2499963894,0.4087092176\
H,0.9453698204,-3.1801964198,0.4099131682\C,0.6614054352,-1.0612877522
,0.2385196271\C,-0.7431406989,1.1919171783,-0.7047786456\C,-0.71923204
37,-1.122405513,-0.0011450739\C,1.3251260138,0.1498855726,-0.006058169
4\C,0.6400010384,1.2674012108,-0.4713434349\C,-1.4208945096,-0.0152001
945,-0.4663868901\H,-1.2514720445,-2.0539380051,0.1758759684\H,2.39654
99168,0.216396734,0.1671220531\H,1.1658428028,2.1979166659,-0.66027835
83\H,-2.4886247024,-0.0764356064,-0.6515019976\C,-1.4571439024,2.33730
85345,-1.1878831731\N,-2.0368251571,3.2671867753,-1.5793583184\H,0.413
9721543,-2.3337714723,2.731818642\H,1.9775074153,-3.1705759847,2.68447
84385\H,1.915512031,-1.3982344738,2.7305975413\\Version=IA64L-G03RevC.
02\State=1-A\HF=-403.1246904\RMSD=6.341e-09\RMSF=1.604e-05\Dipole=1.00
27635,-1.6086177,0.7232293\PG=C01 [X(C9H9N1)]\\@
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n.CH2_CH3_-C6H4NO2

```
1\1\GINC-AC1\FOpt\RB3LYP\Gen\C8H9N1O2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
C6H4NO2.a3.freq\0,1\O,-2.4242693517,-0.2413429662,-2.330109627\N,-2.3
692892014,-0.079106965,-1.1106214934\C,-1.0464113195,-0.1271426202,-0.
4732874806\C,-0.951076908,0.0509157163,0.9057209437\C,0.306358113,0.00
02228435,1.4992250795\C,1.4633668618,-0.2242054826,0.7369988494\C,1.32
66086042,-0.4011406004,-0.648605049\C,0.0791256103,-0.3543829155,-1.26
31498018\C,2.8288978111,-0.235334816,1.387746966\C,3.4742634049,1.1627
222392,1.4328757934\O,-3.3464849286,0.1215168799,-0.3885840061\H,2.744
3672392,-0.6273258125,2.4086570763\H,3.4888043849,-0.920371976,0.84156
25755\H,2.2109206869,-0.5824676237,-1.2543688773\H,0.3921093458,0.1330
875431,2.5747847971\H,-1.8498801435,0.2199083738,1.4858854484\H,-0.036
```

8189887,-0.4933591849,-2.3309693363\H,2.8530937889,1.8649979435,1.9996
137465\H,4.4595759047,1.1178652179,1.9096366974\H,3.6020933675,1.57009
67787,0.4239455883\\Version=IA64L-G03RevC.02\State=1-A\HF=-515.3831906
\RMSD=3.054e-09\RMSF=9.194e-06\Dipole=1.8647339,-0.0208426,0.8896112\PG
G=C01 [X(C8H9N1O2)]\\@

n.CH2_CH3_-C6H4OCH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C9H12O1\CYL509\10-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
C6H4OCH3.a4.freq\0,1\C,-1.2898761987,-0.5071276226,-0.6231159193\C,-1
.2311819475,-0.1631929596,0.7351214455\C,0.0058827437,0.1351833147,1.3
151441941\C,1.1636243861,0.0880504122,0.5318616825\C,1.1262380397,-0.2
493841815,-0.8230845251\C,-0.1273403161,-0.5475154134,-1.382222692\C,2
.3819058003,-0.2566626958,-1.6697556436\O,-2.4274851601,-0.1538620418,
1.3982929942\C,-2.4252725814,0.1852218196,2.7742134525\H,2.3214421218,
-1.0651947225,-2.4100673178\C,2.6255113709,1.0758322254,-2.4009031973\
H,3.2495003793,-0.4826839778,-1.03671786\H,-0.1919444484,-0.8212750593
, -2.4334973491\H,2.119442156,0.3186743991,0.9983178743\H,0.0835050361,
0.3978579237,2.3642219486\H,-2.2567631955,-0.7430531828,-1.0571458526\
H,-1.8274009974,-0.5218529653,3.3652140524\H,-3.4666043929,0.133666592
6,3.0981597118\H,-2.0447245762,1.2021502656,2.9406637201\H,3.539220149
3,1.0321129245,-3.0054395846\H,1.7889859913,1.3171137179,-3.0666142297
\H,2.7282752761,1.900951025,-1.6869918513\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-425.402388\RMSD=5.707e-09\RMSF=1.793e-06\Dipole=0.1551399,
0.1340901,0.4295444\PG=C01 [X(C9H12O1)]\\@

n.CH2_CH3_-C6H4OH

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C8H10O1\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-
C6H4OH.a2.freq\0,1\C,-1.6144269488,0.362574826,-0.3534788249\C,-1.567
0720335,0.1561208039,1.0289298357\C,-0.3320017476,-0.0132775406,1.6606
756306\C,0.8432062626,0.0226132798,0.9090595463\C,0.8201586109,0.22517
05372,-0.4753538579\C,-0.4314044086,0.395166547,-1.0861270814\C,2.0960
347514,0.2214603286,-1.2915895667\O,-2.7571684062,0.13557423,1.7072746
729\C,2.4560310022,-1.169405863,-1.8441518668\H,2.9267996493,0.5889202
345,-0.6755154574\H,1.9984893393,0.9251095846,-2.1285082927\H,-0.48148
11542,0.5613306911,-2.1603814375\H,1.7973289886,-0.1065629107,1.415908
2646\H,-0.2873250631,-0.1674050302,2.7378439421\H,-2.5792176575,0.4998
766353,-0.8319297211\H,-2.5776354654,-0.0128213751,2.6485633153\H,3.38
20513219,-1.1327780681,-2.430096408\H,2.5961504405,-1.8900749181,-1.03
04407402\H,1.6590339185,-1.5527261974,-2.4914237372\\Version=IA64L-G03
RevC.02\State=1-A\HF=-386.0958875\RMSD=4.997e-09\RMSF=1.962e-06\Dipole
=0.3406201,-0.089283,0.3992035\PG=C01 [X(C8H10O1)]\\@

n.CH2_CH3_-CF2CF3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C4H5F5\CYL509\10-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-C
F2CF3.freq\0,1\F,-0.3646774066,0.1472046358,-1.5735821032\C,-0.381097
7266,0.1370476278,-0.2063602028\C,1.0906712442,0.1132977119,0.25395849
11\C,-1.2210144986,-1.0168678796,0.3088252631\F,-0.9019537729,1.332422
8433,0.2052250958\F,1.6885734853,-1.0187433956,-0.162032109\F,1.157024
9849,0.1535593035,1.5978706407\F,1.7673574893,1.1579009057,-0.23747822
21\C,-2.6697135933,-0.9396490151,-0.1806026682\H,-1.1759246197,-0.9969
465097,1.4026982695\H,-0.7453994205,-1.9462299996,-0.0214244424\H,-3.2
437506309,-1.7853392621,0.2096064562\H,-3.1486874975,-0.015988402,0.15
73335681\H,-2.7162334057,-0.9695651305,-1.2731688699\\Version=IA64L-G0
3RevC.02\State=1-A\HF=-654.650233\RMSD=2.394e-09\RMSF=1.234e-04\Dipole
=-0.5477224,-0.5856579,0.2247667\PG=C01 [X(C4H5F5)]\\@

n.CH2_CH3_-CF2H

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H6F2\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-C
F2H.freq\0,1\C,0.2859686228,-0.499011538,-0.538028637\C,0.2649646866,
-0.4640969898,0.976249301\H,1.3045022593,-0.5056143409,1.323607629\C,-
0.4434547574,0.7739171984,1.5321490743\H,0.7912446982,-1.3807247645,-0
.9495680654\F,0.9227309509,0.6125285224,-1.0291404383\F,-0.9944791132,
-0.4856929562,-1.0305142724\H,-0.2265855567,-1.3813802868,1.3226302426
\H,-1.4821346271,0.8126560135,1.1903347014\H,-0.4431297084,0.759812711
1,2.6265832389\H,0.0569650846,1.6888785475,1.2010862199\Version=IA64L
-G03RevC.02\State=1-A\HF=-317.6162587\RMSD=1.587e-09\RMSF=1.157e-04\Di
pole=0.242895,-0.4246359,0.5604056\PG=C01 [X(C3H6F2)]\@
```

n.CH2_CH3_-CF3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C3H5F3\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-C
F3.freq\0,1\F,0.1111595998,0.1757325056,-1.729290281\C,0.1317335775,0
.2071909178,-0.3779321488\F,1.4299406573,0.2201208047,0.0040492276\C,-
0.6159560394,-0.9674430388,0.2121376998\F,-0.4055857075,1.3888269344,0
.0047812784\H,-1.6375661359,-0.9283403626,-0.1804255336\C,-0.613872736
2,-0.9655500481,1.7420976105\H,-0.1487903929,-1.876450902,-0.181287490
2\H,-1.1648015506,-1.8307412687,2.1230104382\H,0.4075781652,-1.0120749
664,2.1320839642\H,-1.0874798435,-0.0597016887,2.1329376273\Version=I
A64L-G03RevC.02\State=1-A\HF=-416.8699002\RMSD=3.209e-09\RMSF=1.290e-0
4\Dipole=-0.3965599,-0.6230985,0.3725937\PG=C01 [X(C3H5F3)]\@
```

n.CH2_CH3_-CCl2H

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C3H6Cl2\CYL509\09-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
CCl2H.freq\0,1\C,0.6579800842,0.0003922015,-0.1448084467\C,0.60167177
9,0.0005623556,1.3795687434\H,1.68487251,0.0008174002,-0.5053100105\Cl
,-0.0997892285,1.4871293679,-0.8483830641\Cl,-0.0981959244,-1.48754776
53,-0.8478814923\H,1.1646696022,0.8824815517,1.710529348\C,-0.79499170
59,-0.0000856649,2.0017867119\H,1.1656052647,-0.880663481,1.7107657205
\H,-0.7134591499,0.0002002501,3.093563975\H,-1.3624494623,0.8864065812
,1.7036422475\H,-1.3614521098,-0.8873428998,1.7040241263\Version=IA64
L-G03RevC.02\State=1-A\HF=-1038.3298355\RMSD=7.338e-09\RMSF=2.842e-05\
Dipole=0.5262898,0.0006048,0.7357132\PG=C01 [X(C3H6Cl2)]\@
```

n.CH2_CH3_-CCl3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C3H5Cl3\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
CCl3.freq\0,1\C,0.1542268626,0.0001801478,-0.0089536761\C,0.093693506
6,-0.0001316789,1.5225548412\Cl,1.8861574038,0.001671488,-0.5311705938
\Cl,-0.6487313773,1.469222785,-0.6885539289\Cl,-0.6463020353,-1.470034
7305,-0.6889525422\H,0.6522129159,0.8821553154,1.8531954516\H,0.653895
2137,-0.8814598916,1.8528923706\C,-1.3106400341,-0.0016107057,2.128903
7351\H,-1.2260370806,-0.0014753779,3.2205447849\H,-1.8773808033,0.8855
031802,1.8328921688\H,-1.8754801074,-0.8899620274,1.8329559266\Versio
n=IA64L-G03RevC.02\State=1-A\HF=-1497.9126185\RMSD=5.426e-09\RMSF=5.44
3e-05\Dipole=-0.1252592,-0.0002059,0.8623556\PG=C01 [X(C3H5Cl3)]\@
```

n.CH2_CH3_-CH2Cl

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C3H7Cl1\CYL509\09-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-
CH2Cl.freq\0,1\H,0.2968422104,-1.00624253,-1.3068578989\C,0.287947132
4,-1.0522192757,-0.2116655529\H,1.3331208162,-1.0086588921,0.115977024
\C,-0.3591099497,-2.3622652188,0.2573739482\C,-0.4574719877,0.15882894
14,0.3332944404\Cl,0.2973051758,1.7228825441,-0.2133553461\H,-0.4485263
```

17,0.1821537204,1.4255858396\H,-1.494182514,0.184818502,-0.0106208371\H,-1.3991719004,-2.4398682818,-0.0811738244\H,0.1854224675,-3.224870502,-0.1408460271\H,-0.3558839207,-2.4424019477,1.3509598109\\Version=IA64L-G03RevC.02\State=1-A\HF=-578.740164\RMSD=9.113e-09\RMSF=2.641e-05\Dipole=-0.3011065,-0.8549879,0.2176578\PG=C01 [X(C3H7C11)]\\@

n.CH2_CH3_-CH2F

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H7F1\CYL509\09-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH2F.freq\0,1\C,0.0481306552,0.0000005887,-0.7216547059\C,0.0689633842,-0.0000007229,0.7980826369\F,1.3846634828,-0.0000003301,1.2554190582\H,-0.4328965864,-0.8901659439,1.2007715029\H,-0.4328976288,0.8901631833,1.2007730949\H,0.5981411651,-0.8804768041,-1.0764289863\H,0.598140438,0.880479032,-1.0764274924\C,-1.3762427037,0.0000004865,-1.284589274\H,-1.3645918312,0.0000012569,-2.379416422\H,-1.9364871617,-0.8853204551,-0.9595382095\H,-1.9364877537,0.8853205883,-0.959536953\\Version=IA64L-G03RevC.02\State=1-A\HF=-218.3703976\RMSD=8.768e-09\RMSF=9.009e-05\Dipole=-0.6127756,0.,-0.3301362\PG=C01 [X(C3H7F1)]\\@

n.CH2_CH3_-CH2OH

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H8O1\CYL509\09-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH2OH.freq\0,1\C,0.0379666061,0.,-0.738968982\C,0.0559864037,0.,0.784310756\O,1.4153657236,0.,1.2098518607\H,0.5915620489,0.8795829792,-1.0906667884\H,0.5915620489,-0.8795829792,-1.0906667884\C,-1.3809700787,0.,-1.3134026152\H,-0.4792456713,-0.887875037,1.1622871788\H,-0.4792456713,0.887875037,1.1622871788\H,1.4250079027,0.,2.1787480304\H,-1.3628055203,0.,-2.4086159601\H,-1.9438292565,-0.8852288458,-0.9919113449\H,-1.9438292565,0.8852288458,-0.9919113449\\Version=IA64L-G03RevC.02\State=1-A'\HF=-194.3475018\RMSD=8.219e-09\RMSF=9.306e-05\Dipole=-0.4516722,0.,0.3725396\PG=CS [SG(C3H2O1),X(H6)]\\@

n.CH2_CH3_-CH2Ph

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C9H12\CYL509\10-Apr-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH2Ph.freq\0,1\C,-1.523089257,0.0000033424,-1.7506799662\C,-1.5102374484,0.0000011791,-0.2084045448\C,-0.1130925631,-0.0000010708,0.3745451749\C,0.5583859042,-1.2026265163,0.6340800276\C,0.5583893543,1.202623609,0.6340785701\C,1.8609974044,-1.2058888515,1.1347101216\C,1.8610001616,1.2058834564,1.1347083741\C,2.5176867848,-0.0000037348,1.3866202977\H,3.5307878081,-0.0000043622,1.7800175797\H,2.3612454566,-2.1505891878,1.332592695\H,2.3612513072,2.1505823298,1.3325899388\H,0.0515796886,-2.1470207087,0.4453774135\H,0.0515846594,2.1470183535,0.4453743618\H,-2.0613555215,0.8796191462,0.1508637051\H,-2.0613574507,-0.8796165769,0.1508612885\H,-0.9704751312,-0.8774473576,-2.1120939378\H,-0.9704728518,0.8774536092,-2.1120915112\C,-2.9385635999,0.000006021,-2.3334095974\H,-2.9184044186,0.0000074076,-3.4292588451\H,-3.5016231959,-0.8847112789,-2.0108628576\H,-3.501620796,0.8847240184,-2.0108605756\\Version=IA64L-G03RevC.02\State=1-A\HF=-350.1942628\RMSD=3.736e-09\RMSF=7.671e-05\Dipole=-0.0897699,0.0000002,-0.0808344\PG=C01 [X(C9H12)]\\@

n.CH2_CH3_-CH_CH2_2

1\1\GINC-AC19\FOpt\RB3LYP\Gen\C5H10\CYL509\15-May-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\CH2CH3-CH_C H2_2.freq\0,1\C,-1.2329250336,0.6089493155,-0.7115463966\C,-1.5843634271,0.4141120348,0.7453534251\C,-0.138225574,0.4972703689,0.3234370584\H,-1.3809717038,-0.2322305103,-1.3852909946\H,-1.4272636035,1.5769410131,-1.1658121989\H,-1.969380471,-0.5565925998,1.0494509879\H,-2.0173714184,1.2497449108,1.2889097006\H,0.3715192524,1.4291216682,0.56942291

```
6\C,0.7556668177,-0.727634012,0.3672002009\H,0.1531514755,-1.618742097
9,0.1407324041\C,1.9359108965,-0.6455069024,-0.6087472825\H,2.56256215
76,-1.5431628358,-0.5540650283\H,2.5731148866,0.2191444026,-0.38588763
9\H,1.5849550348,-0.5397069776,-1.6418515091\H,1.1333023125,-0.8676618
023,1.390209329\\Version=IA64L-G03RevC.02\State=1-A\HF=-196.5259302\RM
SD=5.076e-09\RMSF=1.477e-05\Dipole=0.0289004,0.0079326,0.0165944\PG=C0
1 [X(C5H10)]\@
```

n.CH2_CH3_-CH2CH=CH2

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H10\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH
2CH=CH2.freq\\0,1\H,0.4508009961,-1.0378034657,-1.2209868293\C,0.45021
61034,-1.0860038069,-0.1241466315\H,1.504093759,-1.0394527646,0.184371
5053\C,-0.1614795505,-2.4118588084,0.3387893158\C,-0.2944361203,0.1438
839844,0.4298026831\C,0.3311227156,1.4474575318,0.0144640646\H,-0.3055
455474,0.0778868044,1.5292231806\H,-1.3434727134,0.1167082342,0.105515
3843\H,1.3654523559,1.59788706,0.3308448015\C,-0.2676122966,2.39675783
45,-0.7057282874\H,0.242361991,3.3162269644,-0.981107627\H,-1.29631669
08,2.2919590819,-1.0458878448\H,-1.2065116613,-2.5002240483,0.01726096
54\H,0.386250366,-3.2681236271,-0.0707563079\H,-0.143977965,-2.4964846
518,1.432435905\\Version=IA64L-G03RevC.02\State=1-A\HF=-196.5349731\RM
SD=2.740e-09\RMSF=1.866e-05\Dipole=0.0356424,-0.127888,0.0470426\PG=C0
1 [X(C5H10)]\@
```

n.CH2_CH3_-CH2CH3

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10\CYL509\09-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH
2CH3.freq\\0,1\H,0.7723895691,-1.2319785775,-2.4211906382\C,0.77235906
75,-1.2296109813,-1.325124943\H,1.8177449287,-1.2289435107,-0.99224769
88\H,0.3206262736,-2.1716423121,-0.9902431513\C,0.0127640502,-0.022083
5332,-0.7666447046\H,0.4662066245,0.9047046479,-1.1466407657\C,-0.0128
628717,0.0223715532,0.7667422496\H,-1.0198104678,-0.031145653,-1.14433
96827\H,1.0197127936,0.0315921143,1.144394534\H,-0.4662701444,-0.90443
28306,1.1467100223\C,-0.7721895593,1.2292216867,1.3250043788\H,-0.7724
623731,1.2323144074,2.4211911579\H,-0.3207959462,2.1715312147,0.990108
8402\H,-1.8177653787,1.2286081474,0.9923954974\\Version=IA64L-G03RevC.
02\State=1-A\HF=-158.4580426\RMSD=4.293e-09\RMSF=9.697e-05\Dipole=0.00
00146,-0.000019,0.0000016\PG=C01 [X(C4H10)]\@
```

n.CH2_CH3_-CH_CH3_2

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H12\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-CH
_CH3_2.freq\\0,1\C,0.6203614005,-1.5543566596,-0.1829475038\H,0.573302
3361,-1.6377390008,0.9095969067\H,1.6786149561,-1.5263003953,-0.470454
9678\H,0.1855451079,-2.4711070422,-0.5988508281\C,-0.1299672739,-0.312
8655001,-0.6893873065\C,-1.6152347063,-0.3680143599,-0.2998832811\H,-0
.0818805371,-0.3306158266,-1.7888058668\C,0.5474560547,1.0066817618,-0
.2533299015\H,0.0211789669,1.8417924966,-0.7369724577\H,1.5702017369,1
.0197886458,-0.6559550648\C,0.6067903448,1.2673920529,1.2573747416\H,-
2.1583175047,0.5098068167,-0.6711506359\H,-1.7469072613,-0.406495749,0
.7882353781\H,-2.0966310878,-1.2600465857,-0.7182231609\H,1.1030855183
,2.2228962925,1.4629597595\H,-0.3930367028,1.3167968188,1.7034958141\H
,1.1684095526,0.4881997581,1.785164631\\Version=IA64L-G03RevC.02\State
=1-A\HF=-197.7696866\RMSD=5.943e-09\RMSF=5.205e-05\Dipole=0.0063841,0.
0088775,-0.0319877\PG=C01 [X(C5H12)]\@
```

n.CH2_CH3_-C_CH3_3

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C6H14\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_-C_
```

```
CH3_3.freq\0,1\C,-0.1146031711,0.1985337343,-1.1826771303\C,-0.116012
7359,0.2009159667,0.3697386853\C,1.3236499121,0.2248200931,0.919155048
4\C,-0.856503545,-1.0339639044,0.9191050956\H,0.3612418109,1.129053250
9,-1.5246880075\H,-1.158370248,0.2516600674,-1.5247213371\C,0.56986828
55,-0.9869174583,-1.8744208205\C,-0.8497427734,1.4716823655,0.84214690
15\H,-1.8814374393,-1.0866784816,0.530436942\H,-0.9177681396,-0.995150
8451,2.0137132824\H,-0.3481616068,-1.9673194461,0.6524213508\H,-0.3496
308459,2.3775029266,0.4770553239\H,-0.881215732,1.5261509733,1.9373765
588\H,-1.8842517339,1.4914372461,0.4770226388\H,1.881745202,1.08610932
54,0.5305140209\H,1.8778386557,-0.6820679793,0.6524844503\H,1.32062651
57,0.2972749144,2.0137637296\H,0.5077684536,-0.8793226552,-2.963657659
9\H,1.6321946278,-1.0570578835,-1.6149873493\H,0.0994846467,-1.9420161
937,-1.6150206239\Version=IA64L-G03RevC.02\State=1-A\HF=-237.0836713\
RMSD=4.634e-09\RMSF=5.634e-05\Dipole=0.0012003,-0.0020779,-0.0159531\PG=C01
[X(C6H14)]\@
```

n.CH2_CH3_-CCH

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H6\CYL509\09-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-CCH
.freq\0,1\C,0.4401089598,-0.7145622283,-0.1234562805\C,0.4594563388,-
0.734460862,1.4166621703\H,1.4706367443,-0.717132341,-0.504044811\H,-0
.0225645143,-1.6381973195,-0.4971874823\C,-0.2743747679,0.4397023191,-
0.6723523172\C,-0.8672916184,1.3982279451,-1.1064773672\H,-0.557964992
,-0.7682185631,1.8186196329\H,1.0032498566,-1.6138271024,1.7782049303\
H,0.9492955192,0.1610110947,1.8116868154\H,-1.3900460874,2.2429211884,
-1.4935363181\Version=IA64L-G03RevC.02\State=1-A\HF=-155.9668791\RMSD
=2.984e-09\RMSF=1.768e-05\Dipole=0.1224011,-0.1974998,0.1306433\PG=C01
[X(C4H6)]\@
```

n.CH2_CH3_-CH=C_CH3_2

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C6H12\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-CH
=C_CH3_2.a2.freq\0,1\H,-2.1102138988,-0.5441839309,-2.0183406941\C,-2
.1161494849,-0.5597471117,-0.9190607579\C,-0.7098662251,-0.575539966,-
0.3664905871\C,-0.2833834545,0.3998584821,0.4507304056\C,0.1190508415,
-1.7561164472,-0.811814237\C,1.0671988632,0.5745294864,1.0931037423\C,
1.7589715947,1.8798710798,0.6608201645\H,1.7243358956,-0.2742719445,0.
8757270618\H,0.942805528,0.5906985897,2.1866510479\H,-0.9934676108,1.1
961204232,0.685939493\H,-2.6681976374,-1.4641769295,-0.6258072176\H,-2
.6825547335,0.3099547771,-0.5711593633\H,0.183940021,-1.7916348991,-1.
9083823025\H,-0.3507089328,-2.6996787875,-0.5000590763\H,1.1375979501,
-1.7448200829,-0.4172330434\H,1.1329943865,2.7519066026,0.8856023811\H
,2.7150081162,2.0114710178,1.1808413739\H,1.9535281064,1.8814820244,-0
.4175120427\Version=IA64L-G03RevC.02\State=1-A\HF=-235.8569096\RMSD=3
.683e-09\RMSF=1.577e-05\Dipole=0.0153235,-0.0783738,-0.0385024\PG=C01
[X(C6H12)]\@
```

n.CH2_CH3_-CH=CH2

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C4H8\CYL509\09-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-CH=
CH2.freq\0,1\C,0.4832596032,-0.7693558922,-0.3312686484\C,0.538771158
4,-0.8519269957,1.1954385255\H,1.5071742024,-0.7603774292,-0.735988710
2\H,0.0311098864,-1.6895386917,-0.7326076005\C,-0.2618327178,0.4122782
585,-0.8991463417\C,-0.8684076791,1.3800274921,-0.2102337557\H,-0.2910
934814,0.4532890728,-1.9894315083\H,-0.8793904522,1.4027024639,0.87624
63043\H,-1.3823699188,2.1946123957,-0.7133952687\H,-0.466158334,-0.916
0145702,1.6279192793\H,1.0977050017,-1.7383144281,1.5140274335\H,1.032
2809075,0.0275040108,1.6244913929\Version=IA64L-G03RevC.02\State=1-A\
HF=-157.2203613\RMSD=4.080e-09\RMSF=5.559e-06\Dipole=0.0851128,-0.1354
```

265,-0.0279829\PG=C01 [X(C4H8)]\@

n.CH2_CH3_-CH=CHCH3

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H10\CYL509\10-Apr-2008\0\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-CH
=CHCH3.a2.freq\0,1\H,-2.0825936006,-0.1841694383,-2.3687059784\C,-1.9
879180126,-0.7291535376,-1.4194056191\C,-0.5874062927,-0.6503559829,-0
.8813043588\C,-0.2428762637,-0.1420923454,0.3048418373\C,1.1601692251,
-0.0534003781,0.8422101976\C,1.6035692193,1.393284762,1.1197658197\H,1
.8555819157,-0.5253387245,0.1360829701\H,1.2307727588,-0.6279166721,1.
7783771725\H,-1.0266297249,0.2605910778,0.9517021668\H,0.1976150599,-1
.048995034,-1.5275910285\H,-2.713568919,-0.3085678166,-0.7147195181\H,
-2.2793898415,-1.7682599399,-1.6254717411\H,0.9310080888,1.8827874505,
1.8346670117\H,2.6156060239,1.4226341295,1.5398294118\H,1.5983709861,1
.9875398591,0.1991822733\Version=IA64L-G03RevC.02\State=1-A\HF=-196.5
404397\RMSD=5.103e-09\RMSF=9.742e-06\Dipole=-0.0045348,-0.007763,-0.01
39564\PG=C01 [X(C5H10)]\@

n.CH2_CH3_-CHO

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H6O1\CYL509\09-Apr-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-C
HO.freq\0,1\C,0.4453009371,-0.7408691814,-0.3041183126\C,0.4737058402
, -0.7825750503,1.2218482365\H,1.4609539903,-0.7393546233,-0.7302790611
\H,-0.0336570253,-1.6381448078,-0.7268756653\C,-0.2780458602,0.4594202
251,-0.8716818254\O,-0.8003407951,1.3282300699,-0.208511726\H,-0.30643
32567,0.5041683027,-1.9849827817\H,-0.541155104,-0.803346464,1.6303005
25\H,1.0077731138,-1.6697249768,1.5766169906\H,0.9694791407,0.10470604
92,1.6270252097\Version=IA64L-G03RevC.02\State=1-A\HF=-193.1453441\RM
SD=7.651e-09\RMSF=1.369e-05\Dipole=0.4838393,-0.8045044,-0.3493346\PG=
C01 [X(C3H6O1)]\@

n.CH2_CH3_-CN

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H5N1\CYL509\10-Apr-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-C
N.freq\0,1\C,0.4091145447,-0.687895571,-0.1421961368\C,0.4231727212,-
0.7069392482,1.3972290749\H,1.4332818542,-0.6899808343,-0.5346976856\H
, -0.0785886043,-1.5896459857,-0.53203177\C,-0.2884119992,0.4826657245,
-0.685457042\N,-0.8436504527,1.4143485849,-1.0991851245\H,-0.594421678
6,-0.7280351393,1.7978915098\H,0.9527076714,-1.5970939632,1.7505106722
\H,0.9293223262,0.1773303969,1.795167768\Version=IA64L-G03RevC.02\Sta
te=1-A\HF=-172.0686675\RMSD=1.255e-09\RMSF=1.193e-05\Dipole=0.7166194,
-1.2022712,0.6379213\PG=C01 [X(C3H5N1)]\@

n.CH2_CH3_-COCH3

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C4H8O1\CYL509\10-Apr-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3_-C
OCH3.freq\0,1\C,0.167654534,-0.0000203035,-1.0085830885\C,0.197579040
9,-0.0000188704,0.5172167209\C,1.5711092666,-0.0000444463,1.1700405238
\O,-0.8229113982,-0.0000058086,1.179178223\C,-1.2429483529,0.000083470
2,-1.5920218648\H,0.7402413045,-0.8726079352,-1.3570272984\H,0.7403833
736,0.8724660887,-1.3570445649\H,2.1459815298,0.8810755138,0.858396890
4\H,1.4644397141,-0.0001031607,2.2566891105\H,2.1460050028,-0.88111417
39,0.8582991399\H,-1.2096821489,0.0000754852,-2.6867209863\H,-1.802288
5727,-0.88075119,-1.2629607359\H,-1.8021559488,0.8810067415,-1.2629710
876\Version=IA64L-G03RevC.02\State=1-A\HF=-232.4705552\RMSD=3.480e-09
\RMSF=1.091e-04\Dipole=0.8804619,-0.0000136,-0.5871793\PG=C01 [X(C4H8O
1)]\@

n.CH2_CH3_-CON_CH2CH3_2

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C7H15N1O1\CYL509\10-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3
-CON_CH2CH3_2.freq\0,1\C,0.8296836193,-1.1877035601,1.289278209\C,0.
8960000931,-1.2676600508,2.8144447719\H,1.84614537,-1.1848005145,0.870
1383456\H,0.3399329396,-2.0811943314,0.88138519\C,0.0974244276,0.07318
13885,0.816028304\O,-0.2375832956,0.946833557,1.6132198469\N,-0.166299
1312,0.1957477146,-0.5277612875\C,0.2185060505,-0.7797436794,-1.546805
3545\C,-0.8663190755,1.4043162967,-0.9788049972\H,0.5345792218,-0.2234
215616,-2.438161736\C,-0.9026289545,-1.7581510577,-1.9187392726\H,1.09
8834317,-1.330841665,-1.2080252124\H,-1.5723956118,1.6898391524,-0.196
3096174\H,-1.4419060709,1.1429704624,-1.8742311424\C,0.0828377058,2.56
96478348,-1.2713028638\H,-1.2022148561,-2.3604776706,-1.0543529109\H,-
0.570233389,-2.4377181784,-2.7122452383\H,-1.7894610357,-1.2259305431,
-2.2796769336\H,0.6165722816,2.853938226,-0.3599505878\H,-0.4793939446
,3.4407877453,-1.6277894018\H,0.8195913953,2.3060889802,-2.0395977298\
H,-0.1073780905,-1.3038488254,3.2486942219\H,1.4425445132,-2.164702589
1,3.125391883\H,1.3965200459,-0.388914177,3.2287083266\Version=IA64L-
G03RevC.02\State=1-A\HF=-405.7759178\RMSD=6.139e-09\RMSF=9.516e-06\Dip
ole=0.2155888,-0.7379116,-1.1662257\PG=C01 [X(C7H15N1O1)]\@
```

n.CH2_CH3_-CON_CH3_2

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H11N1O1\CYL509\10-Apr-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3
-CON_CH3_2.freq\0,1\H,-1.8688436208,0.7298809791,-2.2519902767\C,-1.
8777527781,0.7247269487,-1.1534807959\N,-0.5196786022,0.7048776049,-0.
6312908957\H,-2.3955666668,-0.1645386791,-0.7972194887\H,-2.4100191035
,1.6224673177,-0.8105787012\C,-0.1250307264,-0.3462286919,0.167679607\
O,-0.8908876635,-1.2636933425,0.4478468412\C,1.3127947513,-0.335300673
5,0.7003720793\C,1.6047189781,-1.5596320041,1.5675933832\H,1.481138881
9,0.5840595946,1.2773347321\H,2.0143634722,-0.2954424616,-0.1438235502
\C,0.3087614366,1.8319557918,-1.0181684785\H,0.4023361766,1.885730783,
-2.1122106822\H,1.3087329036,1.7552229955,-0.5952267503\H,-0.137474390
5,2.7760287469,-0.6744030723\H,2.6364429689,-1.5274763693,1.9347931268
\H,0.9288423651,-1.6005171554,2.4259047287\H,1.4639485676,-2.483140471
4,0.9997067032\Version=IA64L-G03RevC.02\State=1-A\HF=-327.1443276\RMS
D=9.646e-09\RMSF=4.877e-05\Dipole=0.5823766,1.1527845,-0.4949728\PG=C0
1 [X(C5H11N1O1)]\@
```

n.CH2_CH3_-CONH2

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H7N1O1\CYL509\10-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3
-CONH2.a3.freq\0,1\C,0.1576045305,-0.2713711924,-0.9723518395\C,0.095
0435862,-0.1530894414,0.5514763153\N,1.1746082632,-0.6745985656,1.2165
512799\O,-0.8422967307,0.3626718424,1.1419994022\H,-0.1928423995,-1.28
03388633,-1.2348344337\C,-0.7056102675,0.7794541141,-1.6703124866\H,1.
2007215355,-0.2119344924,-1.3094782133\H,1.117400796,-0.7429405687,2.2
232855839\H,1.8828402598,-1.2156212639,0.7435727044\H,-0.7193911641,0.
6138876496,-2.7526397947\H,-1.7301608178,0.739127633,-1.2922303267\H,-
0.3246793021,1.7886742439,-1.4824016323\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-248.5268516\RMSD=6.622e-09\RMSF=1.553e-05\Dipole=1.0998209,-
0.8067429,-0.3734435\PG=C01 [X(C3H7N1O1)]\@
```

n.CH2_CH3_-CONHCH3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H9N1O1\CYL509\10-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3
-CONHCH3.freq\0,1\C,0.2015479289,-0.0000129394,0.5229222518\O,0.22471
97064,-0.0001125768,1.7485558875\C,1.5073584996,0.0000001643,-0.278246
7354\H,2.0714809183,0.8722377336,0.0729906586\C,1.4298821525,0.0002791
05,-1.8081790164\H,2.0713314679,-0.872463883,0.0726762593\N,-0.9613040
```

279,0.0000161912,-0.1964440583\H,-0.9140749648,-0.0000706689,-1.203622
4413\C,-2.2677123493,-0.0001602475,0.435989448\H,-2.1037400666,0.00010
47979,1.5144076006\H,-2.8437026186,-0.8917863538,0.1598390908\H,-2.844
0957377,0.8910831448,0.1594402721\H,2.4364848697,0.0002980494,-2.23916
20317\H,0.9155712318,-0.8891322828,-2.1925766941\H,0.9156580545,0.8898
802441,-2.192247094\\Version=IA64L-G03RevC.02\State=1-A\HF=-287.835915
3\RMSD=1.997e-09\RMSF=2.935e-05\Dipole=-0.3104207,-0.0000267,-1.423174
6\PG=C01 [X(C4H9N1O1)]\\@

n.CH2_CH3-COOC_CH3_3

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C7H14O2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_
COOC_CH3_3.freq\0,1\C,0.9807322736,-1.6332985527,1.3585456061\C,1.027
8193381,-1.7021008218,2.8834798193\H,1.9897603373,-1.622204169,0.92666
50997\H,0.4916106938,-2.5189948431,0.9328396324\C,0.2436397861,-0.4062
771672,0.8440528069\O,-0.2640751293,0.4372967862,1.5543665768\O,0.2412
315398,-0.4011436911,-0.5051551453\C,-0.406070202,0.6747576252,-1.2795
085596\C,-1.9090007424,0.7040161948,-0.981429828\C,-0.1477080318,0.245
778617,-2.7261534346\C,0.2718718979,2.016350065,-0.9811070053\H,-0.584
9467771,0.9725794922,-3.4189755849\H,-0.5937151124,-0.7342728103,-2.92
4375212\H,0.9271450146,0.1809019792,-2.9241324343\H,-2.4012453251,1.42
04507153,-1.6488996039\H,-2.1013566437,0.9982919959,0.0514579144\H,-2.
3514247987,-0.2826470508,-1.1580449855\H,-0.1304087709,2.7868696978,-1.
.6486193138\H,1.3508890326,1.9451675357,-1.1574290859\H,0.1016804082,2
.3240221571,0.0517637162\H,0.0193300443,-1.7295328364,3.3066914546\H,1
.5646408301,-2.5991876692,3.2092616721\H,1.5330838655,-0.8260247166,3.
30082885\\Version=IA64L-G03RevC.02\State=1-A\HF=-425.6536813\RMSD=5.09
2e-09\RMSF=9.756e-06\Dipole=0.1575718,-0.2626973,-0.6289246\PG=C01 [X(
C7H14O2)]\\@

n.CH2_CH3-COOCH2CH3

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C5H10O2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_
COOCH2CH3.freq\0,1\C,0.7699555172,-1.2848206607,1.0507942092\C,0.8141
089438,-1.3473801523,2.57631333\H,1.7797673459,-1.2758339316,0.6204962
115\H,0.2806581537,-2.1717027275,0.6275569458\C,0.0360207542,-0.061577
5839,0.5333549775\O,-0.4786108986,0.7946725272,1.2202596826\O,0.024997
8318,-0.0423215631,-0.8193193507\C,-0.650000167,1.0808858732,-1.430119
6791\H,-0.1767202356,2.0068522072,-1.0873646638\H,-1.6899532336,1.0972
085323,-1.087881305\C,-0.547676008,0.9115210267,-2.9344290418\H,-1.048
8347278,1.7455113356,-3.4378744985\H,-1.0225365826,-0.0208530879,-3.25
65450287\H,0.4986657144,0.8935822291,-3.2560185358\H,-0.195368087,-1.3
721703911,2.997260043\H,1.3495279279,-2.2433874208,2.9068148102\H,1.31
92440185,-0.469785476,2.9905505912\\Version=IA64L-G03RevC.02\State=1-A
\HF=-347.0221323\RMSD=3.436e-09\RMSF=2.147e-05\Dipole=0.1966595,-0.328
2237,-0.6127051\PG=C01 [X(C5H10O2)]\\@

n.CH2_CH3-COOCH3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H8O2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2_CH3_
OOCH3.freq\0,1\C,-0.0492538951,0.0001321411,0.0900329598\O,-0.0631613
563,0.0000977747,1.3017728063\C,1.1916869417,0.0000277889,-0.782194161
5\C,2.4852453694,-0.0006727202,0.0298646115\H,1.1344425096,0.873547246
8,-1.4444594786\H,1.1338802399,-0.8729282316,-1.4451432481\O,-1.171160
3215,0.0001935981,-0.6680712199\C,-2.4072971036,0.0002891664,0.0633587
202\H,-2.4813811919,-0.8887141423,0.6956752647\H,-3.1946997926,-0.0000
049175,-0.691183366\H,-2.4815546715,0.889668938,0.695132633\H,3.354364
2636,-0.000688752,-0.6360185504\H,2.5438808809,0.8807158542,0.67533786
23\H,2.5433533103,-0.8825852354,0.6746734117\\Version=IA64L-G03RevC.02

\State=1-A\HF=-307.7031867\RMSD=2.705e-09\RMSF=7.263e-06\Dipole=-0.214
8922,0.0000564,-0.6136348\PG=C01 [X(C4H8O2)]\@

n.CH2_CH3-COOH

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C3H6O2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3-C
OOH.freq\0,1\C,-0.2076356425,-0.0000352967,-0.9928701109\C,-0.2386603
934,-0.0001625061,0.5207171374\O,0.7238404353,0.0000142942,1.255494984
\O,-1.512929196,0.0003598581,0.9916701928\C,1.2110558384,-0.0002676375
, -1.5566621222\H,-0.7772134694,0.8733719076,-1.3359653262\H,-0.7775725
313,-0.8731494521,-1.3361028427\H,-1.4396493257,0.0005608695,1.9646980
816\H,1.1870698826,-0.0001706291,-2.6512441288\H,1.7659337504,0.881519
3275,-1.2228331677\H,1.7655829644,-0.8823325996,-1.2229834563\Version
=IA64L-G03RevC.02\State=1-A\HF=-268.3966249\RMSD=6.997e-09\RMSF=8.982e
-05\Dipole=-0.475046,0.0000226,-0.3183116\PG=C01 [X(C3H6O2)]\@

n.CH2_CH3-COPh

1\1\GINC-AC12\FOpt\RB3LYP\Gen\C9H10O1\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2_CH3-C
OPh.freq\0,1\C,-2.7241076675,0.0002955199,0.0329042305\C,-2.71190491
74,0.0003228066,1.4310630725\C,-1.4962889947,0.0002086888,2.1174164871
\C,-0.2944566806,0.0000663914,1.4094552737\C,-0.29656725,0.0000385568,
0.0061635302\C,-1.5252731785,0.000155305,-0.673230219\C,0.962336529,-0
.0001094263,-0.8127754955\O,0.9064733632,-0.0001072025,-2.0336881313\C
,2.3098163003,-0.0002651729,-0.0955401702\C,3.497439919,-0.0004380371,
-1.056277446\H,2.3480892227,-0.8746301152,0.5698314619\H,2.3483094963,
0.874127115,0.5697839494\H,-1.5098708857,0.0001335303,-1.7582481124\H,
0.6427134455,-0.0000216443,1.957176957\H,-1.4835849855,0.00023057,3.20
3942605\H,-3.6694505495,0.0003838626,-0.5030087014\H,-3.6477302417,0.0
004327518,1.9837567331\H,4.4404125009,-0.0005460531,-0.4995178422\H,3.
4765683802,-0.8811347272,-1.704624025\H,3.4767923544,0.8802345375,-1.7
046635548\Version=IA64L-G03RevC.02\State=1-A\HF=-424.2103229\RMSD=3.1
62e-09\RMSF=9.781e-06\Dipole=-0.2013849,0.0000277,1.1023307\PG=C01 [X(
C9H10O1)]\@

n.CH_CH3_2-H

1\1\GINC-AC14\FOpt\RB3LYP\Gen\C3H8\CYL509\10-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-H.f
req\0,1\C,0.0549349818,-0.0998897313,0.5754052281\H,-0.2749521894,0.5
546499635,1.3935393296\C,1.1126349724,0.6266470226,-0.262527963\C,-1.1
613403438,-0.538087171,-0.2476156282\H,1.9711031015,0.9292811241,0.348
2952306\H,0.6977652576,1.53058014,-0.7257305213\H,1.4873458244,-0.0153
630848,-1.0694872994\H,-0.8676856971,-1.2216131263,-1.0540448855\H,-1.
6572655182,0.3243286384,-0.710288432\H,-1.9021745071,-1.0546173281,0.3
736900502\H,0.5084860665,-0.9792670486,1.0524567067\Version=IA64L-G03
RevC.02\State=1-A\HF=-119.1442425\RMSD=5.791e-09\RMSF=1.085e-04\Dipol
e=0.002052,-0.0037313,0.0214936\PG=CS [SG(C3H2),X(H6)]\@

n.CH_CH3_2-BH2

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C3H9B1\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-B
H2.a2.freq\0,1\H,-1.071787612,0.6138098638,-2.2051056267\B,-1.0485511
741,0.0215275957,-1.1631035327\C,0.2620490962,-0.0591084291,-0.3110298
739\H,-2.0783479526,-0.4319003052,-0.74583101\C,0.3689146271,-1.268287
0226,0.6317124532\C,0.2503763901,1.2715527751,0.5021190672\H,-0.497552
9973,-1.3222347968,1.3024477062\H,1.2713419612,-1.2141335294,1.2552106
788\H,0.4101003708,-2.2114019135,0.0739541829\H,-0.6178799797,1.329787
2682,1.1704389112\H,0.2390309017,2.1559269123,-0.1453543272\H,1.148578
9596,1.3301647693,1.1297641882\H,1.1512315381,-0.0226001877,-0.9568169

189\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-144.5689627\\RMSD=4.332e-09
\\RMSF=1.344e-05\\Dipole=0.2299368,0.0494253,0.1502651\\PG=C01 [X(C3H9B1)
J]\\@

n.CH_CH3_2-CH3

1\\1\\GINC-AC30\\FOpt\\RB3LYP\\Gen\\C4H10\\CYL509\\10-Apr-2008\\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CH
3.freq\\0,1\\H,0.4021886146,-0.9145513797,-1.9617201276\\C,0.355956968,-
1.1129078967,-0.8840683224\\H,1.3857119116,-1.2406545023,-0.5248773453\\
H,-0.166582699,-2.0664481368,-0.7408059015\\C,-0.3468475506,0.028329186
3,-0.1347917173\\C,0.3621226642,1.368420963,-0.3783072093\\C,-0.45041390
1,-0.2773787059,1.3663994249\\H,1.3921492138,1.3404296228,0.0011550503\\
H,-0.1559474993,2.1922775717,0.1273409657\\H,0.4083691145,1.6075404234,
-1.4476498513\\H,0.5469583366,-0.3715608938,1.8159728166\\H,-0.986247420
4,-1.2171414132,1.5467831834\\H,-0.9818102925,0.5194350285,1.9007325986
\\H,-1.3696983628,0.111892399,-0.5323244445\\Version=IA64L-G03RevC.02\\S
tate=1-A\\HF=-158.4588091\\RMSD=6.787e-09\\RMSF=6.250e-05\\Dipole=-0.03120
83,0.0025483,-0.0121211\\PG=C01 [X(C4H10)]\\@

n.CH_CH3_2-NH2

1\\1\\GINC-AC28\\FOpt\\RB3LYP\\Gen\\C3H9N1\\CYL509\\11-Apr-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-N
H2.freq\\0,1\\H,-1.701608715,0.4418796997,-1.0902989755\\N,-0.6954166721
,0.6044824741,-1.0536226032\\C,-0.0773764794,-0.3397090331,-0.108373142
7\\H,-0.3479721557,0.4221966382,-1.9950295746\\C,-0.6655666006,-0.097017
4426,1.2836553873\\C,1.4383840337,-0.1272013373,-0.1225233583\\H,-0.2244
851232,-0.7782928942,2.0199821687\\H,-1.7511866191,-0.258100509,1.28865
54734\\H,-0.4761951525,0.9348529519,1.5998856106\\H,1.6783852227,0.90391
33371,0.159949167\\H,1.8546543886,-0.3096258071,-1.1214904078\\H,1.93671
05317,-0.8092568833,0.5755694065\\H,-0.2730313949,-1.3953769746,-0.3784
179636\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-174.4872755\\RMSD=4.688e
-09\\RMSF=2.625e-05\\Dipole=-0.140712,-0.4727835,-0.200166\\PG=C01 [X(C3H
9N1)]\\@

n.CH_CH3_2-OH

1\\1\\GINC-AC23\\FOpt\\RB3LYP\\Gen\\C3H8O1\\CYL509\\18-May-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-O
H.a2.freq\\0,1\\C,-0.179683907,0.3156294651,-0.0847226567\\O,-0.16869639
41,0.4172531446,1.3421492166\\C,1.2427274034,0.3326492361,-0.6491209999
\\C,-0.9810130703,-0.9044265853,-0.5441553277\\H,0.2863054466,-0.3709535
376,1.6812032943\\H,-1.0746889071,-0.9337060842,-1.6361893961\\H,-1.9850
417035,-0.88655672,-0.1085898911\\H,-0.4872916937,-1.8340218398,-0.2283
324622\\H,1.7856281903,1.2110093736,-0.2860332813\\H,1.2382896613,0.3533
157383,-1.7453249701\\H,1.7947142976,-0.5646394735,-0.3362914085\\H,-0.7
005266956,1.2244146918,-0.4096417114\\Version=IA64L-G03RevC.02\\State=1
-A\\HF=-194.353442\\RMSD=3.683e-09\\RMSF=1.441e-05\\Dipole=0.2455106,-0.47
06197,-0.3496282\\PG=C01 [X(C3H8O1)]\\@

n.CH_CH3_2-F

1\\1\\GINC-AC29\\FOpt\\RB3LYP\\Gen\\C3H7F1\\CYL509\\10-Apr-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-F
.freq\\0,1\\C,-0.4170148571,-0.0529760891,-1.3679935586\\C,-0.2923056213
, -0.1801683467,0.1422105423\\C,1.0109872064,-0.8116065708,0.6060642588\\
F,-0.3712324237,1.1086447732,0.6945958495\\H,0.4199701176,0.5276294657,
-1.7715360104\\H,-1.3494280809,0.4557917455,-1.6321837536\\H,-0.41454205
06,-1.0407602563,-1.8423175701\\H,1.8663342278,-0.2407559937,0.22790521
45\\H,1.0939208182,-1.842135865,0.2429687614\\H,1.0605947917,-0.82454018
97,1.6994111376\\H,-1.145758382,-0.744525824,0.542702116\\Version=IA64L
-G03RevC.02\\State=1-A\\HF=-218.3780005\\RMSD=2.723e-09\\RMSF=2.765e-05\\Di

pole=0.0780695,-0.6001311,-0.2871046\PG=C01 [X(C3H7F1)]\@

n.CH_CH3_2-SiH3

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C3H10Si1\CYL509\11-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
SiH3.freq\0,1\H,-1.3336093663,-0.0187999131,-1.7389700999\Si,-1.37260
25649,0.0125949472,-0.2485766768\C,0.3919152028,0.0045200752,0.4625619
493\H,-2.1095369871,1.2388323026,0.1701159807\H,-2.1407568028,-1.17578
90072,0.2201627207\C,1.146375431,-1.2851491915,0.0887910515\C,1.179252
8484,1.2576682216,0.0360869899\H,2.1833664458,1.2582383586,0.480963655
5\H,0.6794849606,2.1826687771,0.3462691082\H,1.3064053268,1.2975721518
, -1.05320464\H,2.1503770808,-1.2932379807,0.5338471687\H,1.271870664,-
1.373419395,-0.9978439605\H,0.6230353289,-2.1832801739,0.4367605722\H,
0.2805383645,0.0286510504,1.5573330247\Version=IA64L-G03RevC.02\State
=1-A\HF=-409.8323853\RMSD=3.802e-09\RMSF=7.824e-06\Dipole=0.3102757,-0
.0009616,0.1471594\PG=C01 [X(C3H10Si1)]\@

n.CH_CH3_2-PH2

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C3H9P1\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-PH
2.freq\0,1\H,-2.1087715801,-0.703624878,0.11528549\P,-1.284354609,0.4
487863591,0.2813700184\H,-1.3713762213,0.4101072573,1.7048271755\C,0.3
884536862,-0.4220377195,0.115500603\C,1.5045236613,0.5154210623,0.5984
321928\C,0.6031501841,-0.8459769075,-1.3445833147\H,1.5763109434,-1.33
95413777,-1.4614045185\H,0.5868394432,0.0212899926,-2.0160280604\H,-0.
1681484727,-1.5473580858,-1.6829417706\H,2.4837694608,0.031047167,0.49
4728108\H,1.379049891,0.7894677382,1.6522245742\H,1.527013651,1.441290
8826,0.0106267616\H,0.3838668266,-1.3189127011,0.746035069\Version=IA
64L-G03RevC.02\State=1-A\HF=-461.0835012\RMSD=8.186e-09\RMSF=5.368e-05
\Dipole=0.3430184,-0.4164369,0.1326544\PG=C01 [X(C3H9P1)]\@

n.CH_CH3_2-SH

1\1\GINC-AC22\FOpt\RB3LYP\Gen\C3H8S1\CYL509\20-May-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CH_CH3_2-S
H.a2.freq\0,1\C,-0.1369210618,0.2042877369,-0.5138527762\S,-0.1733419
838,0.419067419,1.3302289705\C,1.2929458772,0.2095635473,-1.0600668949
\C,-0.9300316268,-1.0264944303,-0.9601027377\H,0.4842744688,-0.7243792
535,1.6279606023\H,-0.9619600249,-1.0808647816,-2.0561314162\H,-1.9567
363994,-0.9973066858,-0.5846015252\H,-0.4605414468,-1.9481241826,-0.59
49881982\H,1.8337845666,1.1094544269,-0.7540117629\H,1.2805183691,0.16
74119937,-2.1570048586\H,1.8525656024,-0.6625049264,-0.7001975719\H,-0
.6543925263,1.1070935819,-0.8605543437\Version=IA64L-G03RevC.02\State
=1-A\HF=-517.3288187\RMSD=7.655e-09\RMSF=1.536e-05\Dipole=0.1734312,-0
.3569343,-0.6072659\PG=C01 [X(C3H8S1)]\@

n.CH_CH3_2-Cl

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C3H7Cl1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
Cl1.freq\0,1\Cl,0.0023070926,0.2173148709,-1.3484783228\C,-0.260974520
4,-0.3480561494,0.3848208364\C,1.0470395808,-0.9027883582,0.9329486595
\C,-0.827687478,0.8033419869,1.2046937378\H,1.8121692364,-0.1211647115
,0.9812945407\H,1.4245014468,-1.719806711,0.3119652977\H,0.8817785983,
-1.2871291273,1.947456405\H,-0.1131632209,1.6310200206,1.2603749397\H,
-1.0334633013,0.4558725322,2.2250741926\H,-1.7599744533,1.1782849518,0
.7735608683\H,-1.0013343038,-1.1464146996,0.2896258302\Version=IA64L-
G03RevC.02\State=1-A\HF=-578.7436049\RMSD=6.063e-09\RMSF=2.914e-05\Dip
ole=-0.0986496,-0.2508354,0.8942814\PG=C01 [X(C3H7Cl1)]\@

n.CH_CH3_2-Br

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C3H7Br1\CYL509\10-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
Br.freq\0,1\Br,0.0951092223,-0.0938464075,-1.0163684984\C,-0.20172090
4,0.4564668548,0.897863039\C,1.1174956242,0.3684596135,1.6500183638\C,
-1.3112721096,-0.3967900613,1.4933996985\H,1.8880811104,0.9906522279,1
.1874454649\H,1.481055895,-0.6632952197,1.6889271023\H,0.96592255,0.71
71243973,2.6805637797\H,-1.022001375,-1.4519518439,1.5275178892\H,-2.2
386531995,-0.3095882376,0.9213337201\H,-1.5076831795,-0.0622527139,2.5
210537441\H,-0.5225602468,1.4951172085,0.798369137\Version=IA64L-G03R
evC.02\State=1-A\HF=-2692.4295868\RMSD=2.619e-09\RMSF=2.924e-05\Dipol
e=-0.130026,0.2169371,0.9564122\PG=CS [SG(C1H1Br1),X(C2H6)]\@
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n.CH_CH3_2-N_CH3_2

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1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H13N1\CYL509\11-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
N_CH3_2.freq\0,1\C,1.1863325454,0.4606046973,1.3808863792\H,2.2573373
805,0.6859603056,1.3501119702\H,1.0515918802,-0.3920699335,2.050058090
1\H,0.6699050394,1.3350358456,1.8267365845\N,0.726360704,0.1449508799,
0.0313770479\C,-0.7233707786,-0.1315985637,-0.0270273333\C,1.134675905
,1.2091663572,-0.8813720963\C,-1.1096702756,-1.277992277,0.9204945975\
C,-1.1638972251,-0.4921884763,-1.4543167385\H,2.2090085877,1.386297510
4,-0.7664050933\H,0.6122943799,2.1698766543,-0.696269749\H,0.960922863
6,0.9218261777,-1.9207206149\H,-0.5604499994,-1.3228467878,-1.83894553
81\H,-1.0779560314,0.3471136963,-2.1501079831\H,-2.213978235,-0.803093
2511,-1.451349804\H,-0.5022738909,-2.1658806719,0.7088228587\H,-2.1631
194682,-1.5400895416,0.7759590264\H,-0.9837570953,-1.0179208678,1.9752
212095\H,-1.2884713657,0.7731842794,0.2852608559\Version=IA64L-G03Rev
C.02\State=1-A\HF=-253.1000893\RMSD=5.837e-09\RMSF=5.741e-06\Dipole=-0
.1052975,0.167689,0.0578912\PG=C01 [X(C5H13N1)]\@
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n.CH_CH3_2-NHCH3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H11N1\CYL509\11-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
NHCH3.freq\0,1\C,1.8090202294,0.2091363748,0.8702471001\H,2.857298536
4,0.1262263025,0.5647584481\H,1.6304177246,-0.5601237264,1.6288615653\
H,1.6675871416,1.1947680737,1.3543085619\N,0.9532657455,-0.0148172032,
-0.2907523903\C,-0.4725393055,0.2590058393,-0.0655216619\C,-1.09489647
57,-0.8235183137,0.8246388596\C,-1.1814876671,0.3224219965,-1.42128812
63\H,1.2751762378,0.5872074289,-1.0466144497\H,-0.7659749164,1.1198269
95,-2.0510497245\H,-2.2508912903,0.5224033802,-1.2948054463\H,-1.06619
27543,-0.6272977098,-1.9560805792\H,-0.6270068813,-0.8592318383,1.8141
451835\H,-0.9781904322,-1.8081507827,0.3577554431\H,-2.163420601,-0.62
99310973,0.9730378064\H,-0.6122436699,1.2357480151,0.4424928946\Versi
on=IA64L-G03RevC.02\State=1-A\HF=-213.7945844\RMSD=3.229e-09\RMSF=1.75
0e-05\Dipole=0.0015983,0.3737678,0.0173631\PG=C01 [X(C4H11N1)]\@
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n.CH_CH3_2-NHCHO

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1\1\GINC-AC8\FOpt\RB3LYP\Gen\C4H9N1O1\CYL509\19-May-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
NHCHO.a2.freq\0,1\H,0.8912329057,0.124696603,-2.547718221\C,0.6230366
601,0.5314190461,-1.5514954762\O,0.8520070024,1.6854711973,-1.22758173
24\N,0.0046224656,-0.395222236,-0.7698475107\C,-0.4026367757,-0.128559
842,0.6134017721\H,-0.0530330611,-1.3450765489,-1.1144792931\C,0.74330
26162,-0.4041932703,1.5967536197\C,-1.6631648228,-0.9325276382,0.94131
28417\H,-1.4700338314,-2.0125459445,0.886748462\H,-2.4757411805,-0.693
6887355,0.2472968489\H,-2.0030802272,-0.7119203484,1.9585946949\H,1.61
76102988,0.2004889219,1.3381610468\H,1.0333913727,-1.4622723842,1.5771
351863\H,0.4426036815,-0.1541640017,2.6209045267\H,-0.6345893037,0.940
4387384,0.6431066387\Version=IA64L-G03RevC.02\State=1-A\HF=-287.83344
```

3\RMSD=7.898e-09\RMSF=4.587e-06\Dipole=-0.4535836,-1.3874252,0.2251117
\PG=C01 [X(C4H9N1O1)]\@

n.CH_CH3_2-NHCOCH3

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H11N1O1\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-NHCOCH3.freq\0,1\H,-0.840328825,1.8121947769,-2.1760111618\C,0.1808539639,1.9380264248,-1.8016581064\C,0.5872460808,0.9095064961,-0.753930659\H,0.279863254,2.9399904961,-1.3717423488\H,0.8777705094,1.8750911165,-2.64262484\N,-0.3910337029,0.0300350978,-0.3806441067\O,1.7217993605,0.8736001428,-0.2909526998\C,-0.1871686856,-0.977054494,0.6629889968\H,-1.3302902068,0.169043404,-0.7272452657\C,-0.453731696,-0.3997679543,2.0603879705\C,-1.048479514,-2.2067531781,0.3641607231\H,-0.8167121865,-2.6210283142,-0.622702028\H,-2.1183528304,-1.9581681,0.3900834549\H,-0.876049959,-2.9861536916,1.1138538269\H,0.1919171733,0.464915161,2.2398965062\H,-0.2490814709,-1.1483816845,2.834861973\H,-1.499329355,-0.0826178524,2.1630926908\H,0.8711140391,-1.2476759056,0.5989739883\Version=IA64L-G03RevC.02\State=1-A\HF=-327.156535\RMSD=5.606e-09\RMSF=4.436e-06\Dipole=-1.3511665,-0.2262132,-0.2307486\PG=C01 [X(C5H11N1O1)]\@

n.CH_CH3_2-NO2

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C3H7N1O2\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-NO2.freq\0,1\O,-1.0028915933,-0.8406194368,-0.9281107925\N,-0.7660254648,0.1938746565,-0.3088975785\C,0.5659001238,0.2730190028,0.427372687\O,-1.512544843,1.1651652876,-0.2355716962\C,1.692486459,0.1672085006,-0.5987878396\C,0.6003047245,-0.8294733997,1.4841247027\H,2.6558377001,0.2620423362,-0.0874239257\H,1.6233455422,0.9624731728,-1.3479241858\H,1.6573668443,-0.8003046105,-1.1068514766\H,1.5363555837,-0.7595532248,2.0475535609\H,0.546573538,-1.813970352,1.0115547064\H,-0.2312979002,-0.7300011513,2.189088503\H,0.5453405928,1.261299805,0.8894884757\Version=IA64L-G03RevC.02\State=1-A\HF=-323.6457411\RMSD=2.412e-09\RMSF=3.352e-05\Dipole=1.3010859,-0.0262108,0.6696878\PG=C01 [X(C3H7N1O2)]\@

n.CH_CH3_2-OCF3

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C4H7F3O1\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-OCF3.freq\0,1\C,1.289394599,0.1427048519,0.1662430739\O,0.0888759367,-0.0140081085,-0.6619220863\C,-1.0668468665,-0.2063032724,-0.0139503386\F,-1.3601086046,0.7955332681,0.8543288459\F,-1.0739063067,-1.3486640165,0.7176459884\F,-2.0523546033,-0.2815834648,-0.9113784056\C,1.6662894025,1.6186089886,0.1923166749\C,2.3539570236,-0.7548196119,-0.4476383131\H,3.2859999121,-0.680192371,0.1229636052\H,2.5563674678,-0.4560908124,-1.4817544497\H,2.0259839691,-1.7984860187,-0.44604531\H,2.5664856141,1.7681301434,0.798911048\H,0.8561022923,2.2154604592,0.619653074\H,1.8682934494,1.9789616083,-0.8220343098\H,1.0503204803,-0.2044359599,1.1764885927\Version=IA64L-G03RevC.02\State=1-A\HF=-531.4038068\RMSD=2.605e-09\RMSF=5.055e-06\Dipole=0.9768403,0.1485428,0.2212987\PG=C01 [X(C4H7F3O1)]\@

n.CH_CH3_2-OCH2CH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C5H12O1\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-OCH2CH3.freq\0,1\H,0.3703545135,-3.1161331728,1.6961648183\C,0.0883851359,-2.5761331889,0.7853610983\C,0.3246701227,-1.083241877,0.9554843793\O,-0.0532513033,-0.4375531702,-0.2486035905\C,0.2310527422,0.960639146,-0.3091648261\C,0.1955414448,1.340463175,-1.7866325259\C,-0.762572

```
3085,1.7812001414,0.520406358\H,-0.2573629182,-0.7045013533,1.81098107
03\H,1.3881062572,-0.8829781494,1.1738397689\H,0.6802654668,-2.9651435
796,-0.0494564399\H,-0.9679198253,-2.7748520381,0.5767666406\H,0.91633
62444,0.741749422,-2.3520752264\H,0.4355769625,2.4007045952,-1.9227284
935\H,-0.8019902745,1.1551416896,-2.2007684602\H,-0.7308945953,1.50880
96954,1.5806220406\H,-1.7829237717,1.6174785798,0.1553156377\H,-0.5358
089222,2.8510925472,0.4461513432\H,1.2498084668,1.1314927465,0.0812891
229\Version=IA64L-G03RevC.02\State=1-A\HF=-272.979948\RMSD=4.927e-09\
RMSF=9.806e-07\Dipole=0.1735747,0.2073281,0.3162315\PG=C01 [X(C5H12O1)
]\@
```

n.CH_CH3_2-OCH3

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H10O1\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
OCH3.freq\0,1\C,-1.4312138408,0.3992890563,-1.2884891504\O,-0.8893021
06,-0.3351790319,-0.2126175909\C,0.282282023,0.2345779234,0.3731013836
\H,-0.7744183777,0.4134726294,-2.1715704409\H,-2.3699551924,-0.0890991
87,-1.564994614\H,-1.6456811949,1.4422035115,-1.0018996994\C,0.4396889
937,-0.4262946157,1.7390672582\C,1.5179562402,0.0333899306,-0.51054390
15\H,1.3054462554,-0.0181375451,2.2719829343\H,0.5823186938,-1.5064910
437,1.6220472678\H,-0.4557079729,-0.2639342348,2.3469665611\H,2.405860
5125,0.465598932,-0.0348773141\H,1.4022001071,0.5107480324,-1.48939313
56\H,1.6965919644,-1.0360743486,-0.6701331562\H,0.1154815559,1.3173717
409,0.5139987843\Version=IA64L-G03RevC.02\State=1-A\HF=-233.6608613\R
MSD=1.556e-09\RMSF=2.160e-06\Dipole=0.2026098,0.3864285,-0.1487059\PG=
C01 [X(C4H10O1)]\@
```

n.CH_CH3_2-OCHO

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H8O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-O
CHO.freq\0,1\C,-0.38955314,0.1876645078,-0.5881673908\O,-0.244286958,
-0.5945936359,0.6404815794\C,0.5918243675,-0.1186160477,1.5738985059\H
,0.5866044533,-0.8034130794,2.4367745589\O,1.2496046873,0.8924971781,1
.5078534653\C,0.7402538775,-0.1674571804,-1.5488159085\C,-1.775463319,
-0.137120983,-1.1262075134\H,-1.8594173016,-1.2026498649,-1.3664599049
\H,-1.966907578,0.4380297332,-2.0385649797\H,-2.5474730084,0.113085727
2,-0.3918746124\H,1.710819078,0.0842307871,-1.1127802091\H,0.628473292
7,0.3945973879,-2.4828448538\H,0.7226680653,-1.2370108087,-1.786040606
6\H,-0.319679551,1.2430799992,-0.3091359091\Version=IA64L-G03RevC.02\
State=1-A\HF=-307.7005464\RMSD=1.944e-09\RMSF=7.851e-06\Dipole=-0.5096
635,-0.3822826,-0.5017964\PG=C01 [X(C4H8O2)]\@
```

n.CH_CH3_2-OCOCH3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H10O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
OCOCH3.freq\0,1\C,-1.1564878923,0.0443090798,0.1007220313\O,0.1450746
299,-0.520938328,-0.2364082659\C,1.235312298,0.0694670047,0.3043671488
\C,2.4971258455,-0.6378063093,-0.1367901607\O,1.195807837,1.0308094991
,1.0422246219\C,-1.4552110199,1.2203588845,-0.823751407\C,-2.154241186
6,-1.0985379693,-0.026761536\H,3.3626809203,-0.15287631,0.3157875764\H
,2.5824000372,-0.6085733292,-1.2281297141\H,2.4623784385,-1.6915063367
,0.1588335293\H,-2.1818741157,-1.4782649172,-1.0541507297\H,-3.1588568
615,-0.7520134788,0.2391811022\H,-1.8868213596,-1.9252855516,0.6389222
016\H,-0.7103510408,2.0100386996,-0.6930272926\H,-2.4417321866,1.63915
29451,-0.5946213264\H,-1.4529626714,0.8978341794,-1.8711343354\H,-1.10
09091638,0.395780588,1.1350916817\Version=IA64L-G03RevC.02\State=1-A\
HF=-347.0258152\RMSD=9.217e-09\RMSF=9.039e-06\Dipole=-0.2876419,-0.520
7571,-0.4430558\PG=C01 [X(C5H10O2)]\@
```

n.CH_CH3_2-Si_CH3_3

```
1\1\GINC-AC18\FOpt\RB3LYP\Gen\C6H16Si1\CYL509\11-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-Si_CH3_3.freq\0,1\H,1.6621841237,-1.5526687335,-1.4707880545\C,1.612
1702831,-1.542016309,-0.3756054869\H,2.6419431309,-1.4894515867,-0.001
2654152\H,1.195203495,-2.5045693531,-0.0543116636\Si,0.5795379416,-0.0
877764018,0.2725338397\C,-1.2326670124,-0.2763470393,-0.3176220668\C,0
.6334994024,-0.1017124552,2.1694054215\C,1.323509279,1.5387675265,-0.3
618895293\C,-1.3540328222,-0.3599909928,-1.8514746222\C,-2.1578875796,
0.8230369909,0.2389309833\H,2.3617260613,1.650624675,-0.0259520653\H,0
.7660258603,2.4099066217,0.0027099298\H,1.3275820567,1.583468003,-1.45
76035111\H,1.6675124207,-0.0553878138,2.5327190057\H,0.1834760671,-1.0
156162365,2.5766624254\H,0.09657084,0.7514343641,2.6005526542\H,-1.864
8384185,1.8160396725,-0.1258909006\H,-2.1473126178,0.857365812,1.33456
56742\H,-3.1982513688,0.6595533465,-0.0743103469\H,-0.7614647095,-1.18
21777571,-2.2692995047\H,-1.0167395784,0.5678979149,-2.3313523029\H,-2
.3973801489,-0.5190838173,-2.1569573125\H,-1.5773176977,-1.238891816,0
.0945794305\Version=IA64L-G03RevC.02\State=1-A\HF=-527.811565\RMSE=2.
105e-09\RMSE=2.049e-05\Dipole=0.0314301,-0.0254441,0.0264859\PG=C01 [X
(C6H16Si1)]\@
```

n.CH_CH3_2-P_CH3_2

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C5H13P1\CYL509\11-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
P_CH3_2.freq\0,1\C,-1.1401308321,1.1565681149,1.3642366139\H,-0.47853
10228,1.9703464599,1.6768157202\H,-1.7524290717,0.8813874001,2.2300223
308\H,-1.8039081377,1.5256006393,0.5719584839\P,-0.1360804203,-0.32897
44685,0.8348862062\C,-1.5472955589,-1.423164719,0.2813653364\C,0.49791
42023,0.2742480993,-0.8405610432\H,-1.1614912041,-2.3567837777,-0.1395
451859\H,-2.19312297,-0.9404034145,-0.463173734\H,-2.157386587,-1.6843
620036,1.1530208802\C,1.5031092484,1.4216120333,-0.6538090087\C,1.1392
696962,-0.8836013952,-1.6214483837\H,1.9778572325,-1.3186555593,-1.063
8301657\H,1.529617472,-0.5276602577,-2.5834768392\H,0.4248463138,-1.68
62846873,-1.8334625227\H,2.3597336198,1.1008364038,-0.0482209056\H,1.0
526645837,2.2914446174,-0.163766065\H,1.8898491585,1.7546929197,-1.625
4332097\H,-0.3636936181,0.6504854875,-1.4129029683\Version=IA64L-G03R
evC.02\State=1-A\HF=-539.7224327\RMSE=2.641e-09\RMSE=1.535e-05\Dipole=
-0.3448966,0.2019411,-0.3514031\PG=C01 [X(C5H13P1)]\@
```

n.CH_CH3_2-SC_CH3_2CN

```
1\1\GINC-AC22\FOpt\RB3LYP\Gen\C7H13N1S1\CYL509\19-May-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_
2-SC_CH3_2CN.a2.freq\0,1\N,-0.3173824933,-1.1708347304,-2.4740955487\
C,-0.1619747265,-1.2315675977,-1.3238914888\C,0.0631516411,-1.30925016
55,0.126813603\S,-0.535234843,0.2623852404,0.943462814\C,0.3036660531,
1.6258082755,-0.0133769463\C,-0.6284924486,2.2193123037,-1.0737724403\
C,0.790062534,2.6805906811,0.986523446\H,1.1713865998,1.1712506945,-0.
5038074307\C,1.5567286693,-1.5650108748,0.4079473062\C,-0.8040217898,-
2.4393687776,0.7214524665\H,2.186045447,-0.7587391609,0.0214178449\H,1
.7120696495,-1.641234161,1.4877475112\H,1.8765658421,-2.5006338344,-0.
0657737443\H,-0.6707152813,-2.4699462514,1.8075031036\H,-0.4949519863,
-3.4039887895,0.3054319571\H,-1.8629383691,-2.2842450805,0.5004387928\
H,-1.5177394353,2.6575630077,-0.6070809456\H,-0.9534139729,1.462680688
5,-1.7918692036\H,-0.1074203357,3.013026763,-1.6248992648\H,-0.0473969
011,3.0989579453,1.557411663\H,1.2701328921,3.507962464,0.4498062995\H
,1.5090911965,2.2619419121,1.6967615553\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-727.5054388\RMSE=2.798e-09\RMSE=1.008e-05\Dipole=0.6238979,0
.0177293,0.9668133\PG=C01 [X(C7H13N1S1)]\@
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n.CH_CH3_2-SCH2COOCH3

```
1\1\GINC-AC8\FOpt\RB3LYP\Gen\C6H12O2S1\CYL509\19-May-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-SCH2COOCH3.a2.freq\0,1\S,1.0678678102,0.4033037218,0.8806500096\C,0.
253933861,-0.8675420622,1.9651451218\C,1.341512983,-1.3960431164,2.906
6793832\C,-0.4231669402,-1.9917320956,1.1792635415\C,-0.3773073426,1.2
977766185,0.1641371599\C,-0.8279017398,0.7294628529,-1.1658597557\O,-1
.7249011073,-0.0737780254,-1.3180110995\O,-0.0876172296,1.2258627616,-
2.1771059423\C,-0.3882197222,0.6967834671,-3.4793390719\H,-0.057693354
6,2.3346017746,0.0356342791\H,-1.2113536488,1.2604905939,0.8685702703\
H,-1.4266706662,0.9067706139,-3.7487208078\H,-0.2267200917,-0.38421419
64,-3.4983481932\H,0.2959096861,1.1993276273,-4.1633959341\H,0.9101476
899,-2.1394142801,3.5873510949\H,2.1442182374,-1.8873482682,2.34416251
67\H,1.7831795054,-0.5945051747,3.5068752203\H,-0.8952011022,-2.697141
8692,1.8762553126\H,-1.1925808,-1.6116392859,0.5025726823\H,0.31320447
74,-2.5427472944,0.5832926146\H,-0.4952847957,-0.3259516652,2.55612885
25\Version=IA64L-G03RevC.02\State=1-A\HF=-784.5130454\RMSD=4.104e-09\
RMSF=7.845e-06\Dipole=-0.0511961,0.1439641,-0.0274358\PG=C01 [X(C6H12O
2S1)]\@
```

n.CH_CH3_2-SCH2Ph

```
1\1\GINC-AC2\FOpt\RB3LYP\Gen\C10H14S1\CYL509\19-May-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
SCH2Ph.a2.freq\0,1\C,-1.4734707897,-0.9917999854,-1.1384407618\S,-1.5
417216533,-1.1547357907,0.7055261613\C,0.2446403855,-1.0560124008,1.17
00436539\C,-0.8700496213,-2.2255269687,-1.814034753\C,-2.9006684579,-0
.7166186197,-1.6233588306\C,0.9343991122,0.23742807,0.8054218847\H,0.7
799508326,-1.9110020842,0.7456031222\H,0.2273102699,-1.1961697747,2.25
65675069\C,1.972227601,0.2491448756,-0.1345486539\C,0.5604789556,1.449
2922398,1.4055410373\C,2.6259235274,1.438750416,-0.46684464\C,1.212235
234,2.6363034838,1.0790760824\C,2.2483915296,2.6355779594,0.1401492347
\H,2.7557807103,3.5622890472,-0.1142722094\H,0.9128300333,3.565105854,
1.5577653439\H,3.4297084987,1.4264844258,-1.1984188705\H,-0.2532972823
,1.4565630599,2.1263808591\H,2.2780391162,-0.6829540673,-0.6050475138\
H,-3.5701286656,-1.5489088309,-1.3752664811\H,-2.9076100556,-0.5962145
702,-2.7133488538\H,-3.307076392,0.1949482758,-1.1745133052\H,-0.82642
89524,-2.0768742398,-2.9011130973\H,-1.4759959804,-3.1157719807,-1.612
8517447\H,0.1496327894,-2.4253466366,-1.4684564245\H,-0.8498133274,-0.
1156102479,-1.3494724348\Version=IA64L-G03RevC.02\State=1-A\HF=-787.6
933837\RMSD=3.918e-09\RMSF=1.737e-06\Dipole=0.45455,0.1429094,-0.41612
85\PG=C01 [X(C10H14S1)]\@
```

n.CH_CH3_2-SCH3

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H10S1\CYL509\19-May-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
SCH3.a2.freq\0,1\S,0.3928356641,0.1982180995,-1.0062084531\C,0.128142
3521,0.0025954456,0.8164108293\C,1.4678010861,-0.4192534487,1.42846115
38\C,-0.9871305347,-0.9914263094,1.1495549656\C,-1.1641650863,1.010858
2932,-1.5092154531\H,-1.0628689801,1.2517840182,-2.5708368609\H,-1.321
7071911,1.9412741703,-0.9541422821\H,-2.0309685615,0.3559776556,-1.383
0660664\H,1.3666853795,-0.5254652829,2.5151036449\H,1.7956277331,-1.38
537582,1.0269355431\H,2.250779978,0.3183708517,1.2266381485\H,-1.12120
28269,-1.0576277543,2.2373703597\H,-1.9473876236,-0.6920088413,0.71719
40153\H,-0.7414734757,-1.990140388,0.772314139\H,-0.140741961,0.995077
9143,1.2005556356\Version=IA64L-G03RevC.02\State=1-A\HF=-556.6427639\
RMSD=4.698e-09\RMSF=1.824e-06\Dipole=-0.4969791,0.1591866,0.4290078\PG
=C01 [X(C4H10S1)]\@
```

n.CH_CH3_2-SO2CH3

1\1\GINC-AC1\FOpt\RB3LYP\Gen\C4H10O2S1\CYL509\19-May-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-SO2CH3.a3.freq\0,1\C,0.0278857944,0.0511405154,-1.1765351928\S,0.102
8755107,0.1594470414,0.661805532\C,1.6082366458,-0.7407890378,1.121346
4986\O,0.3240250566,1.5729284098,1.0147057161\O,-1.0468327431,-0.57752
75484,1.2170678511\H,1.5144363796,-1.7948896436,0.8560700478\H,1.69131
29619,-0.6344613827,2.2055279184\H,2.4713856335,-0.281072059,0.6352979
869\C,-0.1644687228,-1.3931369896,-1.6407326987\C,-1.0969656874,0.9818
19719,-1.6418400101\H,-1.1285164167,0.9898191969,-2.7366028853\H,-0.93
75033752,2.0028448526,-1.2870539245\H,-2.0650531769,0.6301828826,-1.27
09016524\H,0.6736500405,-2.0395302477,-1.3603532217\H,-0.2457943184,-1
.4140855483,-2.733183629\H,-1.081963531,-1.8124095424,-1.2173142767\H,
0.9963709423,0.4450366956,-1.5079949949\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-707.0321809\RMSD=5.252e-09\RMSF=4.732e-06\Dipole=1.027347,-0
.8240943,-1.2248269\PG=C01 [X(C4H10O2S1)]\@

n.CH_CH3_2-SOCH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H10O1S1\CYL509\19-May-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-SOCH3.a4.freq\0,1\C,-0.3685875585,0.0325107634,-1.0399484739\S,-0.4
287518646,0.4313942531,0.7605947191\O,0.8844083916,-0.4661855273,1.347
3245995\C,2.1247122145,0.2466027567,1.3543266252\C,-0.4578089457,-1.47
32951488,-1.2848709076\H,2.8586238273,-0.4412607997,1.7855052827\H,2.0
647319323,1.15164819,1.97027467\H,2.4423274005,0.5235040268,0.34072190
13\C,-1.5154655134,0.8142261588,-1.6913266269\H,-1.5200386351,0.629365
7264,-2.7716094521\H,-1.4156019103,1.8935214274,-1.5332047258\H,-2.486
4590433,0.4952567563,-1.294507278\H,0.3227052506,-2.003791169,-0.73207
15095\H,-0.3337961439,-1.6915278802,-2.3536265045\H,-1.4297111291,-1.8
627042961,-0.9619347839\H,0.5848799698,0.4128970059,-1.4267436027\Ver
sion=IA64L-G03RevC.02\State=1-A\HF=-631.8292163\RMSD=5.747e-09\RMSF=9.
863e-06\Dipole=0.3924334,0.249106,-0.6755411\PG=C01 [X(C4H10O1S1)]\@

n.CH_CH3_2-Ph

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C9H12\CYL509\11-Apr-2008\0\#\B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-Ph.
freq\0,1\H,-3.6271583725,-0.9330190477,-0.1412075331\C,-2.5893007429,
-0.6134489506,-0.097963156\C,-1.560162863,-1.5572426079,-0.1231390818\
C,-0.2285356025,-1.1462682007,-0.0676028028\C,0.1062175953,0.213814829
7,0.014203588\C,-0.9375220587,1.1475698363,0.0384727698\C,-2.272838901
2,0.742576169,-0.0168329401\H,-1.7946094651,-2.6169859107,-0.186220262
6\C,1.5580709149,0.6714125406,0.0752653933\C,2.2719803616,0.1499239693
,1.3367681092\C,2.3354539838,0.2867506051,-1.1978084094\H,-0.700353192
3,2.2076992609,0.1016434129\H,0.5592761475,-1.8956746332,-0.0883286274
\H,-3.0642011566,1.4876796022,0.0035721558\H,3.2956142393,0.5396086453
,1.3906409009\H,2.3326475865,-0.9449558525,1.3358926295\H,1.7420026133
,0.4535604239,2.246095581\H,3.3594472792,0.6772099869,-1.1582869804\H,
1.8507045745,0.687883335,-2.0945015028\H,2.3989516096,-0.8020278228,-1
.3117061287\H,1.5475020133,1.7684928681,0.134225534\Version=IA64L-G03
RevC.02\State=1-A\HF=-350.1932771\RMSD=7.910e-09\RMSF=4.012e-05\Dipole
=0.1006969,0.0331307,0.0043101\PG=C01 [X(C9H12)]\@

n.CH_CH3_2-C6H4CN

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C10H11N1\CYL509\11-Apr-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-C6H4CN.freq\0,1\N,-4.4777723671,-0.5754239292,0.1541020369\C,-3.3201
598003,-0.4658849723,0.1097375928\C,-1.8941343601,-0.3303084921,0.0551
601696\C,-1.0806622885,-1.461023005,-0.1153528527\C,0.3029178712,-1.31
68347688,-0.1668467298\C,0.9122352952,-0.0599528225,-0.0518370951\C,0.
0846090282,1.061991563,0.118360671\C,-1.298762358,0.9376137988,0.17212

98341\H,-1.5362157683,-2.4420302264,-0.2061046608\C,2.4269827999,0.075
9728818,-0.1107420992\C,3.0018914064,0.6327438547,1.205948222\C,2.8777
138223,0.9237014425,-1.3158914892\H,0.5263538856,2.0504123684,0.210647
5944\H,0.9233445724,-2.1997877977,-0.2992683816\H,-1.9260519873,1.8135
521176,0.304079931\H,3.9718802807,0.955974724,-1.3724652507\H,2.518560
3451,1.9563623132,-1.2344513571\H,2.4989718723,0.5107203111,-2.2569530
805\H,4.0966802828,0.663558756,1.1620147287\H,2.7115794919,0.012564354
8,2.060753565\H,2.6481081854,1.6528218828,1.3964487277\H,2.8354069112,
-0.93429818,-0.2474134155\\Version=IA64L-G03RevC.02\State=1-A\HF=-442.
4377848\RMSD=3.890e-09\RMSF=3.697e-05\Dipole=2.0392824,0.2073329,-0.07
6496\PG=C01 [X(C10H11N1)]\\@

n.CH_CH3_2-C6H4NO2

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C9H11N1O2\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_
2-C6H4NO2.freq\\0,1\O,-2.7706571777,2.2890120127,-0.71912815\N,-1.7924
644508,1.9253879568,-1.3731408119\C,-0.8671352545,0.971830925,-0.74676
64485\O,-1.5371147985,2.3060866297,-2.5161948641\C,-1.1283006703,0.521
3276585,0.5467643577\C,-0.246738371,-0.3811962315,1.1313970492\C,0.890
3428843,-0.8403571948,0.4451526944\C,1.1178230776,-0.3634687379,-0.854
1708706\C,0.2486984669,0.5405246625,-1.459574047\H,0.4193123573,0.9121
049359,-2.4624995938\C,1.8539915426,-1.8279642027,1.0863625073\C,2.520
16517,-1.2386688413,2.3446487303\C,1.168293588,-3.172150646,1.39832668
41\H,-0.4492146053,-0.7328419436,2.1391092883\H,1.9916455397,-0.706088
4508,-1.4024501184\H,-2.006689539,0.8797466883,1.0692855459\H,1.895565
2089,-3.8863838888,1.8010449479\H,0.7218450658,-3.6096852261,0.4990061
292\H,0.3729253032,-3.0516007738,2.1431560639\H,3.2544155964,-1.942920
8281,2.7522522003\H,1.7822517766,-1.0359454932,3.1296970387\H,3.036367
4275,-0.2993952664,2.119192233\H,2.6481602326,-2.0247589401,0.35393211
97\\Version=IA64L-G03RevC.02\State=1-A\HF=-554.6962852\RMSD=7.686e-09\
RMSF=4.581e-05\Dipole=1.3097372,-1.3590949,0.9062463\PG=C01 [X(C9H11N1
O2)]\\@

n.CH_CH3_2-C6H4OCH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C10H14O1\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_
2-C6H4OCH3.freq\\0,1\C,-1.5062732459,-0.9662375836,-0.3069813405\C,-1.5
446654415,-0.2429927457,0.8919984314\C,-0.446157965,0.5459237037,1.251
8314444\C,0.6698093206,0.6007322974,0.4125560503\C,0.7287794518,-0.113
460516,-0.7889273077\C,-0.3854072169,-0.8967155933,-1.1265868138\C,1.9
466593138,-0.0515377328,-1.7014534728\O,-2.6876871555,-0.3733475325,1.
6318598685\C,-2.7767441779,0.3382379815,2.8541446766\C,3.2101085981,-0
.6058366685,-1.0161722745\C,2.1919795561,1.3704300982,-2.2408857956\H,
-0.3747007594,-1.4658751957,-2.0539110902\H,1.5106967887,1.2209932294,
0.7144010545\H,-0.4462436454,1.1170699316,2.1735338584\H,-2.3647430081
, -1.5745929463,-0.5749969193\H,-1.9937493232,0.0307619504,3.5605811835
\H,-3.7548346674,0.0941062225,3.2733004134\H,-2.7112644906,1.423521599
2,2.6974702645\H,4.0596918135,-0.6072089528,-1.7098136167\H,3.05251565
11,-1.631726336,-0.6658615564\H,3.4909407423,0.0030873022,-0.148301587
7\H,3.0358146812,1.3802154016,-2.9414415488\H,2.4268466649,2.068575665
2,-1.428306668\H,1.3086537488,1.7532437077,-2.7635635193\H,1.733343888
4,-0.6966507647,-2.5651108024\\Version=IA64L-G03RevC.02\State=1-A\HF=-
464.7154001\RMSD=7.337e-09\RMSF=1.963e-05\Dipole=0.1080624,0.2817763,0
.3648536\PG=C01 [X(C10H14O1)]\\@

n.CH_CH3_2-C6H4OH

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C9H12O1\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_
2-C6H4OH.freq\\0,1\C,-1.5816894402,-0.9479309134,-0.0114026625\C,-1.9123

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171374,-0.1809931407,1.1111829297\C,-1.005318337,0.7670617494,1.589225
4233\C,0.2209651318,0.9412866087,0.9444868283\C,0.5744293029,0.1871701
977,-0.1789592589\C,-0.3550391502,-0.7596273345,-0.6399838891\C,1.9167
178683,0.3916764819,-0.8686477192\O,-3.1319004365,-0.4046811866,1.6936
334702\C,2.7928051957,-0.8743050988,-0.8125922201\C,1.7508704111,0.882
3353155,-2.3195541018\H,-0.1191386121,-1.3667445534,-1.5107775229\H,0.
9162902987,1.6841524451,1.3296948123\H,-1.2536445626,1.3687779112,2.46
23210081\H,-2.294472862,-1.6820554263,-0.3743434322\H,-3.2285848249,0.
1898894287,2.4535543746\H,2.7279931277,1.0787305106,-2.7772849625\H,1.
1619237047,1.8050934629,-2.3604695158\H,1.2398129593,0.1334038457,-2.9
365366452\H,3.7753234603,-0.6870062511,-1.2625193315\H,2.3291852957,-1
.7032132836,-1.3609655554\H,2.9466154112,-1.2037913525,0.2207499903\H,
2.4453570255,1.180169561,-0.3150229593\\Version=IA64L-G03RevC.02\State
=1-A\HF=-425.4090228\RMSD=3.933e-09\RMSF=2.067e-05\Dipole=0.186344,0.3
872534,0.3225699\PG=C01 [X(C9H12O1)]\\@
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n.CH_CH3_2-CF2CF3

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1\1\GINC-AC15\FOpt\RB3LYP\Gen\C5H7F5\CYL509\19-May-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
F2CF3.a2.freq\\0,1\F,-0.7589667967,1.0240789896,-1.0161385497\C,-0.247
7290959,0.4310782993,0.1060819586\C,1.2258524833,0.0855805417,-0.21525
8666\C,-1.1390507408,-0.7240601928,0.5642962793\F,-0.1966368175,1.3863
785083,1.0860112465\F,1.3212962584,-0.6116414597,-1.3612971479\F,1.757
041623,-0.657239252,0.7754886123\F,1.9550516709,1.201048969,-0.3452132
965\C,-2.5298873292,-0.1793465166,0.9305431214\C,-1.2367217517,-1.8480
233826,-0.4794814862\H,-1.6111258953,-1.4610711882,-1.4329335881\H,-1.
9369433922,-2.6111431924,-0.1252583421\H,-0.2750381761,-2.3335578277,-
0.6624094033\H,-3.0299330026,0.2341074505,0.0486152752\H,-2.4665845013
,0.6050448828,1.6890946483\H,-3.1503074833,-0.9901057923,1.3249073909\
H,-0.6649223858,-1.1182786235,1.4712389934\\Version=IA64L-G03RevC.02\S
tate=1-A\HF=-693.9634563\RMSD=3.408e-09\RMSF=1.681e-05\Dipole=-0.55345
68,-0.6046578,0.2191279\PG=C01 [X(C5H7F5)]\\@
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n.CH_CH3_2-CF2H

```
1\1\GINC-AC8\FOpt\RB3LYP\Gen\C4H8F2\CYL509\10-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CF
2H.freq\\0,1\C,0.0791388406,-0.0346399269,-0.7913204204\C,-0.113818753
3,0.0302622176,0.7148159913\C,0.4482066625,1.3448308752,1.2718425491\H
,1.1343876052,-0.0230125185,-1.0946956604\F,-0.5418828726,1.0274612572
,-1.3974785236\F,-0.4883110798,-1.176932862,-1.2956238784\C,0.51001738
65,-1.1985821678,1.3893616582\H,1.5965521771,-1.2255803754,1.234656299
\H,0.087153456,-2.1256665413,0.9923251438\H,0.3308762952,-1.1731238897
,2.4693733651\H,1.5324993474,1.4100917547,1.112874333\H,0.2680917391,1
.4103607929,2.3500027346\H,-0.018207942,2.2097875129,0.7920042799\H,-1
.2008719237,0.0111617187,0.8731824535\\Version=IA64L-G03RevC.02\State=
1-A\HF=-356.9315991\RMSD=6.847e-09\RMSF=5.996e-05\Dipole=0.4336282,0.
0398377,0.6341166\PG=CS [SG(C2H2),X(C2H6F2)]\\@
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n.CH_CH3_2-CF3

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H7F3\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
F3.freq\\0,1\F,0.4431821262,0.4434631841,-1.6486284972\C,0.4074329452,
0.3978366405,-0.2963296592\F,1.6859414287,0.5001681718,0.1363380725\C,
-0.2560628745,-0.8746524952,0.2062194112\F,-0.2445257256,1.5089017105,
0.1222635381\C,-1.6804937504,-0.9985467807,-0.3521206557\C,-0.22517289
87,-0.9307671728,1.739974268\H,-1.6840437721,-0.9757045903,-1.44567378
31\H,-2.3118972372,-0.1801464874,0.0099597434\H,-2.1285736008,-1.94283
3903,-0.0271783741\H,0.7977158349,-0.8619488995,2.1212739491\H,-0.6584
819339,-1.8736483062,2.0882330779\H,-0.8075896573,-0.1092264388,2.1705
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291949\H,0.3572693735,-1.6925101225,-0.1933620151\\Version=IA64L-G03RevC.02\State=1-A\HF=-456.1850621\RMSD=4.747e-09\RMSF=2.375e-05\Dipole=-0.3831239,-0.6742302,0.2880681\PG=C01 [X(C4H7F3)]\\@

n.CH_CH3_2-CC12H

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C4H8Cl2\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CC12H.freq\\0,1\C,0.3450121831,-0.2409218115,-0.4564260216\C,0.4074231908,-0.4930834171,1.0562954724\H,1.2679456788,-0.5510390524,-0.9438492307\Cl,0.14834822,1.5111184631,-0.8736892537\Cl,-0.9636045135,-1.2150937887,-1.2464863567\C,1.6854934463,0.1238041959,1.6474156481\C,-0.8459200252,-0.0447089108,1.8160249548\H,2.5831887068,-0.2126006527,1.1152774869\H,1.7877413001,-0.1731406113,2.6965879956\H,1.6544211989,1.217196146,1.6066254931\H,-0.7628820643,-0.3364303102,2.8683501722\H,-1.7502854955,-0.5038137505,1.4065997532\H,-0.9629336035,1.0430020511,1.7749637552\H,0.4901084986,-1.5861336235,1.1385696283\\Version=IA64L-G03RevC.02\State=1-A\HF=-1077.6437577\RMSD=4.240e-09\RMSF=2.257e-05\Dipole=0.5762652,-0.2943182,0.7006057\PG=C01 [X(C4H8Cl2)]\\@

n.CH_CH3_2-CC13

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H7Cl3\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CC13.freq\\0,1\C,-0.1096053597,0.0088474919,-0.2246693995\C,-0.2429564863,0.0246466193,1.3181888761\Cl,1.6141518094,-0.1415216269,-0.7474244212\Cl,-0.7918247156,1.5289579567,-0.9379222537\Cl,-1.0427592392,-1.3756418623,-0.9298655813\C,0.458361312,1.2326540882,1.9599121977\C,0.2410764815,-1.2821987159,1.9668834736\H,1.5422933254,1.1818983966,1.8171842189\H,0.2596546997,1.2228809813,3.0365970792\H,0.098743205,2.1824532173,1.5580363599\H,1.3175834037,-1.4188957341,1.8243958156\H,-0.2763108369,-2.1584380631,1.5700675827\H,0.0475004617,-1.2325646977,3.0434033061\H,-1.3233734715,0.1184630488,1.4870331061\\Version=IA64L-G03RevC.02\State=1-A\HF=-1537.2246039\RMSD=4.848e-09\RMSF=2.540e-05\Dipole=-0.007412,0.0032167,0.9292141\PG=C01 [X(C4H7Cl3)]\\@

n.CH_CH3_2-CH2Cl

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C4H9Cl1\CYL509\10-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CH2Cl.freq\\0,1\C,-0.8995444085,0.2513772411,-0.5972700021\C,-0.5565268817,0.1712369254,0.8922999143\Cl,1.1713063011,-0.3218882697,1.2240525255\C,-0.0958025979,1.334441154,-1.3287170446\C,-0.7985592174,-1.1096125936,-1.298444681\H,-1.1752041551,-0.5702309079,1.4026442105\H,-0.6830586319,1.139701563,1.3812375466\H,0.2366514228,-1.4663702622,-1.3150428523\H,-1.1470431557,-1.0346943553,-2.3345065512\H,-1.4082399741,-1.8672859906,-0.7918625278\H,0.9706922217,1.0864444236,-1.346604159\H,-0.2066001374,2.3116099772,-0.8436650609\H,-0.4376014519,1.4323433612,-2.3650864259\H,-1.9592046243,0.5559264141,-0.603216234\\Version=IA64L-G03RevC.02\State=1-A\HF=-618.0538415\RMSD=9.932e-09\RMSF=7.865e-06\Dipole=-0.7989812,0.2262677,-0.2946105\PG=C01 [X(C4H9Cl1)]\\@

n.CH_CH3_2-CH2F

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H9F1\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CH2F.freq\\0,1\C,-0.3454399368,-0.2605289106,0.3432003965\C,0.7562869752,0.7614769629,0.0850320333\F,1.9266503278,0.120748503,-0.3209930764\C,-0.6216009365,-1.0987240327,-0.9111941126\C,-1.6084132716,0.4468253301,0.8533007379\H,0.9844860982,1.3362334939,0.992058193\H,0.461719149,1.4625323667,-0.7086513648\H,-1.4125163958,1.0201678241,1.7675485031\H,-2.3957301118,-0.2807368775,1.0784620505\H,-2.0055749941,1.1400383828,0.1004529921\H,0.2966892889,-1.5729550408,-1.2694435419\H,-1.017470381

5,-0.4716627138,-1.7211510042\H,-1.3582243372,-1.8836233382,-0.7058990
94\H,0.0217717527,-0.9310267226,1.1335266232\\Version=IA64L-G03RevC.02
\State=1-A\HF=-257.6859932\RMSD=5.214e-09\RMSF=2.313e-05\Dipole=-0.584
7774,0.1950406,0.2134178\PG=C01 [X(C4H9F1)]\\@

n.CH_CH3_2-CH2OH

1\1\GINC-AC20\FOpt\RB3LYP\Gen\C4H10O1\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-
CH2OH.freq\\0,1\C,-0.3772234345,-0.241629653,0.3366644668\C,0.75708711
51,0.7471096364,0.0638997384\O,1.9435803982,0.0131122955,-0.2253132321
\C,-0.6502317583,-1.1287159586,-0.885031796\C,-1.6390658291,0.50642514
49,0.7874489771\H,0.9014723166,1.3946458374,0.9449472906\H,0.478160949
,1.3994795963,-0.7820720585\H,2.6402526007,0.6477813516,-0.44913918\H,
-1.454707588,1.108395549,1.6856184326\H,-2.4481519553,-0.196157402,1.0
166016802\H,-2.0015912253,1.1807049133,0.0003573966\H,0.2601023832,-1.
6447509456,-1.2023602682\H,-1.011907066,-0.5272089298,-1.7300410272\H,
-1.4154682114,-1.8812256704,-0.6609276732\H,-0.0402019478,-0.885697681
9,1.1616329455\\Version=IA64L-G03RevC.02\State=1-A\HF=-233.662367\RMSD
=8.301e-09\RMSF=2.313e-05\Dipole=0.0322996,0.5684984,-0.0127036\PG=C01
[X(C4H10O1)]\\@

n.CH_CH3_2-CH2Ph

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C10H14\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
H2Ph.freq\\0,1\C,-1.4875826286,-1.4102627199,0.4763721718\C,-0.0511645
797,-1.3988896423,-0.1053117586\C,0.6142008346,-0.0382613556,-0.119073
5638\C,0.7484560602,0.6976512091,-1.3037244701\C,1.1067200721,0.525008
2576,1.0678104406\C,1.3501545373,1.9579215776,-1.305646797\C,1.7079296
422,1.7833247905,1.0725279937\C,1.8314696825,2.5059936858,-0.116418056
8\H,2.3027727732,3.4852691277,-0.1154098875\H,1.4450559382,2.508909788
2,-2.2379671745\H,2.0854809337,2.1980944906,2.0038189134\H,0.380490529
8,0.2757607211,-2.2365072631\H,1.0227158991,-0.0337290526,1.9979610727
\H,0.5629837196,-2.0936218841,0.4841134874\H,-0.0826032782,-1.80417521
48,-1.1261350328\C,-1.9920258243,-2.8528370477,0.6227325268\C,-2.45762
47677,-0.571881744,-0.3666886237\H,-1.3284528391,-3.4479733416,1.26171
92571\H,-2.0475502605,-3.350133874,-0.3545860723\H,-2.9953397676,-2.87
81640458,1.0641131444\H,-2.1201318411,0.4656314587,-0.4580324594\H,-3.
4585301962,-0.5637371671,0.0807959542\H,-2.5511277918,-0.9851038349,-1
.3800966017\H,-1.4389619907,-0.9636292375,1.4807334848\\Version=IA64L-
G03RevC.02\State=1-A\HF=-389.5080308\RMSD=7.431e-09\RMSF=1.999e-06\Dip
ole=-0.0511939,-0.0634861,0.0417523\PG=C01 [X(C10H14)]\\@

n.CH_CH3_2-CH_CH2_2

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C6H12\CYL509\18-May-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-CH
_CH2_2.freq\\0,1\C,-1.604598876,0.6856297198,-0.8568521548\C,-1.658129
3808,0.7777984057,0.6509643325\C,-0.3274537471,0.6721848496,-0.0529808
876\H,-1.9238158629,-0.2464421641,-1.3181273192\H,-1.847119196,1.57082
51471,-1.4389258105\H,-2.013085817,-0.0927092477,1.1983812292\H,-1.937
4425667,1.7260825358,1.102549811\H,0.2617800109,1.5896969895,-0.088237
5142\C,0.5132844118,-0.5915824115,0.0542493141\C,1.3296283563,-0.60366
81628,1.3559271822\C,1.4210936689,-0.7573751769,-1.1742285582\H,2.1346
50375,0.0738110879,-1.2471215094\H,0.8355362981,-0.775480899,-2.100337
502\H,2.0002379543,-1.6869758205,-1.1189293392\H,0.6788709285,-0.51236
36718,2.2328764508\H,1.9072524009,-1.5305804454,1.4550671518\H,2.03967
99608,0.2333685842,1.379087618\H,-0.1794910843,-1.4471554395,0.0812413
638\\Version=IA64L-G03RevC.02\State=1-A\HF=-235.8405315\RMSD=3.057e-09
\RMSF=1.100e-05\Dipole=0.0056257,0.0065979,-0.0002355\PG=C01 [X(C6H12)
]\\@

n.CH_CH3_2-CH2CH=CH2

```
1\1\GINC-AC8\FOpt\RB3LYP\Gen\C6H12\CYL509\11-Apr-2008\0\B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CH
CH=CH2.freq\0,1\C,0.4655526568,0.2666590059,-0.6578613259\C,0.5266822
669,-0.1180351921,0.8402178296\H,1.496296467,0.3037708281,-1.043392005
9\H,0.058294353,1.2828307697,-0.756656599\C,-0.3347880439,-0.686457906
8,-1.5030334683\C,1.5283876897,0.7745593343,1.5861036379\C,-0.85870732
97,-0.0625275234,1.4981594261\C,-1.4017835544,-0.3661397359,-2.2366369
964\H,0.0087208689,-1.7233283434,-1.4976642517\H,-1.9323880056,-1.1052
219224,-2.831334539\H,-1.7834532921,0.6524505779,-2.2750690847\H,2.531
8193139,0.704312411,1.1490952202\H,1.6014716279,0.4912799878,2.6427579
294\H,1.2201647491,1.8275698484,1.5460597116\H,-0.8109927228,-0.385093
9774,2.5449882781\H,-1.5773390263,-0.7027774633,0.9760562303\H,-1.2546
937838,0.9617217636,1.4834468266\H,0.8900373382,-1.1558623716,0.900017
6664\Version=IA64L-G03RevC.02\State=1-A\HF=-235.8491004\RMSD=3.598e-0
9\RMSF=3.370e-06\Dipole=0.1007294,-0.0241696,0.0694063\PG=C01 [X(C6H12
)]\@
```

n.CH_CH3_2-CH2CH3

```
1\1\GINC-AC28\FOpt\RB3LYP\Gen\C5H12\CYL509\19-May-2008\0\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CH
2CH3.a2.freq\0,1\C,0.3518083518,0.4640127112,-0.0507413803\C,0.407348
2286,0.4444889358,1.4844246407\C,1.7687704961,0.4133891405,-0.64136686
3\C,-0.5143856111,-0.6753981157,-0.624043221\C,-1.9979904151,-0.616566
5932,-0.2422241671\H,-0.0907427243,-1.6392570181,-0.3039090471\H,-0.43
04904589,-0.6574615371,-1.7197926606\H,2.3844374983,1.2428807477,-0.27
34627464\H,1.7482274788,0.4702678895,-1.736389284\H,2.2745161782,-0.52
17533844,-0.3665356168\H,-0.5850830384,0.5535312837,1.9347483554\H,1.0
331790296,1.2607329048,1.86457604\H,0.8373704683,-0.4989728721,1.84675
05017\H,-0.1073885035,1.4164966384,-0.3596399933\H,-2.5620093485,-1.41
45684362,-0.7386634862\H,-2.1500008877,-0.7314997709,0.8366321505\H,-2
.445321993,0.3400470831,-0.5406082686\Version=IA64L-G03RevC.02\State=
1-A\HF=-197.771131\RMSD=4.905e-09\RMSF=4.158e-06\Dipole=-0.0144368,0.0
116158,-0.0150288\PG=C01 [X(C5H12)]\@
```

n.CH_CH3_2-CH_CH3_2

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C6H14\CYL509\11-Apr-2008\0\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CH
_CH3_2.freq\0,1\C,-0.5244807287,1.8918762529,-0.1609092293\H,-0.27067
29715,2.2242383399,0.8547357319\H,-1.6139633899,1.8131428254,-0.224560
8164\H,-0.2124845524,2.6828726032,-0.8529867196\C,0.1824241849,0.56743
90223,-0.497763363\C,1.6997850061,0.8082075735,-0.5808585596\H,-0.1616
799065,0.2474943197,-1.4949057766\C,-0.1824241849,-0.5674390223,0.4977
63363\C,0.5244807287,-1.8918762529,0.1609092293\C,-1.6997850061,-0.808
2075735,0.5808585596\H,2.2427789053,-0.0660626374,-0.9523788566\H,2.11
05216514,1.0644695464,0.4050714732\H,1.9218376726,1.6427878744,-1.2562
493166\H,-1.9218376726,-1.6427878744,1.2562493166\H,-2.1105216514,-1.0
644695464,-0.4050714732\H,-2.2427789053,0.0660626374,0.9523788566\H,1.
6139633899,-1.8131428254,0.2245608164\H,0.2706729715,-2.2242383399,-0.
8547357319\H,0.2124845524,-2.6828726032,0.8529867196\H,0.1616799065,-0
.2474943197,1.4949057766\Version=IA64L-G03RevC.02\State=1-AG\HF=-237.
0825063\RMSD=4.160e-09\RMSF=8.796e-06\Dipole=0.,0.,0.\PG=CI [X(C6H14)]
\@
```

n.CH_CH3_2-C_CH3_3

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C7H16\CYL509\11-Apr-2008\0\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-C
CH3_3.freq\0,1\C,-0.0304140891,-0.079326282,1.727967837\C,0.296912647
```

```
2,0.472104568,0.325307508\C,-0.2851336076,1.8974100859,0.2048799814\C,
-0.2785704282,-0.4339003404,-0.8193401734\H,0.3865071639,0.5780400941,
2.5008458124\H,0.3945504399,-1.0770894967,1.8848172719\H,-1.1105959062
,-0.1418142546,1.9012610111\C,1.8305107914,0.5827805599,0.1817665446\C
,0.3136080347,-1.854971696,-0.8529700878\C,-1.8152869588,-0.5321084503
,-0.8297118882\H,2.2312886347,1.3049760951,0.9033254612\H,2.1120921922
,0.925875051,-0.8220643193\H,2.3343189769,-0.372006009,0.3642047864\H,
0.1962459608,2.5695209247,0.9255583233\H,-1.3612915861,1.9243906658,0.
4045793697\H,-0.1180411869,2.3116463028,-0.7977000893\H,1.403982628,-1
.8544271997,-0.9438530477\H,-0.0845314231,-2.4068815427,-1.7126243307\
H,0.0507968169,-2.4251010889,0.0462368698\H,-2.2989980511,0.446549154,
-0.9033979458\H,-2.1958769569,-1.0290518853,0.0707818038\H,-2.14734937
74,-1.1250775728,-1.6900880235\H,0.0171433364,0.0585200915,-1.75928128
27\Version=IA64L-G03RevC.02\State=1-A'\HF=-276.3932387\RMSD=2.895e-09
\RMSF=9.266e-06\Dipole=0.0011894,0.0021936,-0.0158953\PG=CS [SG(C3H2),
X(C4H14)]\@
```

n.CH_CH3_2-CCH

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C5H8\CYL509\10-Apr-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CCH
.freq\0,1\C,0.0552292952,0.5569280982,-0.0087219942\C,0.2631275603,0.
6332215218,1.517626924\C,1.4015183903,0.4853560694,-0.7585166756\C,-0.
8075879336,-0.5762887555,-0.3665996951\C,-1.5109209821,-1.5150386786,-
0.6558283493\H,-2.1291600842,-2.3447387645,-0.9127755403\H,-0.69390128
01,0.7101130914,2.0430005326\H,0.7795442021,-0.261609264,1.8821156881\
H,0.8704631501,1.5089809638,1.773287635\H,1.249154682,0.4574367768,-1.
8419128433\H,2.0155211487,1.3603773277,-0.516856398\H,1.956090766,-0.4
143803299,-0.4702176013\H,-0.4559105651,1.4787506669,-0.3244027318\Ve
rsion=IA64L-G03RevC.02\State=1-A'\HF=-195.2811677\RMSD=4.060e-09\RMSF=6
.882e-05\Dipole=0.1565695,0.1825906,0.0656017\PG=C01 [X(C5H8)]\@
```

n.CH_CH3_2-CH=C_CH3_2

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C7H14\CYL509\11-Apr-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CH
=C_CH3_2.freq\0,1\H,3.2810833926,-0.0127884769,-0.6877946071\C,2.5671
765004,-0.7226327289,-0.2460224012\C,1.2970382498,-0.0236976795,0.1815
556768\C,1.5063813818,1.0736727952,1.197392064\C,0.1104023778,-0.38650
59625,-0.3290000128\C,-1.2632455563,0.1711615067,-0.0441631391\C,-1.88
3010462,0.7601330856,-1.3263934106\C,-2.176180616,-0.9197618041,0.5487
504228\H,0.110055367,-1.2008240132,-1.0585812654\H,2.3731150031,-1.509
7463475,-0.9815182931\H,3.077535486,-1.179138722,0.6141174577\H,2.1868
282375,1.8414900361,0.8030260623\H,1.9834000327,0.6758272283,2.1041709
208\H,0.5808159786,1.5702852682,1.4975865925\H,-2.2826452575,-1.761686
2853,-0.1474965259\H,-3.179837068,-0.5257959982,0.7506808399\H,-1.7670
557738,-1.3123577975,1.4860926353\H,-1.2642149766,1.5689710075,-1.7301
241842\H,-2.8856565456,1.1598882812,-1.1309251343\H,-1.9766978285,-0.0
085757019,-2.1043656756\H,-1.1880973001,0.9802362463,0.6924159783\Ver
sion=IA64L-G03RevC.02\State=1-A'\HF=-275.1710644\RMSD=9.779e-09\RMSF=3.
244e-05\Dipole=0.0671433,0.0653153,0.0690119\PG=C01 [X(C7H14)]\@
```

n.CH_CH3_2-CH=CH2

```
1\1\GINC-AC7\FOpt\RB3LYP\Gen\C5H10\CYL509\18-May-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-CH=
CH2.a2.freq\0,1\H,1.9531986445,1.4881115826,-0.8111209638\C,2.0419582
426,0.6999882826,-0.0654595813\H,3.0310836853,0.5424822662,0.356758067
3\C,0.9916519684,-0.0315139047,0.3078604667\C,-0.4137866242,0.11482006
29,-0.2213290203\H,1.1281313377,-0.8124099495,1.0602040719\C,-0.870739
33,-1.1782906569,-0.9225251172\C,-1.3864783759,0.4970404522,0.91023918
52\H,-0.2062446333,-1.4334514009,-1.7550614528\H,-1.8886688298,-1.0712
```

023175,-1.3162853151\H,-0.8718787065,-2.0242664897,-0.223077037\H,-1.0
902966155,1.4381362443,1.3860489721\H,-1.4090913784,-0.2785957318,1.68
66253389\H,-2.4071840807,0.6129212983,0.526303861\H,-0.414684709,0.926
0090812,-0.9631111408\\Version=IA64L-G03RevC.02\State=1-A\HF=-196.5354
58\RMSD=1.800e-09\RMSF=1.078e-05\Dipole=-0.1137885,-0.0299861,-0.00464
41\PG=C01 [X(C5H10)]\\@

n.CH_CH3_2-CH=CHCH3

1\1\GINC-AC22\FOpt\RB3LYP\Gen\C6H12\CYL509\20-May-2008\0\\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\CH_CH3_2-CH
=CHCH3.a2.freq\\0,1\H,1.4752959519,0.0003330106,-1.5017439229\C,1.5177
909156,0.0002133183,-0.4103899814\C,2.8929464961,0.000285857,0.1953060
095\C,0.3716835889,0.0000161111,0.2750580387\C,-1.0126734647,-0.000065
2661,-0.3256467118\H,0.4101070046,-0.0001017685,1.3682195579\C,-1.7881
345589,-1.2676754177,0.0807181433\C,-1.7884254069,1.2672627026,0.08104
19141\H,-1.2643507512,-2.1731354433,-0.2444701501\H,-2.791523855,-1.27
36917692,-0.3622771644\H,-1.9055075958,-1.3222842599,1.1707777094\H,-1
.2648460614,2.1729266278,-0.2439080331\H,-1.9058180379,1.3215619438,1.
171114908\H,-2.7918131549,1.2731657921,-0.3619581943\H,-0.9088808153,0
.0000861526,-1.4201462697\H,2.8500032069,0.000194869,1.289908318\H,3.4
691807184,-0.8800376472,-0.1210900064\H,3.4690279694,0.88075866,-0.120
9512266\\Version=IA64L-G03RevC.02\State=1-A\HF=-235.854767\RMSD=1.835e
-09\RMSF=4.478e-06\Dipole=0.0308731,0.0000038,-0.0257212\PG=C01 [X(C6H
12)]\\@

n.CH_CH3_2-CHO

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H8O1\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
HO.freq\\0,1\O,1.0227075805,0.8032421514,-1.4117625116\C,1.0627656376,
0.201535056,-0.3615224904\H,2.0139172095,0.141723965,0.2189571262\C,-0
.1103070504,-0.5134899207,0.2846326288\C,-1.3892683379,-0.3826039946,-
0.5433326496\C,-0.2757713175,-0.0184987059,1.7352993553\H,-1.236172785
4,-0.7422953594,-1.5650003692\H,-1.7026627713,0.6648283433,-0.60884908
99\H,-2.2038113153,-0.9571216019,-0.0893119835\H,0.6593586221,-0.10417
22888,2.3014077193\H,-1.0377523591,-0.6081428529,2.2554112237\H,-0.589
6696936,1.0317030392,1.7563602316\H,0.1906188581,-1.5741150647,0.33466
41706\\Version=IA64L-G03RevC.02\State=1-A\HF=-232.4593426\RMSD=8.667e-
09\RMSF=1.582e-05\Dipole=-0.1974047,-0.5347207,0.8573253\PG=C01 [X(C4H
8O1)]\\@

n.CH_CH3_2-CN

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C4H7N1\CYL509\11-Apr-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
N.freq\\0,1\N,0.2300683493,-0.3648705698,-2.1811348123\C,0.2797179177,
-0.1791502434,-1.0360243672\C,0.3323604648,0.0558647427,0.4163767021\C
, -0.3636968943,-1.0925760775,1.1742422776\C,-0.2696674272,1.431956265,
0.7625682778\H,-0.2729507856,-0.9285793701,2.2531159732\H,-1.427893093
1,-1.1355055403,0.9203589022\H,0.0860675136,-2.0598028207,0.9314488464
\H,0.2459771696,2.2370277379,0.2306903758\H,-1.3310290227,1.4697492885
,0.4960552755\H,-0.1782199322,1.6132209716,1.8386992657\H,1.3952853391
,0.0614156011,0.6945977058\\Version=IA64L-G03RevC.02\State=1-A\HF=-211
.3831056\RMSD=3.970e-09\RMSF=8.768e-05\Dipole=0.0020512,0.2501003,1.53
09894\PG=C01 [X(C4H7N1)]\\@

n.CH_CH3_2-COCH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C5H10O1\CYL509\19-May-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-
COCH3.a2.freq\\0,1\C,-0.740955384,0.5730398303,-1.856345293\C,-0.67182
72094,0.1253368955,-0.405683622\C,0.6937099251,0.2194360388,0.28621252

15\O,-1.6519238468,-0.3016728876,0.1757976253\H,-1.6946626433,0.273990
1098,-2.2961226142\H,0.0890142581,0.1627223072,-2.4435531306\H,-0.6524
099431,1.6667917869,-1.9033748785\C,1.4674955142,-1.0916590295,0.02493
61303\C,0.5395326039,0.4870475854,1.7871329585\H,1.5195050548,0.515474
2632,2.276393503\H,-0.0632134442,-0.2977674528,2.2531246399\H,0.037873
9661,1.4432333462,1.9719225643\H,2.4630697292,-1.0407964074,0.47936791
77\H,1.5979175087,-1.2880501182,-1.0455143305\H,0.9347637009,-1.942546
1658,0.4640316995\H,1.2557998891,1.0411235093,-0.1801725447\Version=I
A64L-G03RevC.02\State=1-A\HF=-271.7832112\RMSD=8.614e-09\RMSF=1.314e-0
5\Dipole=0.8750488,0.3290289,-0.4736092\PG=C01 [X(C5H10O1)]\@

n.CH_CH3_2-CON_CH2CH3_2

1\1\GINC-AC8\FOpt\RB3LYP\Gen\C8H17N1O1\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-CON_CH2CH3_2.freq\0,1\H,2.0739032387,-1.2454836116,2.8616971259\C,1.
6066314394,-1.3829588167,1.8794500628\C,1.3528231032,-0.0272663993,1.2
106621079\N,0.7914914031,-0.1332087208,-0.1374536658\C,1.7444288803,-0
.2525749436,-1.2488080607\C,2.1532652461,1.101633294,-1.8344642208\C,-
0.5452051514,-0.0759920552,-0.4523236184\O,-0.9211834182,-0.0978488244
, -1.624104631\C, -1.576012526,0.0444631341,0.682233464\C, -1.9551898283,
1.5286510758,0.8567588525\C, -2.8090376568,-0.8048750612,0.342641886\H,
2.2957583565,0.5268286482,1.1288908385\H,0.7001724014,0.5876162395,1.8
348291769\H,1.2745953785,-0.8628502164,-2.0225091981\H,2.6228044887,-0
.7931864727,-0.8775292075\H,0.6701514181,-1.9337970029,2.0186334837\H,
2.2733132535,-2.0038482446,1.2710140303\H,1.2759710562,1.6104993811,-2
.243640186\H,2.8811743994,0.9643208687,-2.6427452685\H,2.6103178422,1.
7481378547,-1.0756393745\H,-1.0919108507,2.1428062552,1.1398313436\H,-
2.7201721162,1.6418135698,1.6332999885\H,-2.3559293413,1.9250632545,-0
.0822633997\H,-2.5531062693,-1.8681024552,0.2739907531\H,-3.2245455634
, -0.4996056948,-0.6210005202\H,-3.5764578462,-0.6879812909,1.116378670
3\H,-1.1572333608,-0.3234608086,1.6248716129\Version=IA64L-G03RevC.02
\State=1-A\HF=-445.0885403\RMSD=9.477e-09\RMSF=3.476e-06\Dipole=0.7812
356,0.0446029,1.1261956\PG=C01 [X(C8H17N1O1)]\@

n.CH_CH3_2-CON_CH3_2

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H13N1O1\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-CON_CH3_2.freq\0,1\C,1.2196148156,-0.1611146331,-0.4301138169\C,-0.
1154091313,0.4806949916,-0.0142358167\N,-1.2330887691,-0.3202673661,0.
0928881357\O,-0.1665798852,1.6817646213,0.2406433716\C,1.9270380074,-0
.727608591,0.8180893454\C,2.0960163336,0.8826635715,-1.1339855599\C,-1
.2950631374,-1.7561872455,-0.1160651132\C,-2.4915546265,0.2868659012,0
.5039832539\H,-1.9926885303,-2.000239372,-0.9298211539\H,-0.3204759957
, -2.170359915,-0.3650626126\H,-1.6546128789,-2.2581342316,0.7932799522
\H,-3.2704920741,0.0925878055,-0.2453375769\H,-2.8275549065,-0.1289057
472,1.4639445979\H,-2.3391038577,1.35987147,0.6069106227\H,3.058347452
2,0.4393849745,-1.4147179222\H,2.275601762,1.7376552409,-0.4775855928\H,
1.6134216435,1.2590478668,-2.0419987469\H,2.8974766712,-1.1579171629
,0.5459971649\H,1.3375516623,-1.5083487151,1.3121426108\H,2.1014245672
,0.072261593,1.5462600442\H,1.041511382,-0.9810331834,-1.135409066\Ver
sion=IA64L-G03RevC.02\State=1-A\HF=-366.4563222\RMSD=2.171e-09\RMSF=1
.315e-06\Dipole=-0.2721287,-1.3288192,-0.1383841\PG=C01 [X(C6H13N1O1)]
\@

n.CH_CH3_2-CONH2

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H9N1O1\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2
-CONH2.freq\0,1\C,0.6131467829,-0.2575285182,0.3991753516\C,-0.775639
4586,0.2000686553,-0.0624649977\N,-1.7610208103,0.159412868,0.88462139

```
22\O,-0.9890570864,0.5770424824,-1.2069867025\C,1.0456980174,-1.475314
464,-0.433707977\C,1.6050595218,0.9070473444,0.2443887649\H,-1.5961272
679,-0.1449117172,1.8312139318\H,-2.6912629019,0.4553802898,0.62333189
\H,2.615976253,0.5919582487,0.5263180633\H,1.3254586445,1.7593206605,0
.8743169625\H,1.6206553633,1.2460228198,-0.7960031468\H,2.0555683102,-
1.7948596197,-0.1529761571\H,1.0423026679,-1.2182942366,-1.4974438591\
H,0.3668824774,-2.3234159214,-0.2877783953\H,0.5705596357,-0.549068564
1,1.4582177341\Version=IA64L-G03RevC.02\State=1-A\HF=-287.8410234\RMS
D=3.688e-09\RMSF=3.138e-05\Dipole=-0.0789243,-0.3600367,1.341789\PG=C0
1 [X(C4H9N1O1)]\@
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n.CH_CH3_2-CONHCH3

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H11N1O1\CYL509\11-Apr-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_
2-CONHCH3.freq\0,1\H,-2.7519983468,1.5206197454,-1.4062140491\C,-2.56
01931335,0.6379302029,-0.7841524978\N,-1.3114287477,0.7670370102,-0.05
54357868\C,-0.2675935532,-0.1027084746,-0.2150435213\C,0.9728827146,0.
189442687,0.6375005375\O,-0.3078342823,-1.0567720396,-0.9852576185\C,2
.1718577916,0.4555137702,-0.2875325486\C,1.2397047051,-1.0042819846,1.
5690771986\H,-1.2072940244,1.5303189157,0.5967064815\H,-2.4683844119,-
0.2390277468,-1.4265671999\H,-3.4071939327,0.4965629892,-0.1018867144\
H,3.0819701777,0.6235922044,0.2992625853\H,2.005028066,1.3369272845,-0
.917449664\H,2.3324074346,-0.4045062138,-0.9448654782\H,2.1486009392,-
0.8381574179,2.1583081921\H,1.3670667502,-1.9162141465,0.9777615703\H,
0.407583918,-1.1647505785,2.2643057978\H,0.7949377748,1.0841750034,1.2
51654923\Version=IA64L-G03RevC.02\State=1-A\HF=-327.1523274\RMSD=2.76
5e-09\RMSF=1.819e-06\Dipole=-0.2923768,1.1112489,0.7266238\PG=C01 [X(C
5H11N1O1)]\@
```

n.CH_CH3_2-COOC_CH3_3

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C8H16O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
COOC_CH3_3.freq\0,1\H,-1.4358689152,-1.6930724969,-2.6294068909\C,-1.
2326576954,-1.312196877,-1.6221033276\C,0.1811028913,-0.7232078995,-1.
5725455685\C,0.3353973903,0.4956349977,-2.4886174836\O,0.5283288508,-0
.3575553916,-0.1861534594\C,-0.1723333081,0.5655294094,0.5065078384\O,
-1.1197579628,1.1938333115,0.0789325194\C,0.3765329357,0.6886770148,1.
9264265367\C,1.2261617214,-1.7903151006,-1.9080307575\C,-0.0693708828,
2.0047098002,2.5695645617\C,-0.0646495253,-0.5368802218,2.7532779247\H
,1.0802714065,-2.152842475,-2.9311135244\H,1.1439708128,-2.6411156448,
-1.2237441905\H,2.2378663812,-1.3798199493,-1.8263943296\H,-1.98309754
9,-0.5599076599,-1.3742818803\H,-1.3219845575,-2.1482008289,-0.9195137
99\H,0.1985023836,0.189689135,-3.5320495434\H,1.3399124387,0.921588107
2,-2.3892046625\H,-0.4002253518,1.2650798881,-2.2494198605\H,0.3346499
217,2.0863399953,3.5847200004\H,-1.1609359986,2.0589370547,2.623207496
2\H,0.27533608,2.8686802766,1.9922140532\H,0.3488724416,-0.4778069297,
3.7660375187\H,0.2795039426,-1.4686567696,2.2945342474\H,-1.1572193344
,-0.5752170937,2.8369712919\H,1.4707776315,0.6643952917,1.8483332469\
Version=IA64L-G03RevC.02\State=1-A\HF=-464.9673476\RMSD=4.662e-09\RMSF
=1.788e-05\Dipole=0.4846759,-0.5193976,-0.0628331\PG=C01 [X(C8H16O2)]\
\@
```

n.CH_CH3_2-COOCH2CH3

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H12O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
COOCH2CH3.freq\0,1\C,-1.5281375269,0.2627675399,0.237917529\C,-0.2139
074135,-0.4539701311,-0.0459486058\O,-0.1017135813,-1.5463771365,-0.56
08547578\O,0.8437555425,0.3037546853,0.3283388929\C,2.1497634874,-0.25
60326375,0.0617053196\C,3.1828011118,0.742197481,0.5499297925\C,-1.725
```

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9137173,1.3974931628,-0.7888197557\C,-2.6970694633,-0.7261859426,0.234
1250032\H,2.2325244524,-1.2187657452,0.5765142758\H,2.2394241958,-0.44
91894285,-1.0123541735\H,3.0809125647,1.6986171584,0.0269284979\H,4.19
0923205,0.354719177,0.3662822057\H,3.0740523304,0.9241586532,1.6239959
446\H,-2.7839211884,-1.218472156,-0.7392928016\H,-3.6362519517,-0.2034
476258,0.4459882787\H,-2.5610477234,-1.5082707612,0.9879196511\H,-0.89
32733965,2.1067452173,-0.7613839563\H,-2.6510302448,1.9432374377,-0.57
34859468\H,-1.8019709606,0.9922880968,-1.8047064873\H,-1.4318958422,0.
7217427516,1.2302657341\\Version=IA64L-G03RevC.02\State=1-A\HF=-386.33
58063\RMSD=6.934e-09\RMSF=2.950e-06\Dipole=0.2351744,0.6524868,0.25601
62\PG=C01 [X(C6H12O2)]\\@
```

n.CH_CH3_2-COOCH3

```
1\1\GINC-AC11\FOpt\RB3LYP\Gen\C5H10O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-
COOCH3.freq\\0,1\C,0.1390720828,0.3806797642,-1.0955557185\C,0.2041505
278,-0.0463917689,0.3647038528\O,0.9751208639,-0.8561709429,0.83341424
5\O,-0.7474240418,0.5807290311,1.0977558446\C,-0.801105608,0.208628772
3,2.4839726974\H,-1.6101940838,0.7991943589,2.9153027913\C,-1.07846183
44,-0.2853532926,-1.7702591843\C,1.4487742209,0.048240363,-1.815878436
5\H,-1.0073813117,-0.8600451126,2.589004585\H,0.1464697996,0.435366452
6,2.980081863\H,2.3007100629,0.5530067671,-1.3491271143\H,1.394753427,
0.3624997125,-2.8639593947\H,1.6451806715,-1.0277686389,-1.7840817207\
H,-0.9754551956,-1.3768180206,-1.7654205257\H,-1.1560852758,0.04146767
35,-2.812916793\H,-2.0089572101,-0.0239508959,-1.2574265164\H,-0.02519
17951,1.4657599699,-1.1027171567\\Version=IA64L-G03RevC.02\State=1-A\H
F=-347.0168458\RMSD=4.125e-09\RMSF=1.421e-05\Dipole=-0.5306054,0.40473
41,-0.0464522\PG=C01 [X(C5H10O2)]\\@
```

n.CH_CH3_2-COOH

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H8O2\CYL509\11-Apr-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2-C
OOH.freq\\0,1\C,0.2949095063,-0.4138958831,-0.578984737\C,0.0092157441
,0.1887043807,0.787030981\O,0.125603632,1.354662931,1.0947058653\O,-0.
4319932705,-0.7493113844,1.6668623529\C,1.1162946426,0.5514810827,-1.4
372393956\C,-1.0337535642,-0.8104826349,-1.257211161\H,-0.6144386169,-
0.2714036313,2.4978343949\H,2.0662359741,0.804250891,-0.9560740224\H,0.
570108514,1.4858449304,-1.5995423289\H,1.3323398503,0.1006494618,-2.4
118534125\H,-0.8327204027,-1.2779148736,-2.2270964045\H,-1.6590009722,
0.0728403928,-1.4318788117\H,-1.5987826583,-1.5179881615,-0.6435768098
\H,0.8673774471,-1.3339330549,-0.4019324753\\Version=IA64L-G03RevC.02\
State=1-A\HF=-307.7102108\RMSD=2.629e-09\RMSF=2.407e-05\Dipole=-0.1239
546,-0.5731667,-0.1276065\PG=C01 [X(C4H8O2)]\\@
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n.CH_CH3_2-COPh

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C10H12O1\CYL509\11-Apr-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH_CH3_2
-COPh.freq\\0,1\C,-2.9674598149,-0.2349514258,-0.2055445398\C,-3.08921
92036,0.2042281328,1.116333254\C,-1.9496645503,0.5643231364,1.83705843
95\C,-0.6909186448,0.487068657,1.2404098209\C,-0.55690867,0.0467166549
,-0.0857733462\C,-1.7122090561,-0.3128190651,-0.7998277634\C,0.7636302
811,-0.0604276348,-0.7982373677\O,0.7973120332,-0.4146132973,-1.968369
4072\C,2.0657055018,0.2338748124,-0.0435110375\C,2.4549703459,-1.00635
00171,0.7922176264\C,3.1847762796,0.6223956584,-1.0159249789\H,-1.5942
16272,-0.6499834254,-1.8243322061\H,0.1823888879,0.773531253,1.8172134
264\H,-2.039675834,0.9073151686,2.8641677881\H,-3.8528932865,-0.515639
347,-0.7695850506\H,-4.0692537516,0.2660844954,1.5820913916\H,4.111881
4551,0.8220207278,-0.4670060109\H,2.9228385033,1.5203263003,-1.5853403
124\H,3.3680271264,-0.18105961,-1.7346105317\H,3.3747984253,-0.8096165
```

24,1.354191607\H,2.635582837,-1.8648973925,0.1354324402\H,1.6728108846
,-1.2857228096,1.5058509467\H,1.8929999469,1.070194088,0.6456811252\\V
ersion=IA64L-G03RevC.02\State=1-A\HF=-463.5224737\RMSE=3.611e-09\RMSE=
2.569e-06\Dipole=-0.2759583,0.2386172,1.0492991\PG=C01 [X(C10H12O1)]\\
@

n.CH2Cl-H

1\1\GINC-LC118\FOpt\RB3LYP\Gen\C1H3Cl1\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_-H
.freq\\0,1\C,0.,0.,1.1391029998\H,-1.0337728907,0.,1.4851004992\H,0.51
68864454,-0.8952735851,1.4851004992\H,0.5168864454,0.8952735851,1.4851
004992\C1,0.,0.,-0.6641129115\\Version=IA32L-G03RevC.02\State=1-A\HF=
-500.1085335\RMSE=4.027e-09\RMSE=2.190e-05\Dipole=0.,0.,0.8194529\PG=C
03V [C3(C1Cl1),3SGV(H1)]\\@

n.CH2Cl-BH2

1\1\GINC-LC25\FOpt\RB3LYP\Gen\C1H4B1Cl1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_-
BH2.freq\\0,1\C,0.0616881694,-0.2698377493,-0.783742479\H,1.0670884245
,-0.4594047578,-1.1818372609\H,-0.5358106722,-1.1445740125,-1.07199781
01\B,-0.5341674555,1.0207048747,-1.4278086564\H,-0.8932030727,1.961953
4066,-0.7916211482\H,-0.6214853585,1.0336500439,-2.6218458332\C1,0.193
1834671,-0.2868307387,1.029929424\\Version=IA32L-G03RevC.02\State=1-A\
HF=-525.5378615\RMSE=3.085e-09\RMSE=8.962e-06\Dipole=-0.0086859,-0.110
2617,-0.8153503\PG=C01 [X(C1H4B1Cl1)]\\@

n.CH2Cl-CH3

1\1\GINC-LC95\FOpt\RB3LYP\Gen\C2H5Cl1\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_-CH
3.freq\\0,1\H,-0.6373329462,-0.3057686766,-1.4905004182\C,-0.650259678
4,-0.3027734108,-0.3988938882\H,-1.0876347909,-1.2393740857,-0.0478054
672\C,-1.3778029419,0.9089508181,0.1581583614\H,-0.9196556025,1.839348
7658,-0.1897534501\H,-1.3696376271,0.9063645151,1.2520086219\H,-2.4213
7929,0.8894451697,-0.1801696379\C1,1.0943538811,-0.3368870666,0.123566
6772\\Version=IA32L-G03RevC.02\State=1-A\HF=-539.4262582\RMSE=3.386e-0
9\RMSE=9.765e-05\Dipole=-0.8622658,0.0825537,-0.2157114\PG=C01 [X(C2H5
Cl1)]\\@

n.CH2Cl-NH2

1\1\GINC-LC119\FOpt\RB3LYP\Gen\C1H4Cl1N1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_-
NH2.freq\\0,1\C,0.5303722129,0.5410877103,0.3972624972\H,0.4824635892
,0.5046823493,1.4840068793\H,1.5613431741,0.4993280331,0.0508726997\N,
-0.1355824237,1.6681010941,-0.1082775586\H,-0.1064698617,1.7245083918,
-1.1219411466\H,-1.1014466626,1.7294158408,0.1997623988\C1,-0.18053215
,-1.1400687374,-0.1316666414\\Version=IA32L-G03RevC.02\State=1-A\HF=-5
55.4617538\RMSE=5.149e-09\RMSE=5.309e-05\Dipole=0.008501,0.8369843,0.0
032904\PG=C01 [X(C1H4Cl1N1)]\\@

n.CH2Cl-OH

1\1\GINC-AC18\FOpt\RB3LYP\Gen\C1H3Cl1O1\CYL509\20-Aug-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Cl_-
OH.freq\\0,1\C,0.3997285877,0.7331263767,-0.0126895925\O,0.4556616374
,0.7446077078,1.3611641239\H,1.4206323328,0.7242549144,-0.3898020589\H
,-0.1764572217,1.5561052589,-0.4451048003\H,-0.446711999,0.8205684334,
1.711638395\C1,-0.4024192787,-0.7915616782,-0.6876415866\\Version=IA64
L-G03RevC.02\State=1-A\HF=-575.3184757\RMSE=6.795e-09\RMSE=6.666e-05\D
ipole=-0.1899292,0.8133432,0.1661823\PG=C01 [X(C1H3Cl1O1)]\\@

n.CH2Cl-F

```
1\1\GINC-LC117\FOpt\RB3LYP\Gen\C1H2Cl1F1\CYL509\26-Jun-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-F.freq\0,1\H,-0.6386339149,-0.2421294106,-1.4828517906\C,-0.66978443
58,-0.2551263487,-0.3920896939\H,-1.1573044424,-1.151499499,-0.0051261
993\F,-1.3102810952,0.8526220159,0.064791893\Cl,1.0357161669,-0.279365
3604,0.1916111231\Version=IA32L-G03RevC.02\State=1-A\HF=-599.3319433\
RMSD=3.649e-09\RMSF=2.751e-05\Dipole=-0.4114762,-0.470309,-0.4338456\PG
=C01 [X(C1H2Cl1F1)]\@
```

n.CH2Cl-SiH3

```
1\1\GINC-LC144\FOpt\RB3LYP\Gen\C1H5Cl1Si1\CYL509\26-Jun-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-SiH3.freq\0,1\H,0.6723420485,-0.0096939924,-1.5933153149\C,0.680214
6018,0.0015887682,-0.5006432921\H,1.7211418392,-0.0117150655,-0.168356
6317\Si,-0.2685175119,1.4941274286,0.1997504978\H,-1.6738616375,1.4660
780194,-0.2753196795\H,-0.2329247034,1.4631720005,1.68273503\H,0.39492
92856,2.736030548,-0.2866424118\Cl,-0.0708040751,-1.5630110659,0.04989
71642\Version=IA32L-G03RevC.02\State=1-A\HF=-790.7986722\RMSD=4.551e-
09\RMSF=4.721e-05\Dipole=0.3704063,0.5944082,-0.2717782\PG=C01 [X(C1H5
Cl1Si1)]\@
```

n.CH2Cl-PH2

```
1\1\GINC-LC135\FOpt\RB3LYP\Gen\C1H4Cl1P1\CYL509\26-Jun-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-PH2.freq\0,1\C,0.6364418925,0.0172346406,0.4709668391\H,0.6252027343
,0.0095250225,1.5627554917\H,1.6772604984,0.0068361859,0.1411536949\P,
-0.1744697969,1.5888456538,-0.13212167\H,-0.2750926477,1.2215485874,-1
.5015863371\H,-1.5142115898,1.2247147064,0.1727819039\Cl,-0.1008684351
,-1.5528657149,-0.0717106317\Version=IA32L-G03RevC.02\State=1-A\HF=-8
42.0487367\RMSD=4.900e-09\RMSF=1.553e-05\Dipole=0.1989519,0.3511837,0.
1465701\PG=C01 [X(C1H4Cl1P1)]\@
```

n.CH2Cl-SH

```
1\1\GINC-LC142\FOpt\RB3LYP\Gen\C1H3Cl1S1\CYL509\26-Jun-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-SH.freq\0,1\C,0.3041223046,0.5464926388,-0.4976525029\S,0.3025928317
,0.5751383187,1.3420137253\H,1.321278648,0.5309495983,-0.888441332\H,-
0.2506108055,1.3923038927,-0.9031629929\H,0.9506486531,1.7590581905,1.
4361596703\Cl,-0.5110315077,-0.9507929773,-1.0665211726\Version=IA32L
-G03RevC.02\State=1-A\HF=-898.2846419\RMSD=4.465e-09\RMSF=3.677e-05\Di
pole=0.489572,0.8892054,-0.2407893\PG=C01 [X(C1H3Cl1S1)]\@
```

n.CH2Cl-Cl

```
1\1\GINC-LC116\FOpt\RB3LYP\Gen\C1H2Cl2\CYL509\26-Jun-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-Cl.freq\0,1\H,-0.2847556997,-0.5406713548,-1.5291626351\C,-0.311000685
6,-0.545395073,-0.4419186269\H,-0.8327795046,-1.4194184744,-0.05898184
69\Cl,-1.2020338972,0.9117713378,0.0969085103\Cl,1.3775362079,-0.60397
95607,0.152483039\Version=IA32L-G03RevC.02\State=1-A\HF=-959.696347\R
MSD=3.077e-09\RMSF=2.117e-05\Dipole=-0.2953417,-0.5177471,-0.419556\PG
=C01 [X(C1H2Cl2)]\@
```

n.CH2Cl-Br

```
1\1\GINC-LC27\FOpt\RB3LYP\Gen\C1H2Br1Cl1\CYL509\26-Jun-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-Br.freq\0,1\H,0.1282420017,-0.893376808,-1.5756745177\C,0.104339517,
-0.902743524,-0.4894889333\H,-0.4431759998,-1.7579245042,-0.1030300679
\Br,-0.8731131686,0.7041087139,0.0745752157\Cl,1.7792857541,-0.9750613
```

235,0.1179709166\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-3073.3822345\\
RMSD=1.998e-09\\RMSF=1.942e-05\\Dipole=-0.264649,-0.5039359,-0.398536\\PG
=C01 [X(C1H2Br1Cl1)]\\@

n.CH2Cl-N_CH3_2

1\\1\\GINC-LC126\\FOpt\\RB3LYP\\Gen\\C3H8Cl1N1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_
-N_CH3_2.freq\\0,1\\C,1.0795214915,-0.5834825547,1.4112986494\\H,1.12927
04593,-0.4761657891,2.4993817862\\H,2.0997520376,-0.5816173185,1.016008
7768\\H,0.6137735275,-1.5512803554,1.1705588754\\N,0.3364692479,0.539622
4323,0.8508649765\\C,0.4513912235,0.727273352,-0.5170000022\\C,-0.998511
8937,0.7081243914,1.4139011467\\H,1.483726707,0.6769106612,-0.856820357
4\\H,-0.0513542129,1.6310447094,-0.8548982115\\H,-0.9223380253,0.7990201
883,2.5019509331\\H,-1.6605912739,-0.1376440542,1.1734099884\\H,-1.44916
90147,1.6242208384,1.0204505991\\Cl,-0.3995741096,-0.6396080612,-1.6161
938817\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-634.0823226\\RMSD=4.690e
-09\\RMSF=1.840e-05\\Dipole=0.3527571,0.5653961,1.065025\\PG=C01 [X(C3H8C
l1N1)]\\@

n.CH2Cl-NHCH3

1\\1\\GINC-LC120\\FOpt\\RB3LYP\\Gen\\C2H6Cl1N1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2Cl_
-NHCH3.freq\\0,1\\H,-1.459087391,0.5144925379,-2.6960064531\\C,-1.473080
1727,0.7335276065,-1.6242689764\\N,-0.4227524545,-0.0452188704,-0.97216
60914\\C,-0.3528132801,0.1500807134,0.4424555313\\H,-0.3992773978,1.2186
448527,0.6630827274\\H,-1.1098662497,-0.3751916735,1.0411422371\\H,-2.49
35517414,0.542289455,-1.2468290797\\H,-1.261771482,1.8015846101,-1.4991
827781\\H,-0.5125271305,-1.0344570465,-1.1900103817\\Cl,1.24415937,-0.45
01459154,1.1072851199\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-594.7593
21\\RMSD=2.879e-09\\RMSF=3.623e-06\\Dipole=-1.1368643,0.1126402,-0.388757
6\\PG=C01 [X(C2H6Cl1N1)]\\@

n.CH2Cl-NHCHO

1\\1\\GINC-LC121\\FOpt\\RB3LYP\\Gen\\C2H4Cl1N1O1\\CYL509\\26-Jun-2008\\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C
l_-NHCHO.freq\\0,1\\O,-1.7058070586,0.5560222738,-1.3023247197\\C,-1.763
57914,-0.1435317931,-0.3129766772\\N,-0.6978632228,-0.8356041928,0.2219
500835\\C,0.6266323587,-0.6591023524,-0.2538022954\\H,0.5854213016,-0.27
46194811,-1.2700786271\\H,1.1988196981,-1.5832997024,-0.1934816058\\H,-0
.8319512018,-1.2933074009,1.1147155349\\H,-2.6971791829,-0.3253097813,0
.2514127119\\Cl,1.5940040647,0.5701995528,0.7272384114\\Version=IA32L-G
03RevC.02\\State=1-A\\HF=-668.797455\\RMSD=8.321e-09\\RMSF=8.039e-05\\Dipol
e=-0.2470738,-1.301403,0.6495242\\PG=C01 [X(C2H4Cl1N1O1)]\\@

n.CH2Cl-NHCOCH3

1\\1\\GINC-LC122\\FOpt\\RB3LYP\\Gen\\C3H6Cl1N1O1\\CYL509\\26-Jun-2008\\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C
l_-NHCOCH3.freq\\0,1\\C,0.7415623144,-0.990661916,-0.3740229472\\H,1.654
7892965,-0.4453391779,-0.1493272335\\H,0.9077466108,-1.7889433906,-1.09
51571555\\N,-0.2384055519,-0.0754478668,-0.8242781024\\H,-1.1144005606,-
0.4521708143,-1.1620532176\\C,-0.1918433802,1.2680080881,-0.4695922352\\
O,0.7777368924,1.7550725438,0.0830957055\\C,-1.4347613982,2.0602827532,
-0.8313141799\\H,-1.1629703385,3.1115071418,-0.9391070719\\H,-2.16749645
07,1.9768658755,-0.0193560926\\H,-1.90594257,1.7058125127,-1.7541721216
\\Cl,0.2673807366,-1.8615265284,1.1925841258\\Version=IA32L-G03RevC.02\\
State=1-A\\HF=-708.122103\\RMSD=7.130e-09\\RMSF=4.272e-06\\Dipole=-0.92907
77,-0.1291399,-1.2450539\\PG=C01 [X(C3H6Cl1N1O1)]\\@

n.CH2Cl-NO2

```
1\1\GINC-LC124\FOpt\RB3LYP\Gen\C1H2Cl1N1O2\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl1-NO2.freq\0,1\O,-1.104929785,0.1457826225,-1.1187618486\N,-0.9963540206,-0.2585925037,0.0229949682\C,0.3507210155,-0.1912167889,0.7391027481\O,-1.8772867903,-0.7447401929,0.7243952681\H,0.1784550843,0.4142738511,1.6275724726\H,0.5879832343,-1.218606077,1.0108551841\Cl,1.6447909609,0.5031435911,-0.2399456634\Version=IA32L-G03RevC.02\State=1-A\HF=-704.594216\RMSD=6.892e-09\RMSF=1.002e-04\Dipole=0.6820242,-0.1281843,0.7922685\PG=C01 [X(C1H2Cl1N1O2)]\@
```

n.CH2Cl-OCF3

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H2Cl1F3O1\CYL509\20-Aug-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CH2Cl-OCF3.freq\0,1\C,-1.0325779692,-0.3108812076,-0.8970284724\O,-0.8237764961,0.2640594672,0.3695584232\C,0.2707425597,-0.1466685293,1.0730588555\F,1.424353596,0.1887149152,0.4779086275\F,0.2821547999,-1.4862233539,1.2381939426\F,0.2133951728,0.4323833831,2.2678197963\H,-0.6867392788,-1.3435156196,-0.9315005789\H,-2.1001618007,-0.2382497688,-1.0889893478\Cl,-0.1959415655,0.5882772689,-2.2263212385\Version=IA64L-G03RevC.02\State=1-A\HF=-912.3578713\RMSD=5.056e-09\RMSF=5.586e-05\Dipole=-0.5294376,-0.5380437,-0.0831775\PG=C01 [X(C2H2Cl1F3O1)]\@
```

n.CH2Cl-OCH2CH3

```
1\1\GINC-LC129\FOpt\RB3LYP\Gen\C3H7Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-OCH2CH3.freq\0,1\C,0.5614225671,-0.6553663365,0.4103221781\H,0.5404212268,-0.6692580219,1.508089832\H,1.6007603974,-0.6693532257,0.056329188\O,-0.1601226119,0.4105672584,-0.1167612927\C,0.3789082455,1.673126082,0.2761891464\C,-0.4757893041,2.762186852,-0.3480859149\H,1.4256390479,1.7553029288,-0.0599550068\H,0.3778740886,1.7558781597,1.3755262294\H,-0.0930222804,3.7497901248,-0.069111414\H,-1.5117813187,2.6793908622,-0.005579175\H,-0.4654461536,2.6788046332,-1.4391341265\Cl,-0.1988654802,-2.1908690067,-0.1448604496\Version=IA32L-G03RevC.02\State=1-A\HF=-653.9392017\RMSD=8.328e-09\RMSF=2.472e-05\Dipole=0.6388076,0.9084773,0.4662468\PG=C01 [X(C3H7Cl1O1)]\@
```

n.CH2Cl-OCH3

```
1\1\GINC-LC131\FOpt\RB3LYP\Gen\C2H5Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-OCH3.freq\0,1\C,-0.7522585265,-0.000078737,-2.1090112971\O,-0.7540058701,0.000045428,-0.6892867905\C,0.5391413698,-0.0001106148,-0.1735195755\H,-0.2552094174,-0.8947913115,-2.5145282986\H,-1.7986498445,0.0000634545,-2.4198986327\H,-0.2549199462,0.8944024431,-2.5146839084\H,1.0997800562,-0.8993423165,-0.4617439907\H,1.1000708046,0.8988798853,-0.4619307998\Cl,0.4364516617,0.000091796,1.6224861877\Version=IA32L-G03RevC.02\State=1-A\HF=-614.6197453\RMSD=6.927e-09\RMSF=2.682e-05\Dipole=0.3574357,-0.0001678,-1.1570328\PG=C01 [X(C2H5Cl1O1)]\@
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n.CH2Cl-OCHO

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1\1\GINC-LC132\FOpt\RB3LYP\Gen\C2H3Cl1O2\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-OCHO.freq\0,1\C,0.0286816703,0.0002927578,-0.575417944\O,0.0239930459,0.0001997719,0.8525216607\C,1.2509855052,0.0005038482,1.4165825716\O,2.2955931443,0.0008671773,0.8163241276\H,0.5188213124,-0.8960165002,-0.9556469174\H,0.5175207428,0.8973671696,-0.9555226368\H,1.137505369,0.000366644,2.5099021702\Cl,-1.6710905882,-0.0008842672,-1.1174403935\Version=IA32L-G03RevC.02\State=1-A\HF=-688.6532314\RMSD=9.161e-09\RMSF=5.048e-05\Dipole=0.0187626,0.0002327,0.1747868\PG=C01 [X(C2H3Cl1O2)]\@
```

n.CH2Cl-OCOCH3

1\1\GINC-LC133\FOpt\RB3LYP\Gen\C3H5Cl1O2\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-OCOCH3.freq\0,1\C,-0.1248014725,0.0004285519,-1.0114195094\O,-0.1425
582496,-0.0000930154,0.4107176908\C,1.0928484581,0.000430109,0.9892683
625\C,0.9770022111,-0.0015372628,2.4921496232\O,2.1170393748,0.0015788
365,0.3457520679\H,0.364419356,0.8967346843,-1.3929634311\H,0.36519073
33,-0.8951795917,-1.3936262323\H,1.9753215193,0.0066631837,2.930368789
1\H,0.4294945292,-0.8891899083,2.8253118318\H,0.4131980268,0.874990257
3,2.827253368\Cl,-1.8243393145,-0.0001078578,-1.5687113678\Version=IA
32L-G03RevC.02\State=1-A\HF=-727.979979\RMSD=3.561e-09\RMSF=3.904e-05\
Dipole=0.0654056,-0.0015361,0.5415332\PG=C01 [X(C3H5Cl1O2)]\@

n.CH2Cl-Si_CH3_3

1\1\GINC-LC145\FOpt\RB3LYP\Gen\C4H11Cl1Si1\CYL509\26-Jun-2008\0\#\B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C
l_-Si_CH3_3.freq\0,1\H,1.1154492025,-1.1320503674,-2.4185715691\C,1.1
319049646,-1.1107903776,-1.322207099\H,2.1819758697,-1.083891588,-1.00
73012384\H,0.7002393531,-2.0510714841,-0.9621710407\Si,0.1727594725,0.
373411669,-0.6575294112\C,-1.6265250617,0.3313065669,-1.227980346\C,0.
2225281541,0.3435516523,1.2563763955\C,1.0017360959,1.993597521,-1.185
9221086\H,-1.6933703915,0.3364329961,-2.3226233487\H,-2.1853544313,1.1
993054697,-0.8580806546\H,-2.1328945393,-0.5699343301,-0.8654277284\H,
2.0416739779,2.0479369405,-0.8422447563\H,0.4727284255,2.8681695651,-0.
7886661507\H,1.012530542,2.0856419511,-2.2789347266\H,1.24596336,0.36
88354704,1.6411416956\H,-0.3186980421,1.1868459029,1.6945912014\Cl,-0.
5433376976,-1.1664691804,1.9465940601\Version=IA32L-G03RevC.02\State=
1-A\HF=-908.7826829\RMSD=3.792e-09\RMSF=5.717e-06\Dipole=0.326959,0.66
25085,-0.5679775\PG=C01 [X(C4H11Cl1Si1)]\@

n.CH2Cl-P_CH3_2

1\1\GINC-LC136\FOpt\RB3LYP\Gen\C3H8Cl1P1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
-P_CH3_2.freq\0,1\C,1.7239834647,-0.5532873514,0.7621693114\H,1.71679
63585,-0.5500201689,1.8572164189\H,2.7682857981,-0.5018533059,0.436325
0084\H,1.2832862181,-1.4897477261,0.4055850174\P,0.8239162556,0.945637
9901,0.1260407657\C,0.7960980858,0.5818959643,-1.6983744576\C,-0.93332
98211,0.5409950534,0.6019135109\H,0.1818725764,1.328029239,-2.21335341
11\H,0.4057898861,-0.4163043408,-1.921062654\H,1.8157962707,0.66332740
48,-2.0894877539\H,-1.0276940576,0.5860836617,1.6891129709\H,-1.601193
2046,1.2888783398,0.1688165914\Cl,-1.6130702386,-1.0888579384,0.104822
7141\Version=IA32L-G03RevC.02\State=1-A\HF=-920.691699\RMSD=3.265e-09
\RMSF=4.850e-06\Dipole=0.3834978,0.2316437,-0.0371055\PG=C01 [X(C3H8Cl
1P1)]\@

n.CH2Cl-SC_CH3_2CN

1\1\GINC-LC141\FOpt\RB3LYP\Gen\C5H8Cl1N1S1\CYL509\26-Jun-2008\0\#\B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C
l_-SC_CH3_2CN.freq\0,1\C,1.2197982213,0.7532700467,0.3338806607\H,1.2
148531186,0.7710920519,1.4238577497\S,0.4701065624,-0.7863680103,-0.32
62356112\C,-1.3224495674,-0.5594826307,0.1668098149\C,-1.5141120084,-0.
.629279247,1.6942953288\C,-2.0848009658,-1.7012640721,-0.537625624\C,-
1.7876529945,0.7408420608,-0.3370398465\H,-1.1477838379,-1.5916386215,
2.0625192172\H,-0.976666231,0.1711250121,2.2101161051\H,-2.5772800598,
-0.5346768813,1.9431858179\H,-1.9738158081,-1.6430225258,-1.6232815182
\H,-3.1494484812,-1.6412275156,-0.2898366341\H,-1.7019050212,-2.666884
1335,-0.1925015688\N,-2.1348322216,1.7855681012,-0.7090191751\H,0.7108
115162,1.6304175964,-0.0679342861\Cl,2.9387446615,0.8213652663,-0.1885

378166\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-1108.4636345\\RMSD=4.671
e-09\\RMSF=2.057e-05\\Dipole=-0.5444137,-0.9675266,0.9594544\\PG=C01 [X(C
5H8C11N1S1)]\\@

n.CH2C1-SCH2COOCH3

1\\1\\GINC-LC138\\FOpt\\RB3LYP\\Gen\\C4H7C11O2S1\\CYL509\\26-Jun-2008\\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C
1_-SCH2COOCH3.freq\\0,1\\S,1.3335078932,0.6803923401,-0.5731077389\\C,1.
2559445929,0.7606575014,1.231105679\\H,2.2809037196,0.7034373394,1.5971
897071\\H,0.6555482684,-0.0588636512,1.6231071404\\C,-0.4464093935,0.422
2149812,-0.9634937925\\C,-0.8987591943,-0.9759447382,-0.5961851364\\O,-1
.0242420948,-1.3818082473,0.5415426357\\O,-1.1269842048,-1.7234821172,-
1.6912870884\\C,-1.5260893215,-3.0837330269,-1.4388401933\\H,-1.03258730
73,1.1590591723,-0.4073115524\\H,-0.5536140285,0.6031381215,-2.03405885
01\\H,-2.4521714863,-3.1084581784,-0.859089568\\H,-0.74456189,-3.6126045
541,-0.8874895056\\H,-1.6739394565,-3.5302069106,-2.4220541751\\C1,0.534
4697755,2.2977279901,1.9036392298\\Version=IA32L-G03RevC.02\\State=1-A\\
HF=-1165.4774377\\RMSD=5.478e-09\\RMSF=8.245e-07\\Dipole=-0.2313525,-0.88
2253,-0.7362817\\PG=C01 [X(C4H7C11O2S1)]\\@

n.CH2C1-SCH2Ph

1\\1\\GINC-LC139\\FOpt\\RB3LYP\\Gen\\C8H9C11S1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1_
-SCH2Ph.freq\\0,1\\C,-1.3663355775,-1.0808122809,-0.8865828912\\S,-1.345
450025,-1.1165010628,0.9436376533\\C,0.4883113943,-1.1150208669,1.20130
94253\\H,-0.8235038886,-0.2126938806,-1.2619083026\\C,1.2125733634,0.105
6550423,0.6848357331\\H,0.9086633995,-2.0291119149,0.7690275902\\H,0.581
5995628,-1.1998320303,2.2896206379\\C,2.1252924611,-0.0069590935,-0.371
1953712\\C,0.9943431979,1.3691984913,1.2536621928\\C,2.8100749885,1.1138
294997,-0.8478549172\\C,1.6773485721,2.4877993901,0.7816542695\\C,2.5881
568258,2.3638957806,-0.2718399989\\H,3.1195697818,3.2374537838,-0.63944
48043\\H,1.4997275959,3.4589697777,1.2358117774\\H,3.5156762647,1.006712
4208,-1.6674073673\\H,0.2779553219,1.4726443898,2.0648217082\\H,2.308998
5794,-0.9814772122,-0.819025284\\H,-0.9459935425,-1.9983233605,-1.30261
26438\\C1,-3.0643578841,-0.9597553379,-1.4724127304\\Version=IA32L-G03R
evC.02\\State=1-A\\HF=-1168.6520254\\RMSD=5.835e-09\\RMSF=2.841e-06\\Dipole
=1.2879541,0.1176213,-0.0323802\\PG=C01 [X(C8H9C11S1)]\\@

n.CH2C1-SCH3

1\\1\\GINC-LC140\\FOpt\\RB3LYP\\Gen\\C2H5C11S1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1_
-SCH3.freq\\0,1\\S,0.2059638902,0.,-1.0922371898\\C,0.2080751951,0.,0.73
8442365\\C,2.0183638898,0.,-1.3377727686\\H,2.1836127958,0.,-2.418312199
\\H,0.6971826959,0.8949159343,1.128029543\\H,2.4816931767,0.895904365,-0
.9130992046\\H,0.6971826959,-0.8949159343,1.128029543\\H,2.4816931767,-0
.895904365,-0.9130992046\\C1,-1.4820836055,0.,1.3564840576\\Version=IA3
2L-G03RevC.02\\State=1-A\\HF=-937.6012311\\RMSD=5.980e-09\\RMSF=2.839e-05
\\Dipole=1.2403847,0.,0.0339674\\PG=CS [SG(C2H1C11S1),X(H4)]\\@

n.CH2C1-SO2CH3

1\\1\\GINC-LC143\\FOpt\\RB3LYP\\Gen\\C2H5C11O2S1\\CYL509\\26-Jun-2008\\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C
1_-SO2CH3.freq\\0,1\\C,-0.5378883295,-0.0000015867,-2.2559901156\\S,-0.6
279672542,0.0000007291,-0.446715579\\C,1.1687780117,-0.0000023538,-0.01
30442431\\O,-1.2013197912,1.2796335194,-0.0190495392\\O,-1.2013249243,-1
.2796287554,-0.0190465358\\H,1.6169095411,-0.9010561454,-0.4351333942\\H
,1.6169131594,0.9010486229,-0.4351355304\\H,-0.0314462681,-0.9033807455
, -2.6021413416\\H,-0.0314426708,0.903374759,-2.6021434669\\H,-1.57496349
03,0.0000000812,-2.600804041\\C1,1.4051367897,-0.0000007462,1.749516575

9\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-1087.981322\\RMSD=7.498e-09\\RMSF=2.942e-05\\Dipole=1.1870088,-0.0000044,-1.713212\\PG=C01 [X(C2H5C1102S1)]\\@

n.CH2C1-SOCH3

1\\1\\GINC-LC118\\FOpt\\RB3LYP\\Gen\\C2H5C1101S1\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-SOCH3.freq\\0,1\\C,-0.7304454274,0.1807881051,-0.8963010374\\S,-0.7373842651,0.2052531901,0.9035125526\\O,0.9049750045,0.2719458813,1.2578954825\\C,1.4549179282,1.5950687358,1.3068327424\\H,-0.1044186879,0.9763875507,-1.3014721886\\H,2.5029757894,1.4626136989,1.5883834535\\H,0.9457586834,2.2135349118,2.0546477642\\H,1.4052252491,2.0924780635,0.3298680956\\H,-1.7671735316,0.3394405415,-1.2037206991\\Cl,-0.1629914295,-1.3646596414,-1.6735447857\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-1012.7884934\\RMSD=4.114e-09\\RMSF=3.525e-05\\Dipole=-0.073106,1.268965,0.0088744\\PG=C01 [X(C2H5C1101S1)]\\@

n.CH2C1-Ph

1\\1\\GINC-LC137\\FOpt\\RB3LYP\\Gen\\C7H7C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-Ph.freq\\0,1\\C,0.8986215013,-1.4349690874,0.1627446663\\H,1.9434256854,-1.4275592942,-0.1502272939\\H,0.4351312078,-2.3719327925,-0.1485453523\\C,0.1496219903,-0.2395819254,-0.3443910861\\C,-1.249797099,1.9938616289,-1.3047422518\\C,-1.2283621015,-0.313855709,-0.5854838605\\C,0.8181472878,0.9669619185,-0.5889069682\\C,0.1236413108,2.0776147914,-1.0666955015\\C,-1.9248769368,0.7955335944,-1.0632582159\\H,-1.756028963,-1.2454900659,-0.3950842241\\H,1.8871708531,1.0346260435,-0.4011890872\\H,0.6540637963,3.0070787074,-1.2549453805\\H,-2.9931466179,0.7244538372,-1.2488303031\\H,-1.7914673519,2.8583416122,-1.6790117768\\Cl,0.9469926866,-1.5089946656,2.0013078085\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-731.1602441\\RMSD=9.292e-09\\RMSF=1.369e-05\\Dipole=-0.1493873,0.2368823,-0.9267053\\PG=C01 [X(C7H7C11)]\\@

n.CH2C1-C6H4CN

1\\1\\GINC-LC70\\FOpt\\RB3LYP\\Gen\\C8H6C11N1\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-C6H4CN.freq\\0,1\\C,1.254391155,-2.0132802631,0.464951011\\H,2.2973092128,-2.0058223901,0.1458281642\\H,0.786941138,-2.9463708033,0.1480735255\\C,0.5061503531,-0.8128942185,-0.0366097155\\C,-0.8914797954,1.4292977398,-0.9781975\\C,-0.8736000625,-0.8828753149,-0.2715182302\\C,1.1774372469,0.393653627,-0.2761504958\\C,0.4912885841,1.5091281001,-0.743356117\\C,-1.5729470485,0.2243760997,-0.7386829253\\H,-1.4043754463,-1.8125201963,-0.084477367\\H,2.2465207679,0.4597367879,-0.0927370623\\H,1.0150120419,2.4407823548,-0.9305539527\\H,-2.6407179727,0.1655158335,-0.9222853515\\C,-1.604949332,2.5738690586,-1.465722433\\N,-2.1836390761,3.5022103755,-1.8612770869\\Cl,1.2980610109,-2.0790848933,2.2962829463\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-823.4023081\\RMSD=6.525e-09\\RMSF=1.891e-05\\Dipole=0.7754473,-1.2459161,-0.2391893\\PG=C01 [X(C8H6C11N1)]\\@

n.CH2C1-C6H4NO2

1\\1\\GINC-LC75\\FOpt\\RB3LYP\\Gen\\C7H6C11N1O2\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-C6H4NO2.freq\\0,1\\O,-2.7549250504,-0.3801980945,-2.4614748526\\N,-2.7023945191,-0.2154935165,-1.2433611993\\C,-1.3756471067,-0.2593181454,-0.6049588526\\C,-1.2842205956,-0.0786115139,0.7735519807\\C,-0.0275708637,-0.1270390709,1.3686245504\\C,1.1223841011,-0.3536954405,0.5992565629\\C,0.9958486267,-0.5296877752,-0.7859208133\\C,-0.2525903578,-0.4844894545,-1.3982754654\\C,2.4740545318,-0.4071348317,1.2512935074\\O,-3.6773423502,-0.0172866529,-0.5195668331\\H,2.4136657487,-0.7486759703,2.285325

8041\H,3.1664436746,-1.0449347869,0.7005406019\H,1.8824849289,-0.70122
81692,-1.3900359397\H,0.0622127353,0.0149282081,2.4420719595\H,-2.1837
008557,0.0922625736,1.351770065\H,-0.3702343493,-0.6212169189,-2.46601
34882\Cl,3.2641458201,1.2433561794,1.3180455327\Version=IA32L-G03RevC
.02\State=1-A\HF=-935.6603109\RMSD=5.123e-09\RMSF=2.292e-05\Dipole=1.1
393817,-0.7430265,0.6801086\PG=C01 [X(C7H6Cl1N1O2)]\@

n.CH2Cl-C6H4OCH3

1\1\GINC-LC76\FOpt\RB3LYP\Gen\C8H9Cl1O1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
C6H4OCH3.freq\0,1\C,-1.5623039421,-0.6522854153,-0.3761129747\C,-1.49
95020876,-0.3055369888,0.9830358797\C,-0.2621796986,0.000309993,1.5630
831625\C,0.8927340181,-0.042165096,0.7802073032\C,0.8457895736,-0.3861
856753,-0.5732938408\C,-0.4042389652,-0.6892006,-1.1380258391\C,2.0915
064755,-0.4308944017,-1.3978844529\O,-2.6899569376,-0.2998181087,1.645
8900165\C,-2.6946526365,0.05310387,3.020900602\H,2.0305238945,-1.16794
16244,-2.1995334754\H,2.9784744435,-0.6269466499,-0.7944193326\H,-0.46
69085383,-0.9547625208,-2.1906482942\H,1.8485717954,0.200980511,1.2385
123818\H,-0.1861756639,0.2680983111,2.6105535258\H,-2.5302784807,-0.88
86743259,-0.8064303092\H,-2.0957146458,-0.6463335125,3.6188677687\H,-3
.7370527659,-0.0014714627,3.3394672006\H,-2.3205312433,1.0734405354,3.
1762901679\Cl,2.4444606049,1.1681930291,-2.2547787532\Version=IA32L-G
03RevC.02\State=1-A\HF=-845.6836344\RMSD=8.056e-09\RMSF=5.681e-06\Dipo
le=-0.3873378,-0.6019087,1.1102599\PG=C01 [X(C8H9Cl1O1)]\@

n.CH2Cl-C6H4OH

1\1\GINC-LC77\FOpt\RB3LYP\Gen\C7H7Cl1O1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
C6H4OH.freq\0,1\C,-1.9002514379,0.5315134089,-0.1446716671\C,-1.84879
62532,0.3208834682,1.2385422827\C,-0.6134702898,0.1435147182,1.8716103
023\C,0.5594332365,0.1759215582,1.1212368782\C,0.5268521142,0.38632420
51,-0.2622583547\C,-0.7211512925,0.5610236828,-0.879326297\C,1.7894030
015,0.4228472642,-1.0616111722\O,-3.0344899339,0.3033860544,1.91490522
96\H,2.6432068562,0.7546303464,-0.4696925419\H,1.6987237148,1.05234542
6,-1.9475730282\H,-0.7685977384,0.7204850572,-1.953894261\H,1.51431744
66,0.0326746602,1.6212067499\H,-0.5702239367,-0.0172486251,2.947311589
3\H,-2.8661907032,0.6698241929,-0.6195765978\H,-2.8614279771,0.1405481
676,2.8553048631\Cl,2.2784704316,-1.2372069114,-1.7090270849\Version=
IA32L-G03RevC.02\State=1-A\HF=-806.3770194\RMSD=5.827e-09\RMSF=4.122e-
06\Dipole=-0.2522518,0.6813306,0.9423313\PG=C01 [X(C7H7Cl1O1)]\@

n.CH2Cl-CF2CF3

1\1\GINC-LC82\FOpt\RB3LYP\Gen\C3H2Cl1F5\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CF2CF3.freq\0,1\F,-0.0718172666,0.2462657011,-1.5502717744\C,-0.08715
85368,0.2498642129,-0.1928147133\C,1.3849154144,0.2067320519,0.2806184
51\C,-0.8975637755,-0.9226135676,0.3436224262\F,-0.6087945374,1.430690
3681,0.2272863706\F,1.9686080361,-0.9318283289,-0.1358361467\F,1.43677
08356,0.2412375164,1.6247075667\F,2.0693527234,1.2445766532,-0.2041466
85\H,-0.8934695911,-0.8973212281,1.4336725658\H,-0.4583354091,-1.85708
2438,-0.0066807752\Cl,-2.5997901019,-0.8545864533,-0.2159531032\Versi
on=IA32L-G03RevC.02\State=1-A\HF=-1074.9198653\RMSD=5.143e-09\RMSF=3.7
11e-05\Dipole=0.2513307,-0.5035954,0.411487\PG=C01 [X(C3H2Cl1F5)]\@

n.CH2Cl-CF2H

1\1\GINC-LC83\FOpt\RB3LYP\Gen\C2H3Cl1F2\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CF2H.freq\0,1\C,0.3750269238,-0.6543357044,-0.8232853972\C,0.37228626
26,-0.651192375,0.6941396688\H,1.4008160069,-0.6525314259,1.0600839922

\H,0.8878021559,-1.5498156423,-1.2003959004\F,1.0194041745,0.442380419
7,-1.3063785127\F,-0.8965348837,-0.6542391453,-1.3075623572\H,-0.14784
00104,-1.538914876,1.059116799\Cl,-0.4547341699,0.79300935,1.375384547
6\\Version=IA32L-G03RevC.02\State=1-A\HF=-737.8885586\RMSD=5.977e-09\R
MSF=5.195e-05\Dipole=0.5822022,-1.0173778,0.1774533\PG=C01 [X(C2H3Cl1F
2)]\@

n.CH2Cl-CF3

1\1\GINC-LC84\FOpt\RB3LYP\Gen\C2H2Cl1F3\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CF3.freq\0,1\F,0.1879475844,0.296707066,-2.0109009101\C,0.2311832393,
0.3635690036,-0.660988859\F,1.5206906221,0.3634254041,-0.2877710771\C,
-0.5279841629,-0.8290907889,-0.1014079848\F,-0.3141703342,1.5317941573
, -0.2868735758\H,-1.5592666292,-0.786290004,-0.452896532\H,-0.05320133
59,-1.745298343,-0.4536360147\Cl,-0.5386433732,-0.8472129758,1.69122249
221\\Version=IA32L-G03RevC.02\State=1-A\HF=-837.1397524\RMSD=4.231e-09
\RMSF=4.655e-05\Dipole=-0.3247806,-0.5097488,-0.3928987\PG=C01 [X(C2H2
Cl1F3)]\@

n.CH2Cl-CCl2H

1\1\GINC-LC80\FOpt\RB3LYP\Gen\C2H3Cl3\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CCl2H.freq\0,1\C,0.7789301491,0.0003507828,-0.4196800438\C,0.7644506888
,0.0005924018,1.1034680214\H,1.8177495699,0.0008513696,-0.7518766959\C
1,0.0339591803,1.4859025508,-1.1051294192\Cl,0.0355552034,-1.486232222
2,-1.1046380725\H,1.2841764959,0.8931596409,1.4582096653\H,1.285132082
, -0.8913013761,1.4585016679\Cl,-0.8722992764,-0.0001626075,1.841087344
4\\Version=IA32L-G03RevC.02\State=1-A\HF=-1458.6016667\RMSD=9.843e-09\
RMSF=3.336e-05\Dipole=1.1364519,0.0006586,0.2549108\PG=C01 [X(C2H3Cl3)
]\@

n.CH2Cl-CCl3

1\1\GINC-LC81\FOpt\RB3LYP\Gen\C2H2Cl4\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CCl3.freq\0,1\C,0.2979010535,0.0003737859,-0.2534588234\C,0.2846712607,
0.0001289118,1.281915934\Cl,2.0453473874,0.0018002701,-0.7307653285\Cl
, -0.4939124184,1.4682161931,-0.9116458003\Cl,-0.4916098901,-1.46853203
81,-0.9120310463\H,0.8010332636,0.894087073,1.6324953015\H,0.802888112
6,-0.8928696464,1.6322053909\Cl,-1.3597871531,-0.0017334611,1.99941609
54\\Version=IA32L-G03RevC.02\State=1-A\HF=-1918.1833375\RMSD=4.135e-09\
\RMSF=9.404e-05\Dipole=0.5033354,0.0004868,0.3515046\PG=C01 [X(C2H2Cl4
)]\@

n.CH2Cl-CH2Cl

1\1\GINC-LC91\FOpt\RB3LYP\Gen\C2H4Cl2\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CH2Cl.freq\0,1\H,0.3700104312,-0.5935328599,-1.3730310042\C,0.386878210
1,-0.5887368749,-0.2827658539\H,1.4193194947,-0.5960926096,0.067942849
1\C,-0.3867877595,0.589022742,0.2827053316\Cl,0.3847238867,2.133221757
5,-0.2763709394\H,-0.3701461036,0.5934419589,1.3730025456\H,-1.4193321
428,0.5959956542,-0.0677912947\Cl,-0.3847470858,-2.1333116014,0.276385
0592\\Version=IA32L-G03RevC.02\State=1-A\HF=-999.0190116\RMSD=7.679e-0
9\RMSF=3.993e-05\Dipole=0.0001757,0.0005956,-0.0001235\PG=C01 [X(C2H4C
l2)]\@

n.CH2Cl-CH2F

1\1\GINC-LC92\FOpt\RB3LYP\Gen\C2H4Cl1F1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl_
CH2F.freq\0,1\C,0.4125250692,0.0000006403,-0.4488066028\C,0.386463880

5,-0.0000006409,1.0713416059\F,1.7039004869,-0.000000156,1.5136709072\H,-0.1189262742,-0.8928124419,1.4548158357\H,-0.118927415,0.8928098811,1.4548173152\H,0.9132952032,-0.8908454325,-0.8310272644\H,0.9132940553,0.8908479918,-0.8310257918\Cl,-1.277516097,0.0000000833,-1.0944604869\\Version=IA32L-G03RevC.02\State=1-A\HF=-638.6488028\RMSD=7.553e-09\RMSF=2.738e-05\Dipole=0.1370815,0.,0.0698831\PG=C01 [X(C2H4C11F1)]\@

n.CH2Cl-CH2OH

1\1\GINC-LC93\FOpt\RB3LYP\Gen\C2H5C11O1\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-CH2OH.freq\0,1\C,0.4033454043,0.,-0.457135895\C,0.3742340858,0.,1.0642165638\O,1.7348282933,0.,1.4770110503\H,0.9063993806,0.8904400853,-0.8368021023\H,0.9063993806,-0.8904400853,-0.8368021023\H,-0.1648718301,-0.8898052627,1.4216019937\H,-0.1648718301,0.8898052627,1.4216019937\H,1.7539735628,0.,2.4457169808\Cl,-1.2812430559,0.,-1.1219934811\\Version=IA32L-G03RevC.02\State=1-A\HF=-614.627745\RMSD=4.931e-09\RMSF=2.284e-05\Dipole=0.3105103,0.,0.7962459\PG=CS [SG(C2H1C11O1),X(H4)]\@

n.CH2Cl-CH2Ph

1\1\GINC-LC94\FOpt\RB3LYP\Gen\C8H9C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-CH2Ph.freq\0,1\C,-1.1245052424,0.0000019631,-1.4531025911\C,-1.1701188011,0.000001167,0.0765241305\C,0.2327050708,-0.0000006152,0.6509508056\C,0.9031523672,-1.2044459483,0.9038112391\C,0.903155525,1.2044430343,0.9038109231\C,2.2081713195,-1.206775067,1.3975872794\C,2.2081744812,1.2067688684,1.3975869583\C,2.8649505804,-0.0000039283,1.6452391258\H,3.8801108975,-0.0000052131,2.0328388476\H,2.7098701699,-2.1508372755,1.5932025223\H,2.7098758051,2.1508298156,1.5932019493\H,0.3943363384,-2.1484499832,0.7196035486\H,0.3943419678,2.1484483586,0.7196030134\H,-1.7248562618,0.8816215815,0.4158530748\H,-1.724858073,-0.881618482,0.4158520862\H,-0.6209420861,-0.8881646311,-1.8394440074\H,-0.6209401599,0.8881678967,-1.8394430414\Cl,-2.7971206119,0.0000041817,-2.1732773658\\Version=IA32L-G03RevC.02\State=1-A\HF=-770.476233\RMSD=5.950e-09\RMSF=1.386e-05\Dipole=0.849168,-0.0000012,0.465033\PG=C01 [X(C8H9C11)]\@

n.CH2Cl-CH-CH2_2

1\1\GINC-LC101\FOpt\RB3LYP\Gen\C4H7C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-CH-CH2_2.freq\0,1\C,-1.5831433945,0.7324412365,-0.560278664\C,-1.9512390244,0.5204050578,0.8860576034\C,-0.4954034947,0.6272205884,0.477049014\H,-1.7087233728,-0.101856138,-1.2458600178\H,-1.7677426777,1.7048827867,-1.0071789168\H,-2.3302821275,-0.4558523771,1.17835828\H,-2.3822940563,1.3463339763,1.4446533542\H,0.0167679386,1.5494186756,0.7417630798\C,0.3623770796,-0.600568446,0.5545166458\H,-0.2066418531,-1.5054862271,0.3292805629\H,0.8355801502,-0.7114524288,1.5324063705\Cl,1.7381052354,-0.5589987581,-0.6539700181\\Version=IA32L-G03RevC.02\State=1-A\HF=-616.8081218\RMSD=7.047e-09\RMSF=4.154e-05\Dipole=-0.7849206,0.1051488,0.5484005\PG=C01 [X(C4H7C11)]\@

n.CH2Cl-CH2CH=CH2

1\1\GINC-LC89\FOpt\RB3LYP\Gen\C4H7C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-CH2CH=CH2.freq\0,1\H,0.4406465173,-0.5797634002,-1.3105306166\C,0.498577136,-0.5842130593,-0.2206367575\H,1.5492285921,-0.5928678355,0.0781748064\C,-0.2539391634,0.6021071633,0.384023247\C,0.3790558494,1.9052340683,-0.0317378338\H,-0.2402891715,0.5054942828,1.4776970618\H,-1.3021611295,0.5685937472,0.0675975043\H,1.3953527317,2.0790648774,0.3255886084\C,-0.2079828284,2.8263431384,-0.7964948999\H,0.2956509613,3.7502404874,-1.0676839716\H,-1.2202887197,2.6955208124,-1.1738466774\Cl,-0.200

7297496,-2.1719476962,0.3289459265\\Version=IA32L-G03RevC.02\\State=1-A
\\HF=-616.8164946\\RMSD=2.073e-09\\RMSF=2.151e-05\\Dipole=0.2899507,0.7985
711,-0.2029749\\PG=C01 [X(C4H7C11)]\\@

n.CH2C1-CH2CH3

1\\1\\GINC-LC88\\FOpt\\RB3LYP\\Gen\\C3H7C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-CH
2CH3.freq\\0,1\\C,-0.1874523123,0.2964479584,-0.4713165776\\H,0.30377840
88,1.1825168181,-0.8802165459\\C,-0.1906438835,0.3052434702,1.051981862
7\\H,-1.1996803511,0.2355376456,-0.8778989139\\H,0.8440203423,0.31502587
87,1.4137354583\\H,-0.6455710261,-0.6231967359,1.4160308064\\C,-0.954017
8515,1.5185683973,1.5988291344\\H,-0.9501513938,1.5151137104,2.69395314
55\\H,-0.5007420195,2.460472033,1.2675119472\\H,-2.000040851,1.516132910
3,1.2698267483\\C1,0.7141806573,-1.1366565421,-1.1399946566\\Version=IA
32L-G03RevC.02\\State=1-A\\HF=-578.7401638\\RMSD=4.118e-09\\RMSF=7.129e-05
\\Dipole=-0.4346305,0.6911373,0.4497272\\PG=C01 [X(C3H7C11)]\\@

n.CH2C1-CH-CH3_2

1\\1\\GINC-LC102\\FOpt\\RB3LYP\\Gen\\C4H9C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-C
H-CH3_2.freq\\0,1\\C,0.5340992415,-1.7532284947,-0.444084389\\H,0.514706
7071,-1.8026356281,0.6497030031\\H,1.5833084256,-1.7349894461,-0.762275
2342\\H,0.0806133604,-2.6720585838,-0.8321529616\\C,-0.2269423263,-0.521
472042,-0.9517550277\\C,-1.7102349452,-0.5622492192,-0.5614757196\\H,-0.
1678538231,-0.5186393115,-2.0526934666\\C,0.4494353303,0.792489122,-0.5
523814714\\H,-0.0804985776,1.6533860841,-0.9659181339\\H,1.4898193283,0.
8200805183,-0.8837814723\\H,-2.2538908524,0.3012603005,-0.9629823246\\H,
-1.8293476523,-0.5587388617,0.5270957456\\H,-2.185214715,-1.4696733299,
-0.9506685955\\C1,0.5041302273,1.0734571842,1.2524619459\\Version=IA32L
-G03RevC.02\\State=1-A\\HF=-618.0538415\\RMSD=2.181e-09\\RMSF=2.999e-05\\Di
pole=-0.0913524,-0.2548484,-0.8390191\\PG=C01 [X(C4H9C11)]\\@

n.CH2C1-C-CH3_3

1\\1\\GINC-LC115\\FOpt\\RB3LYP\\Gen\\C5H11C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-C
CH3_3.freq\\0,1\\C,-0.2336375388,0.4046347534,-0.8865381429\\C,-0.2190
120122,0.379295121,0.6516533006\\C,1.2234106556,0.4063003161,1.18711137
67\\C,-0.9634973306,-0.8564488333,1.1871028696\\H,0.28308235,1.288285102
7,-1.2683096646\\H,-1.2572584324,0.3988737693,-1.2683155267\\C,-0.958054
3257,1.659211825,1.1012636112\\H,-1.9975507074,-0.8861950059,0.82187788
62\\H,-0.9956395398,-0.8370753486,2.2826112558\\H,-0.4696153627,-1.78282
51262,0.8784438913\\H,-0.4552545246,2.5636139197,0.7376121519\\H,-0.9889
738425,1.7127527051,2.1954979227\\H,-1.992688838,1.6758793829,0.7376060
824\\H,1.7661175486,1.2869959709,0.8218924056\\H,1.7788206922,-0.4845489
034,0.8784527625\\H,1.222693888,0.4438194436,2.2826198814\\C1,0.58888294
58,-1.0198550002,-1.6790321847\\Version=IA32L-G03RevC.02\\State=1-A\\HF=
-657.3677435\\RMSD=5.902e-09\\RMSF=3.662e-05\\Dipole=-0.3597755,0.6230794
,0.5168652\\PG=C01 [X(C5H11C11)]\\@

n.CH2C1-CCH

1\\1\\GINC-LC79\\FOpt\\RB3LYP\\Gen\\C3H3C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CH2C1-CC
H.freq\\0,1\\C,0.3332975484,-0.5445506863,-0.5356696335\\H,1.3766674181,
-0.5464451116,-0.8596638532\\H,-0.1358238487,-1.4788619839,-0.852819866
9\\C,-0.3807553904,0.6098594139,-1.0438096591\\C,-0.9705204322,1.5638543
893,-1.4889843999\\H,-1.4954312224,2.4093689634,-1.8728059601\\C1,0.3742
62194,-0.5975906217,1.2938865785\\Version=IA32L-G03RevC.02\\State=1-A\\H
F=-576.2410901\\RMSD=2.904e-09\\RMSF=4.077e-05\\Dipole=-0.0178221,0.02185
61,-0.7908324\\PG=C01 [X(C3H3C11)]\\@

n.CH2C1-CH=C_CH3_2

1\1\GINC-LC98\FOpt\RB3LYP\Gen\C5H9C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_-CH
=C_CH3_2.freq\0,1\H,-2.4097944386,-0.7866706981,-2.0459089526\C,-2.42
34776949,-0.8351382267,-0.94836429\C,-1.0194338717,-0.8380161347,-0.39
50658607\C,-0.6207950939,0.1294536921,0.4483678301\C,-0.1614916737,-1.
9837200287,-0.8696042632\C,0.7121906084,0.2600486043,1.0964904601\H,1.
3443386328,-0.6192808693,0.9853846443\H,0.6256310804,0.5051596126,2.15
67253292\H,-1.3276695408,0.9194417211,0.6976559904\H,-2.9527362328,-1.
7611123961,-0.6841930644\H,-3.0091911757,0.0109217592,-0.5769922773\H,
-0.1090315009,-1.9862151962,-1.9665123806\H,-0.60444762,-2.9456824471,
-0.5775486861\H,0.8621400188,-1.9545604711,-0.4901642375\C1,1.68581218
42,1.6601312675,0.382977081\Version=IA32L-G03RevC.02\State=1-A\HF=-65
6.1389803\RMSD=7.375e-09\RMSF=7.682e-07\Dipole=-0.6773412,-0.9097306,0
.0829202\PG=C01 [X(C5H9C11)]\@

n.CH2C1-CH=CH2

1\1\GINC-LC96\FOpt\RB3LYP\Gen\C3H5C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_-CH
=CH2.freq\0,1\C,0.3690632986,-0.5895124796,-0.677535457\H,1.407325342
4,-0.5817220509,-1.0237323517\H,-0.0886874224,-1.5229185209,-1.0197594
086\C,-0.379328652,0.5978009653,-1.2094566756\C,-0.9825576755,1.559693
2943,-0.5161012198\H,-0.3981090569,0.6229197522,-2.3005995229\H,-0.985
2592061,1.5686764702,0.5692945018\H,-1.4952984708,2.3725442864,-1.0215
466631\C1,0.4421745286,-0.698081801,1.1302884446\Version=IA32L-G03Rev
C.02\State=1-A\HF=-577.4994281\RMSD=5.526e-09\RMSF=1.932e-05\Dipole=-0
.0431315,0.0651606,-0.8043262\PG=C01 [X(C3H5C11)]\@

n.CH2C1-CH=CHCH3

1\1\GINC-LC97\FOpt\RB3LYP\Gen\C4H7C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_-CH
=CHCH3.freq\0,1\H,-2.3705846526,-0.4476647496,-2.5326307923\C,-2.2780
254504,-1.0139246803,-1.5962920343\C,-0.883244586,-0.9228002612,-1.052
3585043\C,-0.5555836502,-0.4378702392,0.1494018056\C,0.841102406,-0.39
14858591,0.6642893592\H,1.5501224243,-0.8500421479,-0.02695478\H,0.940
2880111,-0.8572023297,1.6472992808\H,-1.3288776061,-0.0548956177,0.814
4816769\H,-0.0875568738,-1.2883484035,-1.7042190613\H,-3.0149068436,-0
.6234758464,-0.8870832014\H,-2.5448957367,-2.0531725366,-1.830439104\C
1,1.4182893506,1.3394875218,0.9134883661\Version=IA32L-G03RevC.02\Sta
te=1-A\HF=-616.8218886\RMSD=3.749e-09\RMSF=6.877e-06\Dipole=-0.5015191
,-0.8863843,-0.3219129\PG=C01 [X(C4H7C11)]\@

n.CH2C1-CHO

1\1\GINC-LC99\FOpt\RB3LYP\Gen\C2H3C11O1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_-
CHO.freq\0,1\C,0.3434578386,-0.5728896538,-0.6383517892\H,1.370472790
7,-0.5674471989,-1.0211776627\H,-0.1435154509,-1.4784001835,-1.0181633
53\C,-0.3882679766,0.6413980469,-1.1809012058\O,-0.9098467362,1.510256
2444,-0.5311928737\H,-0.3990586742,0.6557986028,-2.2952089992\C1,0.395
2785913,-0.6531206785,1.1470359396\Version=IA32L-G03RevC.02\State=1-A
\HF=-613.4177954\RMSD=9.350e-09\RMSF=2.637e-05\Dipole=0.4048008,-0.676
3699,-1.1167167\PG=C01 [X(C2H3C11O1)]\@

n.CH2C1-CN

1\1\GINC-LC104\FOpt\RB3LYP\Gen\C2H2C11N1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_
-CN.freq\0,1\C,0.3149721415,-0.5308814281,-0.5386251545\H,1.351111131
6,-0.5324251694,-0.8835942739\H,-0.1787793685,-1.442834,-0.8808854746\

C,-0.3845940248,0.6431728647,-1.0488195485\N,-0.9374414657,1.570877967
5,-1.4726390432\C1,0.3416170469,-0.5702726602,1.27044831\\Version=IA32
L-G03RevC.02\State=1-A\HF=-592.3365379\RMSD=3.817e-09\RMSF=3.153e-05\D
ipole=0.6222337,-1.0461324,-0.1815404\PG=C01 [X(C2H2C11N1)]\\@

n.CH2C1-COCH3

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C3H5C11O1\CYL509\20-Aug-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CH2C1
-COCH3.freq\\0,1\C,0.4409124369,0.1000182658,-0.693321516\C,0.44730766
63,-0.0825179472,0.8284725898\C,1.8296734979,0.0121248219,1.4556167738
\O,-0.5539583958,-0.2801211299,1.476005231\H,1.0189598207,-0.706258180
1,-1.1565406701\H,0.9258334097,1.0458200608,-0.9548141941\H,2.21058486
86,1.038249287,1.375187457\H,2.5477818617,-0.6404536019,0.9448998163\H
1.7653841392,-0.263237398,2.509889592\C1,-1.1967199141,0.0934763546,-
1.4159571138\\Version=IA64L-G03RevC.02\State=1-A\HF=-652.7436777\RMSD=
2.701e-09\RMSF=4.545e-06\Dipole=1.574446,0.171244,-0.1314194\PG=C01 [X
(C3H5C11O1)]\\@

n.CH2C1-CON_CH2CH3_2

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C6H12C11N1O1\CYL509\03-Sep-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CH
2C1-CON_CH2CH3_2.freq\\0,1\C,1.1614048126,0.6857263661,0.8365935087\H,
1.0676333492,0.2195043398,1.8212696594\H,0.7244165189,1.6848263147,0.8
868023587\C,0.4706901832,-0.1823446664,-0.2352932716\O,1.1027711867,-0
.7823366214,-1.0909288158\N,-0.8978719887,-0.2435144514,-0.1519008593\
C,-1.7142022836,0.4309734802,0.859619563\C,-1.5979771433,-1.0682570066
,-1.1471589283\H,-2.532993206,-0.2476179822,1.1273321889\C,-2.28552975
4,1.7759861217,0.3949955611\H,-1.1305782283,0.5652034335,1.7744014262\
H,-1.0518172856,-0.9858988637,-2.0889931613\H,-2.5929432713,-0.6337274
505,-1.2952006975\C,-1.7063203426,-2.5375951994,-0.7325936504\H,-1.486
4597626,2.4888744526,0.1642059456\H,-2.9185600955,2.2118334109,1.17640
30977\H,-2.8956717866,1.655322091,-0.5064316368\H,-0.7083902853,-2.973
7972683,-0.6324889547\H,-2.2563661757,-3.1068533314,-1.4907938999\H,-2
.2341997869,-2.6492836486,0.2219658368\C1,2.9123806829,0.8887043564,0.
5161933932\\Version=IA64L-G03RevC.02\State=1-A\HF=-826.0477967\RMSD=8.
771e-09\RMSF=7.573e-06\Dipole=0.0931742,-0.5486776,-2.0342424\PG=C01 [X
(C6H12C11N1O1)]\\@

n.CH2C1-CON_CH3_2

1\1\GINC-AC22\FOpt\RB3LYP\Gen\C4H8C11N1O1\CYL509\20-Aug-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2
C1-CON_CH3_2.freq\\0,1\H,-2.1996991856,0.987687635,-2.4232942524\C,-2.
1535859918,0.9042370561,-1.3303773917\N,-0.7648255956,0.8719539229,-0.
8891295856\H,-2.6388145578,-0.0166000471,-1.010977135\H,-2.6808073212,
1.7635915692,-0.8938602937\C,-0.3624958576,-0.1495554574,-0.0594642551
\O,-1.1001196182,-1.0622380499,0.272681806\C,1.1030722689,-0.070862270
3,0.4149905635\H,1.2826333426,0.8480443591,0.9781017944\H,1.7895794645
,-0.0944746498,-0.4348729388\C,0.0287717783,2.0370624684,-1.2457165489
\H,-0.0867607401,2.2450031749,-2.3164033188\H,1.0896311014,1.878736253
3,-1.0536247714\H,-0.2949100485,2.9306161716,-0.6917856014\C1,1.541135
9337,-1.4396275475,1.4830926448\\Version=IA64L-G03RevC.02\State=1-A\HF=
-747.4158123\RMSD=7.950e-09\RMSF=4.762e-06\Dipole=0.2181276,1.7772749
,-1.039224\PG=C01 [X(C4H8C11N1O1)]\\@

n.CH2C1-CONH2

1\1\GINC-AC\FOpt\RB3LYP\Gen\C2H4C11N1O1\CYL509\22-Aug-2008\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT Freq=noraman\\n.CH2C1-CONH2.freq\\0,1\C,
-0.2964011787,-0.4688553129,0.7088742522\C,1.155699546,-0.0660086821,0
.4337705026\N,1.7136578048,-0.4581269883,-0.735495585\O,1.7279952952,0

.589368351,1.2912657394\H,-0.8820569124,0.4389761503,0.8579739095\H,-0.3211532943,-1.05795823,1.6263491106\H,2.6711752371,-0.1943173959,-0.9181092909\H,1.2059722526,-1.000492784,-1.4182069403\Cl,-1.1369007502,-1.443261108,-0.5757026981\\Version=IA64L-G03RevE.01\State=1-A\HF=-668.8053597\RMSD=1.380e-09\RMSF=8.630e-06\Thermal=0.\Dipole=0.06572,-0.3272743,-0.6805517\PG=C01 [X(C2H4Cl1N1O1)]\@

n.CH2Cl-CONHCH3

1\1\GINC-LC107\FOpt\RB3LYP\Gen\C3H6Cl1N1O1\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-CONHCH3.freq\0,1\C,-0.0208612136,-0.0000880731,0.832958872\O,0.047934989,-0.0001621841,2.0563334756\C,1.3072388182,0.000035292,0.069461588\H,1.8709749485,0.8868375044,0.3611162733\H,1.8710557148,-0.886760098,0.3609788521\N,-1.1676307872,-0.0000295618,0.115827582\H,-1.1015874919,0.0000217128,-0.8926142133\C,-2.4767362752,-0.0001272167,0.7450140912\H,-2.323456579,0.0000227435,1.8250172109\H,-3.0476564112,-0.8918071657,0.4620146709\H,-3.0478733845,0.8913374683,0.4617845091\Cl,1.2182724015,0.0001724839,-1.7484920876\\Version=IA32L-G03RevC.02\State=1-A\HF=-708.1171097\RMSD=2.300e-09\RMSF=1.788e-05\Dipole=-0.5481578,0.0000151,-0.5626793\PG=C01 [X(C3H6Cl1N1O1)]\@

n.CH2Cl-COOC_CH3_3

1\1\GINC-LC112\FOpt\RB3LYP\Gen\C6H11Cl1O2\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-COOC_CH3_3.freq\0,1\C,0.8710518533,-1.4503391324,1.0003160782\H,1.888088025,-1.4297194458,0.604824378\H,0.3727617894,-2.3394275156,0.6079516603\C,0.119976002,-0.2005900732,0.5347118725\O,-0.3800851755,0.6308782972,1.2523376051\O,0.127952283,-0.2131846315,-0.809674941\C,-0.5175931207,0.8600191397,-1.6033578262\C,-2.020008725,0.8878271824,-1.308165676\C,-0.2493360692,0.4141557588,-3.0419922181\C,0.1618549671,2.2002966576,-1.3080933867\H,-0.6824928345,1.1343090416,-3.7439523325\H,-0.6952058852,-0.5671720567,-3.2334985957\H,0.8265253797,0.3481878131,-3.2334274396\H,-2.5099705664,1.5997274703,-1.9817590111\H,-2.2169425559,1.1900847154,-0.2782971346\H,-2.4617733663,-0.0997930206,-1.4798774011\H,-0.2373911824,2.9667422253,-1.9817098869\H,1.2413513985,2.1277435482,-1.4797191259\H,-0.0129457953,2.5158854012,-0.2782318996\Cl,0.9593334418,-1.5915491,2.7821107302\\Version=IA32L-G03RevC.02\State=1-A\HF=-845.9260704\RMSD=4.969e-09\RMSF=1.134e-05\Dipole=0.0156604,-0.0286986,-1.5136243\PG=C01 [X(C6H11Cl1O2)]\@

n.CH2Cl-COOCH2CH3

1\1\GINC-LC110\FOpt\RB3LYP\Gen\C4H7Cl1O2\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-COOCH2CH3.freq\0,1\C,0.120893445,1.2132103587,0.7631475683\H,-0.7233038796,1.8262628818,0.4397466783\H,1.0381057069,1.679138999,0.396096409\C,-0.0106755382,-0.1851924568,0.1655148344\O,-0.0826035861,-1.2267055099,0.7677475068\O,-0.033973525,-0.0633886366,-1.177506677\C,-0.156310148,-1.3026545464,-1.9223593134\H,-1.0764877205,-1.80644977,-1.6106888208\H,0.6845253154,-1.9515392742,-1.6583574803\C,-0.1669351115,-0.9483185658,-3.3966531225\H,-0.2581853238,-1.8613350911,-3.994851826\H,0.7584346468,-0.4393223864,-3.6844552113\H,-1.0108476145,-0.2937863474,-3.6366952551\Cl,0.1646199926,1.2062067895,2.5511399451\\Version=IA32L-G03RevC.02\State=1-A\HF=-767.2938557\RMSD=6.112e-09\RMSF=5.225e-06\Dipole=-0.0128695,0.282455,-1.4510332\PG=C01 [X(C4H7Cl1O2)]\@

n.CH2Cl-COOCH3

1\1\GINC-LC111\FOpt\RB3LYP\Gen\C3H5Cl1O2\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-COOCH3.freq\0,1\C,-0.4588836045,0.0001216356,0.0990362584\O,-0.46506

73733,0.0001344942,1.3037207213\C,0.7617122996,0.0000681269,-0.8163518
583\H,0.7337110203,0.8843105084,-1.4570148006\H,0.7333402498,-0.883849
6867,-1.4574411495\O,-1.5628426038,0.0002201855,-0.6783531363\C,-2.815
1519197,0.0003609387,0.0329422587\H,-2.8964178633,-0.8899278124,0.6615
985728\H,-3.5867597092,0.000299198,-0.7369193851\H,-2.8963441494,0.890
8189554,0.661371103\C1,2.3064523303,-0.0004584004,0.0842179427\Version
n=IA32L-G03RevC.02\State=1-A\HF=-727.9746818\RMSD=4.222e-09\RMSF=1.733
e-05\Dipole=-1.0195674,0.0002769,-0.9097857\PG=C01 [X(C3H5C11O2)]\@

n.CH2C1-COOH

1\1\GINC-LC113\FOpt\RB3LYP\Gen\C2H3C11O2\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_
-COOH.freq\0,1\C,-0.4819796884,0.0000348551,-0.6896093685\C,-0.475958
4284,-0.000019601,0.8326259116\O,0.4810861329,0.0000140376,1.562046541
5\O,-1.7608096619,0.000420687,1.2671558704\H,-1.0153905258,0.884244792
, -1.0462809626\H,-1.0157406266,-0.8839403712,-1.0463343906\H,-1.720425
445,0.0005779759,2.2420918053\C1,1.1609984429,-0.0002618658,-1.3906585
298\Version=IA32L-G03RevC.02\State=1-A\HF=-688.6673229\RMSD=5.282e-09
\RMSF=9.580e-05\Dipole=-1.165057,0.000198,0.1107585\PG=C01 [X(C2H3C11O
2)]\@

n.CH2C1-COPh

1\1\GINC-LC114\FOpt\RB3LYP\Gen\C8H7C11O1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2C1_
-COPh.freq\0,1\C,-3.105706288,0.0003596077,0.156668296\C,-3.086789744
7,0.0004301426,1.5547156226\C,-1.8685765127,0.0002033242,2.2363061325\
C,-0.6698723799,-0.0000930552,1.5237781027\C,-0.6795110044,-0.00017369
,0.1197455044\C,-1.9108652776,0.0000624183,-0.5555643677\C,0.567248008
, -0.0005031026,-0.7133264628\O,0.5221104754,-0.0001202935,-1.927477755
\C,1.9016165416,-0.0002753903,0.0452861953\H,1.9696136306,-0.885161318
8,0.684338829\H,1.9692998366,0.8845902128,0.684402476\H,-1.9014295076,
-0.0000010857,-1.6404535683\H,0.2667816612,-0.0002625265,2.0729990448\
H,-1.8509013434,0.0002590331,3.3225077668\H,-4.0531109656,0.0005359993
, -0.3750500212\H,-4.0198787083,0.0006628864,2.1116455238\C1,3.32691067
88,0.0000163305,-1.0380130676\Version=IA32L-G03RevC.02\State=1-A\HF=-
844.4829097\RMSD=2.783e-09\RMSF=4.507e-05\Dipole=-1.0517954,-0.0001404
,1.5490799\PG=C01 [X(C8H7C11O1)]\@

n.CHClCH3-H

1\1\GINC-LC97\FOpt\RB3LYP\Gen\C2H5C11\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2
-H.freq\0,1\C,-0.0847841216,0.8008918739,-0.1595137722\H,-0.377187964
7,1.4668429568,0.6546386233\C,-1.276565549,0.3636801121,-0.9932020752\
H,-0.9703173802,-0.3144771259,-1.7950997789\H,-1.7436555981,1.24688765
48,-1.4468457576\H,-2.024838686,-0.1438850889,-0.3774290287\C1,0.74155
54777,-0.6199186845,0.6261873377\H,0.6776545315,1.2958173235,-0.764153
715\Version=IA32L-G03RevC.02\State=1-A\HF=-539.4262586\RMSD=6.815e-09
\RMSF=1.923e-05\Dipole=-0.454969,0.6457169,-0.416172\PG=C01 [X(C2H5C11
)]\@

n.CHClCH3-BH2

1\1\GINC-LC81\FOpt\RB3LYP\Gen\C2H6B1C11\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3
_2-BH2.freq\0,1\H,-1.6909236712,-0.0739308835,-1.663204306\B,-1.71815
93095,0.1785918828,-0.4986837739\C,-0.4225401379,0.1962608415,0.383035
7195\H,-2.7668778332,0.3612796262,0.0493853235\C,-0.3150385452,-1.1303
297982,1.1595549269\H,-1.1815456004,-1.2480942786,1.82136786\H,0.59136
8589,-1.1382389989,1.7725587344\H,-0.2736730344,-1.9894748758,0.482703
4497\C1,1.104033318,0.4574609316,-0.6073543353\H,-0.4306462094,1.02307

7899,1.1000876303\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-564.8523083\\
RMSD=4.168e-09\\RMSF=1.577e-05\\Dipole=-0.5940046,-0.2148952,0.6141827\\P
G=C01 [X(C2H6B1C11)]\\@

n.CHClCH3-CH3

1\\1\\GINC-LC27\\FOpt\\RB3LYP\\Gen\\C3H7C11\\CYL509\\26-Jun-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3_2
-CH3.freq\\0,1\\H,1.2854855507,-0.6782569669,-1.7240164832\\C,1.24004509
99,-0.9029315103,-0.6548725842\\H,2.2658594641,-1.0069489669,-0.2791415
826\\H,0.7262558894,-1.8606789664,-0.5228224471\\C,0.5314525893,0.203600
0104,0.114839227\\C,0.4282147178,-0.0617658197,1.6107987234\\H,1.4367929
993,-0.1479247374,2.0346324447\\H,-0.1078900596,-0.9963914835,1.8051265
444\\H,-0.0934431955,0.7505001154,2.1243250456\\Cl,-1.160642677,0.431870
2059,-0.5762175168\\H,1.0195904193,1.1644914237,-0.0669979322\\Version=
IA32L-G03RevC.02\\State=1-A\\HF=-578.7436049\\RMSD=7.756e-09\\RMSF=2.590e-
05\\Dipole=0.8443703,-0.1644035,0.3635903\\PG=C01 [X(C3H7C11)]\\@

n.CHClCH3-NH2

1\\1\\GINC-LC117\\FOpt\\RB3LYP\\Gen\\C2H6C11N1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
3_2-NH2.freq\\0,1\\H,-1.2535862958,1.3049087567,-0.9037355248\\N,-0.2409
360219,1.3892510502,-0.8676382858\\C,0.3368814882,0.5265131632,0.079789
6278\\H,0.134941247,1.2587241981,-1.8020171203\\C,-0.2201466426,0.726299
3098,1.4768715975\\H,0.2457185337,0.0377224543,2.184509218\\H,-1.3016860
018,0.5541748459,1.4909763594\\H,-0.0248370645,1.7571862657,1.792777688
\\Cl,0.1037061523,-1.3391838894,-0.3575677503\\H,1.4225880729,0.61177740
88,0.0496417826\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-594.7807883\\RM
SD=2.952e-09\\RMSF=4.050e-05\\Dipole=-0.1205891,0.86888,-0.0030561\\PG=C0
1 [X(C2H6C11N1)]\\@

n.CHClCH3-OH

1\\1\\GINC-LC107\\FOpt\\RB3LYP\\Gen\\C2H5C11O1\\CYL509\\26-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
3_2-OH.freq\\0,1\\C,0.4308106539,-0.4190920376,0.0279561866\\O,0.4500531
308,-0.5955856246,1.3968210842\\C,-0.4490002632,-1.4791263394,-0.595107
3181\\H,1.060052278,0.0501959787,1.7884516918\\H,-0.5007329675,-1.352390
4256,-1.6785955326\\H,-1.4567243029,-1.4206185252,-0.1756513695\\H,-0.02
81021685,-2.4647377764,-0.366946017\\Cl,-0.2352327917,1.2785181804,-0.4
07541124\\H,1.4331772292,-0.3932630601,-0.4107215491\\Version=IA32L-G03
RevC.02\\State=1-A\\HF=-614.6404482\\RMSD=2.327e-09\\RMSF=1.548e-05\\Dipole
=0.6513404,-0.5243656,0.0541301\\PG=C01 [X(C2H5C11O1)]\\@

n.CHClCH3-F

1\\1\\GINC-LC43\\FOpt\\RB3LYP\\Gen\\C2H4C11F1\\CYL509\\26-Jun-2008\\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-F.freq\\0,1\\C,0.3024022523,0.2530032681,-0.427716016\\C,1.5931786153
, -0.3952640933,0.0141487094\\F,0.2286277064,1.5273166255,0.0635984601\\H
,2.4325387694,0.2009786324,-0.3604013741\\H,1.6728078607,-1.4112907563,
-0.3801874807\\H,1.6406545071,-0.4288100704,1.1058440641\\Cl,-1.13887103
39,-0.6791538056,0.1797836224\\H,0.1836718763,0.2924522114,-1.512559092
1\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-638.6565853\\RMSD=4.902e-09\\R
MSF=6.638e-05\\Dipole=0.773602,-0.2041265,-0.414643\\PG=C01 [X(C2H4C11F1
)\\@

n.CHClCH3-SiH3

1\\1\\GINC-LC113\\FOpt\\RB3LYP\\Gen\\C2H7C11Si1\\CYL509\\27-Jun-2008\\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C
H3_2-SiH3.freq\\0,1\\H,-1.1768282598,0.1715863825,-2.4881817817\\Si,-1.2
621192422,0.2186112233,-1.000754878\\C,0.5076802791,0.160127103,-0.2895

577061\H,-1.9389056433,1.4735877023,-0.590343564\H,-2.0272656278,-0.95
89541078,-0.5190263088\C,1.3030252911,-1.0878769353,-0.663717149\H,2.2
985062611,-1.0744714913,-0.2076137655\H,1.4273058714,-1.1303649969,-1.
7532399634\H,0.7918843182,-2.0003206292,-0.3408808872\C1,0.3749180379,
0.2921727067,1.5422041304\H,1.0571324041,1.0579429948,-0.587966523\\Ve
rsion=IA32L-G03RevC.02\State=1-A\HF=-830.1142221\RMSD=6.727e-09\RMSF=8
.296e-06\Dipole=0.2230832,-0.1114621,-0.7663018\PG=C01 [X(C2H7C11Si1)]
\\@

n.CHClCH3-PH2

1\1\GINC-LC105\FOpt\RB3LYP\Gen\C2H6C11P1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-PH2.freq\0,1\H,-2.025054465,0.0658786362,-0.1598733987\P,-1.17600
50013,1.1957706874,0.0006901651\H,-1.2428406106,1.1748710752,1.4200061
361\C,0.4550718867,0.2775192046,-0.176650774\C,0.7205504064,-0.1226563
866,-1.6261368967\H,1.6987636615,-0.6030415968,-1.7212908078\H,0.70710
71147,0.7682682259,-2.264754976\H,-0.0403100577,-0.821069593,-1.988753
2217\C1,0.6028708619,-1.2001286235,0.9026225683\H,1.239870965,0.951542
6332,0.1764561546\\Version=IA32L-G03RevC.02\State=1-A\HF=-881.364394\R
MSD=8.783e-09\RMSF=2.493e-05\Dipole=0.0653048,0.3203087,-0.3857483\PG=
C01 [X(C2H6C11P1)]\\@

n.CHClCH3-SH

1\1\GINC-LC98\FOpt\RB3LYP\Gen\C2H5C11S1\CYL509\27-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-SH.freq\0,1\C,0.3631202118,-0.3159791496,-0.3051684109\S,0.4064840
514,-0.1113002516,1.5318058463\C,-0.3916529759,-1.5505217996,-0.768802
4777\H,1.0258204806,-1.2910776221,1.7671468178\H,-0.4014169641,-1.5993
531667,-1.8628404452\H,-1.4209887607,-1.5368572927,-0.4018440101\H,0.1
039850124,-2.451296571,-0.3880763102\C1,-0.4131911945,1.1858931586,-0.
9701027678\H,1.3843022999,-0.301789322,-0.6877072095\\Version=IA32L-G0
3RevC.02\State=1-A\HF=-937.6036911\RMSD=4.537e-09\RMSF=8.494e-06\Dipol
e=0.4019539,-1.0390445,-0.2158596\PG=C01 [X(C2H5C11S1)]\\@

n.CHClCH3-Cl

1\1\GINC-LC151\FOpt\RB3LYP\Gen\C2H4Cl2\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-Cl.freq\0,1\C1,0.7288459702,0.6386792151,-1.260731782\C,0.355376090
6,0.0610543441,0.4115771788\C,-0.183294279,1.1920959691,1.2652560424\H
,0.5524689329,2.00116631,1.3076873461\H,-0.3721029886,0.8278147837,2.2
797980784\H,-1.1155108574,1.580867228,0.8479905513\C1,-0.8102275699,-1.
.3197918283,0.3610561503\H,1.2861412369,-0.3498357759,0.7980104362\\Ve
rsion=IA32L-G03RevC.02\State=1-A\HF=-999.016506\RMSD=5.839e-09\RMSF=9.
287e-05\Dipole=0.2565715,0.4157983,0.7470036\PG=C01 [X(C2H4Cl2)]\\@

n.CHClCH3-Br

1\1\GINC-LC32\FOpt\RB3LYP\Gen\C2H4Br1Cl1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-Br.freq\0,1\Br,0.1047612348,-0.728740134,-1.0108213819\C,-0.15082
93988,-0.0476431966,0.8366098363\C,1.1363841644,-0.1572551537,1.627936
5547\H,1.9238409935,0.4530416291,1.1791828192\H,1.4667607824,-1.199990
0627,1.6546278737\H,0.9629890603,0.1874704293,2.6531018092\C1,-0.76360
41489,1.6444180878,0.8154257635\H,-0.9522921166,-0.6603346956,1.242319
5386\\Version=IA32L-G03RevC.02\State=1-A\HF=-3112.7017876\RMSD=3.929e-
09\RMSF=9.472e-05\Dipole=0.2534008,-0.3856185,0.7445097\PG=C01 [X(C2H4
Br1Cl1)]\\@

n.CHClCH3-N_CH3_2

1\1\GINC-LC152\FOpt\RB3LYP\Gen\C4H10Cl1N1\CYL509\26-Jun-2008\0\#\B3LYP

```
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C  
H3_2-N_CH3_2.freq\\0,1\\C,1.5396373658,-0.1346654464,1.391219194\\H,2.63  
3892791,-0.1171481169,1.3773860634\\H,1.2150650222,-0.9719247046,2.0161  
723289\\H,1.1723042126,0.7991188688,1.8429566504\\N,1.0435245516,-0.3170  
050111,0.0305148182\\C,-0.2879532717,-0.7032753225,-0.0715952553\\C,1.53  
88061546,0.6943160804,-0.8990645306\\C,-0.7812064658,-1.1157634201,-1.4  
458894388\\H,2.6267852332,0.7561038341,-0.8034228609\\H,1.1080918222,1.6  
863281582,-0.6941343319\\H,1.306918748,0.4157565363,-1.9288006779\\H,-0.  
1325972848,-1.9083818821,-1.8388409253\\H,-0.791056405,-0.2802882394,-2  
.1491279354\\H,-1.8009935814,-1.4979816704,-1.3681132545\\C1,-1.54033981  
98,0.7263057528,0.5176132487\\H,-0.5130081801,-1.4534168527,0.684876172  
3\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-673.3984807\\RMSD=2.328e-09\\R  
MSF=7.245e-06\\Dipole=1.0996027,-0.6107325,-0.3525773\\PG=C01 [X(C4H10C1  
1N1)]\\@
```

n.CHClCH3-NHCH3

```
1\\1\\GINC-LC120\\FOpt\\RB3LYP\\Gen\\C3H8C11N1\\CYL509\\26-Jun-2008\\0\\#B3LYP/  
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH  
3_2-NHCH3.freq\\0,1\\C,1.911527452,-0.6774650786,0.7983523343\\H,2.94156  
44926,-0.8873866837,0.4967293519\\H,1.5770633715,-1.488931172,1.4531430  
948\\H,1.8841612878,0.2615343309,1.3689219261\\N,1.0654514419,-0.6410576  
393,-0.3893085686\\C,-0.3092776998,-0.5087403299,-0.2139755581\\C,-1.095  
9652332,-0.5671326814,-1.5088462343\\H,1.4238011466,-0.0071636569,-1.09  
83392129\\H,-0.769974741,0.2197648067,-2.1971598158\\H,-2.1627037295,-0.  
4336719214,-1.3198392681\\H,-0.9320509046,-1.5409687743,-1.9844474526\\C  
1,-0.8111980299,1.1823046856,0.6481012726\\H,-0.667361622,-1.2149245705  
,0.5352464708\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-634.0904656\\RMSD  
=7.796e-09\\RMSF=1.081e-05\\Dipole=0.637538,-0.7883647,-0.5187949\\PG=C01  
[X(C3H8C11N1)]\\@
```

n.CHClCH3-NHCHO

```
1\\1\\GINC-LC105\\FOpt\\RB3LYP\\Gen\\C3H6C11N1O1\\CYL509\\26-Jun-2008\\0\\#B3LY  
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_  
CH3_2-NHCHO.freq\\0,1\\H,1.4472569996,-0.3503089999,-2.5043189262\\C,1.3  
950547105,-0.1783458955,-1.4127975623\\O,2.3113842135,0.2870627586,-0.7  
669912431\\N,0.1912894637,-0.5908316162,-0.8858987828\\C,-0.1660972284,-  
0.360960606,0.4729839124\\H,-0.5432288734,-0.8544797023,-1.5317213123\\C  
, -0.9826730906,-1.4952724739,1.0684105607\\H,-0.3926915783,-2.418221008  
7,1.0386200398\\H,-1.9097896953,-1.6506773967,0.5063038664\\H,-1.2455211  
838,-1.2743248807,2.105342215\\C1,-1.1421385552,1.2211259842,0.64288928  
78\\H,0.7525234669,-0.1643366466,1.0222961833\\Version=IA32L-G03RevC.02  
\\State=1-A\\HF=-708.1165332\\RMSD=3.001e-09\\RMSF=2.693e-05\\Dipole=-0.755  
9836,-1.2754459,-0.4917261\\PG=C01 [X(C3H6C11N1O1)]\\@
```

n.CHClCH3-NHCOCH3

```
1\\1\\GINC-LC49\\FOpt\\RB3LYP\\Gen\\C4H8C11N1O1\\CYL509\\26-Jun-2008\\0\\#B3LYP  
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C  
H3_2-NHCOCH3.freq\\0,1\\H,-1.2532980592,1.9179619285,-2.3747177282\\C,-0.  
.2366227887,2.006891973,-1.9768960236\\C,-0.0738062128,1.3149809539,-0.  
6315204878\\H,0.019377621,3.0608886367,-1.8600693724\\H,0.4548606328,1.5  
627611874,-2.7036774893\\N,-0.7980571209,0.1329519888,-0.5193181498\\O,0  
.6243359022,1.7628396755,0.2594399931\\C,-0.6404256282,-0.8465136205,0.  
5070704226\\H,-1.178912735,-0.2238197432,-1.3868272483\\C,-0.6107821101,  
-0.3162222374,1.9313031295\\H,0.2596137663,0.3152777294,2.0980569994\\H,  
-0.5997712115,-1.157635703,2.6286875948\\H,-1.5152692457,0.2782801168,2  
.1054930268\\C1,0.8950891587,-1.8921774116,0.2170629412\\H,-1.4415833985  
, -1.5749018947,0.3829490781\\Version=IA32L-G03RevC.02\\State=1-A\\HF=-74  
7.4362134\\RMSD=2.448e-09\\RMSF=2.899e-06\\Dipole=-1.3638671,0.0112912,-0  
.8185582\\PG=C01 [X(C4H8C11N1O1)]\\@
```

n.CHClCH₃-NO₂

1\1\GINC-LC45\FOpt\RB3LYP\Gen\C2H4Cl1N1O2\CYL509\26-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_C
H3_2-NO2.freq\0,1\O,-0.6612663417,-0.6373153807,-1.9114892651\N,-0.73
79602508,-0.3591135485,-0.7203476294\C,0.5895741755,-0.312459715,0.041
6045376\O,-1.761240017,-0.1490044706,-0.0851037042\C,0.54301985,-1.277
4073464,1.207946363\H,1.4986451796,-1.2554300619,1.7375563965\H,0.3689
186479,-2.2938230546,0.8372600366\H,-0.2603518121,-1.0010965195,1.8937
360946\Cl,0.8705908347,1.3792009425,0.5737730639\H,1.3429522667,-0.552
5103676,-0.7048228576\Version=IA32L-G03RevC.02\State=1-A\HF=-743.9150
309\RMSD=3.540e-09\RMSF=3.227e-05\Dipole=0.9645755,-0.6230164,0.617974
1\PG=C01 [X(C2H4Cl1N1O2)]\@

n.CHClCH₃-OCF₃

1\1\GINC-LC106\FOpt\RB3LYP\Gen\C3H4Cl1F3O1\CYL509\26-Jun-2008\0\#\B3LYP
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_
CH3_2-OCF3.freq\0,1\C,1.2669821997,0.0650365138,-0.2314052016\O,0.098
0717158,-0.400819339,-0.8852705749\C,-1.1398299727,0.0097594637,-0.497
3721716\F,-1.4015967184,1.2724843729,-0.8996317216\F,-1.3195529329,-0.
0260903807,0.8333709877\F,-2.0255328141,-0.7986023731,-1.0761981552\C,
1.2925755083,1.542779425,0.1157916615\H,2.2823771565,1.7965085366,0.50
27047096\H,0.547760576,1.7911024674,0.8741977004\H,1.0989744333,2.1323
365808,-0.7855270845\Cl,1.6133341447,-0.9441195717,1.25748303\H,2.0614
094241,-0.1989371422,-0.9263779645\Version=IA32L-G03RevC.02\State=1-A
\HF=-951.6765037\RMSD=5.457e-09\RMSF=3.110e-05\Dipole=0.5373114,0.7146
226,-0.3213149\PG=C01 [X(C3H4Cl1F3O1)]\@

n.CHClCH₃-OCH₂CH₃

1\1\GINC-LC57\FOpt\RB3LYP\Gen\C4H9Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_
CH3_2-OCH2CH3.freq\0,1\H,-0.3300230735,-3.2964638077,1.4576826231\C,-0.4
081162125,-2.7626840651,0.5043078439\C,-0.4069302012,-1.2632643173,0.7
450161862\O,-0.5313055913,-0.624530656,-0.5348323912\C,-0.3503132863,0
.7345869846,-0.5979000482\C,-1.1740804298,1.5751272515,0.3646505138\H,
-1.2448572558,-0.9719255534,1.3923409225\H,0.5269010835,-0.9404813715,
1.2213457649\H,0.4375667485,-3.0506726369,-0.127472065\H,-1.3324550605
, -3.0745144208,0.0073566962\H,-0.8844468374,1.4069938125,1.4048454453\H,
-2.2331424949,1.3174233351,0.2422630347\H,-1.040830972,2.6362723023,
0.1409263975\Cl,1.4656522695,1.1913604389,-0.3482854334\H,-0.527715209
,1.0138910049,-1.6362242956\Version=IA32L-G03RevC.02\State=1-A\HF=-69
3.2651982\RMSD=9.299e-09\RMSF=2.065e-05\Dipole=-0.917563,-0.2013349,0.
4434499\PG=C01 [X(C4H9Cl1O1)]\@

n.CHClCH₃-OCH₃

1\1\GINC-LC133\FOpt\RB3LYP\Gen\C3H7Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_
CH3_2-OCH3.freq\0,1\C,-1.1382670914,-0.3673442953,-1.7394033933\O,-0.80
20089266,-0.8420929867,-0.4391258845\C,0.407930234,-0.4230712119,0.048
4024335\H,-0.3467320806,-0.6076278748,-2.4634622055\H,-2.0599848168,-0
.8777348683,-2.0241558934\H,-1.3017436119,0.7159274113,-1.7275126449\C
,0.7411972486,-1.1974994847,1.3045767615\H,1.6912479638,-0.861003143,1
.7251241156\H,0.8133115786,-2.2620782485,1.0552513266\H,-0.0492115823,
-1.0619444907,2.0471894729\Cl,0.3768263399,1.4170391344,0.4664267967\H
,1.1979738363,-0.4709702261,-0.7101374486\Version=IA32L-G03RevC.02\St
ate=1-A\HF=-653.9495313\RMSD=3.467e-09\RMSF=1.636e-05\Dipole=0.1270822
, -0.7392598,-0.567739\PG=C01 [X(C3H7Cl1O1)]\@

n.CHClCH₃-OCHO

```
1\1\GINC-LC35\FOpt\RB3LYP\Gen\C3H5Cl1O2\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-OCHO.freq\0,1\C,-0.5529655399,-0.3512778597,-0.6298077363\O,-0.534
6005995,-0.9790216502,0.6478617228\C,0.5150364835,-0.8146190751,1.4937
63885\H,0.2899340882,-1.3765308527,2.4125929001\O,1.5145348391,-0.1779
880581,1.2990203071\C,0.6286190451,-0.6820918663,-1.5237532025\H,1.552
0454187,-0.2532012374,-1.1366821902\H,0.438831206,-0.2929347685,-2.527
8050627\H,0.7310915311,-1.7717292082,-1.5850090529\Cl,-0.7590459995,1.
4547562645,-0.4539064053\H,-1.4917341018,-0.6924499559,-1.0629616221\
Version=IA32L-G03RevC.02\State=1-A\HF=-727.9727887\RMSD=7.204e-09\RMSF
=4.741e-05\Dipole=-0.3330054,-0.951347,-0.355117\PG=C01 [X(C3H5Cl1O2)]
\@
```

n.CHClCH3-OCOCH3

```
1\1\GINC-LC134\FOpt\RB3LYP\Gen\C4H7Cl1O2\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-OCOCH3.freq\0,1\C,-0.9482280842,0.031557146,-0.1960807518\O,0.313
6619885,-0.5450578328,-0.4560977675\C,1.3861038105,0.3106545882,-0.560
8937855\C,2.6573429094,-0.4764452976,-0.7426493346\O,1.2876128038,1.51
11142058,-0.5100557588\C,-2.0155901324,-0.8358509748,-0.825717167\H,3.
4802448073,0.2068663169,-0.9540621464\H,2.5463328511,-1.201918374,-1.5
542279839\H,2.871400417,-1.0389609341,0.1727982014\H,-1.8641880445,-0.
8583492796,-1.9106703792\H,-3.0077496944,-0.4301207363,-0.6137518307\H
,-1.9569164591,-1.856662095,-0.4389288975\Cl,-1.1998525323,0.129690141
6,1.6184885547\H,-0.959600187,1.0664689398,-0.5341879485\Version=IA32
L-G03RevC.02\State=1-A\HF=-767.3047547\RMSD=6.530e-09\RMSF=4.613e-06\D
ipole=0.1204296,-0.7597717,-0.8334917\PG=C01 [X(C4H7Cl1O2)]\@
```

n.CHClCH3-Si_CH3_3

```
1\1\GINC-LC27\FOpt\RB3LYP\Gen\C5H13Cl1Si1\CYL509\27-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-Si_CH3_3.freq\0,1\H,1.8349372437,-1.1672312018,-1.7889129042\C,1
.8664025195,-1.1637339904,-0.6926557004\H,2.9192529419,-1.0944167159,-
0.3930137711\H,1.4800694177,-2.1276390415,-0.3452360713\Si,0.868086275
3,0.2711907881,0.0225463284\C,-0.9568699646,0.1143748117,-0.5668044359
\C,0.9283266551,0.2627828703,1.9107197785\C,1.5343651934,1.9145412429,
-0.6504396608\C,-1.8996318836,1.228539071,-0.1194525482\H,2.5947361867
,2.0317483701,-0.394854128\H,1.0008161436,2.7767304216,-0.2337325988\H
,1.4546019436,1.9678906174,-1.7430692751\H,1.9641393445,0.3261809533,2
.2656955352\H,0.4913535652,-0.6568860078,2.314498628\H,0.381549231,1.1
104911123,2.3400844285\H,-1.5474522973,2.1886825401,-0.5177438629\H,-1
.9414343386,1.3065710729,0.971700143\H,-2.9183783816,1.0636919109,-0.4
864994868\Cl,-1.6308432732,-1.5115018593,0.0038838862\H,-0.9786183299,
0.0340225103,-1.6587958984\Version=IA32L-G03RevC.02\State=1-A\HF=-948
.0971958\RMSD=2.679e-09\RMSF=2.423e-06\Dipole=0.4951272,0.7718779,-0.1
710982\PG=C01 [X(C5H13Cl1Si1)]\@
```

n.CHClCH3-P_CH3_2

```
1\1\GINC-LC27\FOpt\RB3LYP\Gen\C4H10Cl1P1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-P_CH3_2.freq\0,1\C,-0.693273017,1.1173540629,1.7968838814\H,0.016
1251962,1.9264178432,2.0009827865\H,-1.2028392284,0.8781606601,2.73649
07848\H,-1.4306360314,1.4661824676,1.0670772438\P,0.2281157716,-0.3916
505581,1.2182986125\C,-1.1956801447,-1.4847371926,0.7257400061\C,0.868
0169654,0.1927145221,-0.4494794565\H,-0.8221190346,-2.4046545148,0.265
0760774\H,-1.8834537343,-0.990012809,0.0325219858\H,-1.7427963055,-1.7
68394067,1.6312299942\C,1.6164723573,-0.9030954609,-1.2044087738\H,2.4
246099178,-1.2946097521,-0.575674293\H,2.0528159726,-0.5107777806,-2.1
278084569\H,0.9516134338,-1.7313373049,-1.4681971053\Cl,-0.4058496349,
```

0.9259194175,-1.5767688724\H,1.5411700663,1.0297379426,-0.2435213179\\
Version=IA32L-G03RevC.02\State=1-A\HF=-960.0066811\RMSD=4.264e-09\RMSF
=5.413e-06\Dipole=0.1138354,-0.2243837,0.3390424\PG=C01 [X(C4H10C11P1)
]\@

n.CHClCH3-SC_CH3_2CN

1\1\GINC-AC1\FOpt\RB3LYP\Gen\C6H10C11N1S1\CYL509\03-Sep-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CHC
lCH3-SC_CH3_2CN.freq\\0,1\N,-1.4930211324,-1.3900530989,-2.2883730215\
C,-0.9728615515,-1.3584316508,-1.2499546993\C,-0.306116521,-1.35281571
05,0.0615451996\S,-0.7768159674,0.1870279066,1.0189739362\C,-0.0295743
22,1.6363202568,0.1993404097\C,-0.2417288667,1.7836319778,-1.301261140
2\C1,1.76105699,1.8701414991,0.5871170782\C,1.214633872,-1.5224686607,
-0.107920674\C,-0.8886959701,-2.503717494,0.9150074589\H,1.6532920992,
-0.7302457695,-0.716823746\H,1.6952383469,-1.5061426162,0.8737589984\H
,1.420132744,-2.4849306865,-0.5905716521\H,-0.4021537188,-2.5181477903
,1.8946223333\H,-0.7005252585,-3.4585254871,0.4136807349\H,-1.96775720
58,-2.3936569109,1.0543280082\H,-1.3074963887,1.7017688734,-1.53490356
99\H,0.2923889402,1.0193740679,-1.8692076931\H,0.1213326394,2.76432621
8,-1.6229717407\H,-0.5161574661,2.4565874928,0.7315868397\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-1147.7811117\RMSD=3.218e-09\RMSF=1.650e-05
\Dipole=0.1764105,-0.2037066,0.6091668\PG=C01 [X(C6H10C11N1S1)]\\@

n.CHClCH3-SCH2COOCH3

1\1\GINC-LC142\FOpt\RB3LYP\Gen\C5H9C11O2S1\CYL509\27-Jun-2008\0\#B3LYP
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_
CH3_2-SCH2COOCH3.freq\\0,1\S,1.1491302817,0.6035996438,0.6676386438\C,
0.3230611253,-0.8466169716,1.3983454295\C,1.3482795106,-1.7181678083,2
.1088170577\C,-0.2073791845,1.2783101823,-0.3722913046\C,-0.4570635506
,0.4244373297,-1.598799633\O,-0.9004360425,-0.7058072403,-1.5749130692
\O,-0.1135618785,1.0723755053,-2.7274868937\C,-0.2930465419,0.32752854
42,-3.9463143004\H,0.0943358413,2.2886551338,-0.6529059205\H,-1.116050
3692,1.3254820094,0.2351024912\H,-1.341540963,0.0452036103,-4.07044954
11\H,0.3213280501,-0.5762911145,-3.9332659443\H,0.0235173882,0.9975392
659,-4.7456218732\H,0.8522898087,-2.5812521263,2.5610251438\H,2.089788
1786,-2.0766776831,1.3867904533\H,1.8627113496,-1.1617399913,2.8980818
094\C1,-1.0083683526,-0.3683737747,2.583053031\H,-0.2013265822,-1.3816
530122,0.6077797607\\Version=IA32L-G03RevC.02\State=1-A\HF=-1204.79506
7\RMSD=4.489e-09\RMSF=8.939e-06\Dipole=0.3570481,0.1041827,-0.996592\P
G=C01 [X(C5H9C11O2S1)]\\@

n.CHClCH3-SCH2Ph

1\1\GINC-LC133\FOpt\RB3LYP\Gen\C9H11C11S1\CYL509\27-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_
H3_2-SCH2Ph.freq\\0,1\C,-1.5950072536,-1.2186970806,-1.0256718306\S,-1
.5749681229,-1.0842886336,0.7861227117\C,0.22375993,-1.2384588244,1.19
08087647\C,-2.9865861096,-1.6294155083,-1.4934295374\C,1.0866220985,-0
.0210297413,0.9571955405\H,0.619744618,-2.1079153881,0.6558366815\H,0.
2042394506,-1.5006396726,2.2548678827\C,2.1544924311,-0.0758059632,0.0
550341468\C,0.8627693182,1.1678224767,1.6651782113\C,2.9831456235,1.03
11325934,-0.1391715804\C,1.6870122107,2.2741225394,1.4730743914\C,2.75
13507257,2.2092841162,0.5694354601\H,3.3936193582,3.0729435492,0.41962
22657\H,1.4995600276,3.1891382156,2.0287374808\H,3.8064769233,0.971114
5392,-0.8459745958\H,0.0301826389,1.2273752352,2.3620128071\H,2.340465
4576,-0.9918378058,-0.501467126\H,-3.2461645475,-2.6066275223,-1.07325
84186\H,-3.0106801559,-1.6923729739,-2.5849003758\H,-3.7361885876,-0.8
989681506,-1.1746443534\C1,-1.1097271542,0.3316518291,-1.8999084571\H,
-0.8417574432,-1.9454006295,-1.335073264\\Version=IA32L-G03RevC.02\Sta
te=1-A\HF=-1207.970563\RMSD=3.170e-09\RMSF=1.540e-06\Dipole=0.3042072,

-0.6748558,0.1577117\PG=C01 [X(C9H11Cl1S1)]\@

n.CHClCH3-SCH3

1\1\GINC-LC10\FOpt\RB3LYP\Gen\C3H7Cl1S1\CYL509\27-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-SCH3.freq\0,1\S,0.6949475477,-0.2516532599,-1.2439404156\C,0.3845678149,-0.5161794941,0.5282825106\C,-0.7513989326,-1.4741064496,0.8627114733\C,-0.9135586086,0.3906044606,-1.8244020179\H,-0.7586937186,0.6969841421,-2.8619925342\H,-1.2076691118,1.263940082,-1.2365875843\H,-1.6976344907,-0.3698446569,-1.7940997599\H,-0.8080216866,-1.6290433145,1.9444828256\H,-1.7154963249,-1.0841747219,0.5255218657\H,-0.5702712893,-2.4375287621,0.3745747416\Cl,0.1168051729,1.0634339252,1.4495860853\H,1.3352762768,-0.8941684398,0.9086318471\Version=IA32L-G03RevC.02\State=1-A\HF=-976.9226575\RMSD=8.115e-09\RMSF=4.948e-06\Dipole=-0.5201011,-0.6105171,-0.250277\PG=C01 [X(C3H7Cl1S1)]\@

n.CHClCH3-SO2CH3

1\1\GINC-LC70\FOpt\RB3LYP\Gen\C3H7Cl1O2S1\CYL509\27-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-SO2CH3.freq\0,1\C,-0.3264285955,-0.2095639395,-0.9425367235\S,-0.2537900759,-0.1314175088,0.9111184128\C,1.2125126215,-1.0887486929,1.3586713905\O,-0.0402476541,1.2622553173,1.3184806835\O,-1.4416436654,-0.8773768077,1.3580993478\H,1.118012609,-2.1026648751,0.9646160702\H,1.2202682065,-1.1101187963,2.4511336771\H,2.1059333907,-0.5935137581,0.9784820267\C,-1.4974269268,0.6326770073,-1.4210870995\H,-1.5847919468,0.5562467471,-2.5080830013\H,-1.3540173879,1.6796949146,-1.1431271411\H,-2.4193250321,0.2629124281,-0.9615904917\Cl,1.2320691489,0.3288992173,-1.6796453455\H,-0.447426195,-1.2663775383,-1.1882805256\Version=IA32L-G03RevC.02\State=1-A\HF=-1127.3059048\RMSD=6.321e-09\RMSF=2.681e-05\Dipole=0.5088407,-0.9056045,-0.7055162\PG=C01 [X(C3H7Cl1O2S1)]\@

n.CHClCH3-SOCH3

1\1\GINC-LC25\FOpt\RB3LYP\Gen\C3H7Cl1O1S1\CYL509\27-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-SOCH3.freq\0,1\C,-0.8396361002,-0.0685385924,-0.7578902439\S,-0.8283678464,0.4577517088,0.9760155581\O,0.3481775706,-0.5348839083,1.6543730069\C,1.6604819094,0.0534267234,1.7336569719\C,-0.8330352301,-1.5789677999,-0.9462616977\H,2.2679249459,-0.6781629185,2.2737533324\H,1.6377089456,0.9955424442,2.2922626971\H,2.0812589419,0.2259460147,0.7387344624\H,0.0609726267,-2.0168139263,-0.4970956347\H,-0.8557997872,-1.8270512247,-2.0109276664\H,-1.7130851484,-2.0095189063,-0.4573830754\C1,0.518569245,0.6732161198,-1.7772746446\H,-1.7530561855,0.3849064191,-1.1539383232\Version=IA32L-G03RevC.02\State=1-A\HF=-1052.1079321\RMSD=2.828e-09\RMSF=1.174e-05\Dipole=-0.0818982,-0.2410111,0.1003819\PG=C01 [X(C3H7Cl1O1S1)]\@

n.CHClCH3-Ph

1\1\GINC-LC59\FOpt\RB3LYP\Gen\C8H9Cl1\CYL509\27-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-Ph.freq\0,1\H,-3.8099722298,-1.2535489877,-0.1320688582\C,-2.7566605914,-0.9914504605,-0.0807810543\C,-1.7894715892,-1.87872065,-0.5513088592\C,-0.4373834829,-1.5354518407,-0.4879813526\C,-0.0354482255,-0.3083216633,0.0514760408\C,-1.0157932646,0.5787635824,0.5184972508\C,-2.3653211362,0.2402374705,0.4519045649\H,-2.0839793369,-2.8362104045,-0.9724151422\C,1.4357576808,0.0142300436,0.1538429688\C,1.9270489424,0.2674875472,1.5760385677\H,-0.7209167507,1.5453048343,0.9177147601\H,0.313084533,-2.2286702743,-0.8613246394\H,-3.1145741112,0.9394550076,0.8133718793\H,3.0003876399,0.4769122934,1.5849560719\H,1.736071077,-0.6234184691,2.186220718\H,1.404618816,1.1132394653,2.032252163\Cl,1.85191622

06,1.4903776101,-0.885688512\H,2.0163346136,-0.7901270112,-0.302131010
8\\Version=IA32L-G03RevC.02\State=1-A\HF=-770.4763403\RMSD=7.681e-09\R
MSF=4.315e-06\Dipole=-0.3545329,-0.6931609,0.562397\PG=C01 [X(C8H9C11)
J]\\@

n.CHC1CH3-C6H4CN

1\1\GINC-LC140\FOpt\RB3LYP\Gen\C9H8C11N1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-C6H4CN.freq\0,1\N,-4.7872462692,-0.4257415636,0.2222999901\C,-3.6
357844069,-0.2644360457,0.1847207528\C,-2.2164404952,-0.0648094692,0.1
404538138\C,-1.344178238,-1.1339046884,0.4127597264\C,0.0297856214,-0.
9352321854,0.3718109951\C,0.5637159245,0.3238824022,0.0594793406\C,-0.
311942611,1.3800461962,-0.2187780394\C,-1.6916553078,1.1965159789,-0.1
777268683\H,-1.7520272009,-2.1107259171,0.6514926574\C,2.0547496702,0.
569934717,0.0590335663\C,2.7197950525,0.3454372667,1.4146248558\H,0.08
78182095,2.3587990934,-0.4709717996\H,0.6963543972,-1.7700997573,0.565
9447957\H,-2.3636976784,2.0205070805,-0.3941316759\H,3.7913773117,0.55
51496401,1.3575369397\H,2.5850506073,-0.6844144744,1.757686871\H,2.268
2902836,1.016772976,2.1546868866\C1,2.8785419235,-0.4997313479,-1.1980
488528\H,2.2540739964,1.5850301848,-0.2897829666\\Version=IA32L-G03Rev
C.02\State=1-A\HF=-862.7188268\RMSD=7.374e-09\RMSF=6.485e-06\Dipole=1.
3649291,0.6662265,0.597111\PG=C01 [X(C9H8C11N1)]\\@

n.CHC1CH3-C6H4NO2

1\1\GINC-LC82\FOpt\RB3LYP\Gen\C8H8C11N1O2\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-C6H4NO2.freq\0,1\O,-2.8809436331,2.7616179456,-0.643246978\N,-2.
1212920183,2.0911337672,-1.341672781\C,-1.232787369,1.1349778024,-0.66
12018531\O,-2.0520360647,2.1611968103,-2.5682262328\C,-1.2877550824,1.
0316247954,0.7252012788\C,-0.4420163146,0.1236659227,1.3588200512\C,0.
4418492285,-0.6737068566,0.6208022\C,0.4757343376,-0.5409599553,-0.776
1171754\C,-0.3581889817,0.3617043435,-1.4248114515\H,-0.3427885151,0.4
787805639,-2.5012693318\C,1.3059979578,-1.687144301,1.3362529851\C,1.0
074959342,-3.1336680879,0.9495612151\H,-0.4712670949,0.0362697784,2.44
16153355\H,1.1734605828,-1.1357449815,-1.3574869882\H,-1.9762795667,1.
6543792422,1.2826925219\H,1.6473757572,-3.821244409,1.5092637066\H,1.1
689801124,-3.3001648067,-0.1193516093\H,-0.040097329,-3.3612268795,1.1
795306965\C1,3.0880014819,-1.3359292356,1.027213819\H,1.1954943096,-1.
5596678987,2.4148223967\\Version=IA32L-G03RevC.02\State=1-A\HF=-974.97
69237\RMSD=9.217e-09\RMSF=3.842e-05\Dipole=0.2632854,-1.3885483,0.8869
556\PG=C01 [X(C8H8C11N1O2)]\\@

n.CHC1CH3-C6H4OCH3

1\1\GINC-LC149\FOpt\RB3LYP\Gen\C9H11C11O1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-C6H4OCH3.freq\0,1\C,-1.746396739,-0.2710769549,-0.189771192\C,-1.
.7183957455,0.0803666902,1.170264676\C,-0.5155482096,0.4949791032,1.75
02740586\C,0.6403311296,0.5538883719,0.9661857208\C,0.6261279831,0.217
3627614,-0.3883867022\C,-0.5914596568,-0.2018284143,-0.9525395514\C,1.
884346945,0.3328729732,-1.2063062782\O,-2.9072679453,-0.0196590858,1.8
299836023\C,-2.9393549227,0.306772369,3.2106849625\C,1.7648469402,1.21
36413158,-2.4460234288\H,-0.6296887723,-0.4942994793,-1.99817216\H,1.5
714792362,0.8723217466,1.4296316582\H,-0.4624619391,0.7675232975,2.797
9756074\H,-2.6875899978,-0.5987126373,-0.6199662701\H,-2.2778242077,-0.
.3463934945,3.7948271242\H,-3.9716101607,0.1535401192,3.5302943947\H,-
2.6576518115,1.3537700175,3.3844574734\H,2.7176677158,1.2648201553,-2.
9803234692\H,1.476291321,2.226531724,-2.1403946958\H,1.0037714589,0.83
37996766,-3.1336502521\C1,2.4735887627,-1.348788689,-1.7422447887\H,2.
6977654087,0.6919099795,-0.5726804138\\Version=IA32L-G03RevC.02\State=

1-A\HF=-884.9995508\RMSD=4.494e-09\RMSF=8.681e-07\Dipole=-0.46602,0.9588167,0.8361542\PG=C01 [X(C9H11Cl1O1)]\@

n.CHClCH3-C6H4OH

1\1\GINC-LC25\FOpt\RB3LYP\Gen\C8H9Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-C6H4OH.freq\0,1\C,-1.7576064347,-1.4509752537,0.2648682515\C,-2.24
02589709,-0.4013733414,1.0516718447\C,-1.5204493708,0.7975923156,1.128
9137681\C,-0.3324661098,0.9424728173,0.418968353\C,0.1643359331,-0.097
3040478,-0.3779811965\C,-0.5648090044,-1.2926250962,-0.4347507513\C,1.
4299859373,0.0504480035,-1.180170562\O,-3.4131170126,-0.6023786357,1.7
223960028\C,1.4469137948,1.2375431837,-2.1380519067\H,-0.1939254234,-2
.1172374866,-1.0391725794\H,0.2228956395,1.872337884,0.5034379327\H,-1
.8888898669,1.6141984987,1.7474568043\H,-2.3215824346,-2.3769374629,0.
217158477\H,-3.625556287,0.1934028821,2.2345344211\H,2.3856602762,1.27
26138582,-2.6979343889\H,1.329122066,2.1840422994,-1.6025130273\H,0.61
61888753,1.138738751,-2.8470635292\Cl,2.9062818936,0.1880124932,-0.056
7855886\H,1.6203564171,-0.8730140073,-1.7305239301\Version=IA32L-G03R
evC.02\State=1-A\HF=-845.692873\RMSD=7.635e-09\RMSF=1.585e-06\Dipole=-
0.8847954,0.4821339,-0.2338009\PG=C01 [X(C8H9Cl1O1)]\@

n.CHClCH3-CF2CF3

1\1\GINC-LC73\FOpt\RB3LYP\Gen\C4H4Cl1F5\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CF2CF3.freq\0,1\F,-0.7908096185,1.2137150564,-1.2893575185\C,-0.23
37007255,0.572685412,-0.2154656874\C,1.2051933935,0.1912851503,-0.6500
184963\C,-1.1809696535,-0.5789059095,0.148410738\F,-0.1342066246,1.466
4783344,0.8001834207\F,1.1605409115,-0.846209336,-1.5082283514\F,1.964
7961492,-0.1461813825,0.3959660009\F,1.7786441658,1.2309710649,-1.2710
407596\C,-2.5833297377,-0.067774776,0.4596798854\H,-2.9860741934,0.459
2993899,-0.4102504822\H,-2.5638773068,0.6165060508,1.3114752851\H,-3.2
383551567,-0.9088989264,0.6972690439\Cl,-0.5338577897,-1.5216512566,1.
5583896422\H,-1.1899554298,-1.2715380479,-0.6944615311\Version=IA32L-
G03RevC.02\State=1-A\HF=-1114.2370638\RMSD=2.476e-09\RMSF=3.604e-05\Di
pole=-0.7729872,-0.1105283,-0.2847409\PG=C01 [X(C4H4Cl1F5)]\@

n.CHClCH3-CF2H

1\1\GINC-LC77\FOpt\RB3LYP\Gen\C3H5Cl1F2\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CF2H.freq\0,1\C,0.6823339076,0.1614603359,-0.9071002298\C,0.463973
7386,0.187682766,0.6009993615\H,1.7566813223,0.1822761518,-1.135861584
\F,0.1006097089,1.2374368058,-1.5014979557\F,0.154449916,-0.9690098093
, -1.4541640941\C,1.115502637,-1.0025757696,1.2926560827\H,2.1947324949
, -1.0060755881,1.0939591791\H,0.6896257284,-1.9390611651,0.9238514578\H,
0.9656547296,-0.9460385065,2.3731383946\Cl,-1.3141926861,0.240060470
6,0.96782163\H,0.8681830666,1.1326241461,0.9735720034\Version=IA32L-G
03RevC.02\State=1-A\HF=-777.2073551\RMSD=5.510e-09\RMSF=7.777e-05\Dipo
le=1.197153,-0.0844402,0.4252639\PG=C01 [X(C3H5Cl1F2)]\@

n.CHClCH3-CF3

1\1\GINC-LC43\FOpt\RB3LYP\Gen\C3H4Cl1F3\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CF3.freq\0,1\F,0.2465512687,0.9645835903,-1.3179290196\C,0.2117325
351,0.8564390991,0.0212836896\F,1.4668553812,0.9657778043,0.484363917\H,
-0.4612634368,-0.4374535827,0.480856216\F,-0.4944423647,1.9076650392
,0.5010194469\C,-1.891962112,-0.5555783252,-0.0262019047\H,-1.91342579
2,-0.5675815859,-1.1188946341\H,-2.4785505151,0.2972244714,0.330283279
6\H,-2.3466623301,-1.4761242973,0.3463315212\Cl,0.531781801,-1.8549773
612,-0.0583933529\H,-0.4233724651,-0.441584498,1.5722497301\Version=I

A32L-G03RevC.02\State=1-A\HF=-876.4587502\RMSD=3.781e-09\RMSF=7.243e-05\Dipole=-0.783973,-0.0462313,0.3637335\PG=C01 [X(C3H4C11F3)]\@

n.CHClCH3-CCl2H

1\1\GINC-LC133\FOpt\RB3LYP\Gen\C3H5Cl3\CYL509\26-Jun-2008\0\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-CCl2H.freq\0,1\C,0.3493897881,0.2157533963,-0.5826159055\C,0.3853349963,-0.0269811451,0.9327612891\H,1.2264337381,-0.2123947873,-1.0624509337\Cl,0.4261375204,1.9990502542,-0.895179323\Cl,-1.0810076793,-0.5094366762,-1.3903329791\C,-0.8588770873,0.3809222847,1.7056601482\H,-0.6995699332,0.2178387711,2.7743313323\H,-1.7275478751,-0.1993316953,1.3866188856\H,-1.062450592,1.4440103261,1.5406081729\Cl,0.757411687,-1.7937854281,1.2102136685\H,1.2648425026,0.5026316211,1.3061361232\Version=IA32L-G03RevC.02\State=1-A\HF=-1497.921551\RMSD=5.542e-09\RMSF=3.565e-05\Dipole=0.2093609,0.3473227,0.4224413\PG=C01 [X(C3H5Cl3)]\@

n.CHClCH3-CCl3

1\1\GINC-LC151\FOpt\RB3LYP\Gen\C3H4Cl4\CYL509\26-Jun-2008\0\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-CCl3.freq\0,1\C,0.2632233571,0.0767576534,-0.3852649943\C,0.1094016304,0.0536216287,1.1598805069\Cl,2.0353856822,-0.0232762226,-0.7621005614\Cl,-0.3545397316,1.6216816987,-1.0663227755\Cl,-0.5797004454,-1.300650371,-1.1674888203\C,0.6347235689,-1.2082619932,1.8375975999\H,1.6964595519,-1.3492781292,1.6202300827\H,0.0808729667,-2.090032044,1.5075293787\H,0.5114793842,-1.1041987976,2.9183397617\Cl,-1.6286581658,0.2946810358,1.6287224467\H,0.6348119888,0.9393908429,1.5228471816\Version=IA32L-G03RevC.02\State=1-A\HF=-1957.4985601\RMSD=7.844e-09\RMSF=4.124e-05\Dipole=0.550751,-0.2173061,0.5540739\PG=C01 [X(C3H4Cl4)]\@

n.CHClCH3-CH2Cl

1\1\GINC-LC112\FOpt\RB3LYP\Gen\C3H6Cl2\CYL509\26-Jun-2008\0\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-CH2Cl.freq\0,1\C,-0.237863323,-0.0542512343,-0.5666284153\C,0.0960956999,-0.1663515841,0.9179351238\Cl,1.7963226176,-0.7662439016,1.1530394501\C,0.5480283378,1.0058826772,-1.3221718214\H,-0.5577012492,-0.8819733303,1.4157136758\H,0.0248295673,0.8031016808,1.4140655719\H,1.6148887685,0.7615585108,-1.2910049319\H,0.4015941654,1.993692119,-0.8734160382\H,0.2304604829,1.0481674733,-2.3672185279\Cl,-2.0324262045,0.3307086456,-0.6489797143\H,-0.1378750468,-1.0321262542,-1.0419645813\Version=IA32L-G03RevC.02\State=1-A\HF=-1038.3363529\RMSD=7.123e-09\RMSF=2.439e-05\Dipole=0.1169377,0.1453292,-0.1505168\PG=C01 [X(C3H6Cl2)]\@

n.CHClCH3-CH2F

1\1\GINC-LC150\FOpt\RB3LYP\Gen\C3H6Cl1F1\CYL509\26-Jun-2008\0\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-CH2F.freq\0,1\C,-0.5121429892,0.0312567708,-0.3136972931\C,0.5961237404,1.0276238385,-0.6081047225\F,1.7033398313,0.3887181294,-1.1343313815\C,-1.7986266732,0.710543819,0.1381398451\H,0.8913619445,1.5612121946,0.3028251912\H,0.2304545547,1.7537480125,-1.3477255059\H,-1.6332909587,1.3082983092,1.0404416545\H,-2.570331835,-0.0315949441,0.3563315164\H,-2.1708147036,1.3710480175,-0.6548682443\Cl,0.0524525098,-1.1467873875,0.965642437\H,-0.6812546185,-0.5823357369,-1.2019705836\Version=IA32L-G03RevC.02\State=1-A\HF=-677.96613\RMSD=7.108e-09\RMSF=1.904e-05\Dipole=-0.8377175,0.8215145,-0.3165907\PG=C01 [X(C3H6Cl1F1)]\@

n.CHClCH3-CH2OH

1\1\GINC-LC117\FOpt\RB3LYP\Gen\C3H7Cl1O1\CYL509\26-Jun-2008\0\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-CH2OH.freq\0,1\C,-0.506941776,0.0173521846,-0.3194422707\C,0.6246

819005,0.9846643903,-0.6342257856\O,1.7125891316,0.2620757966,-1.18057
06627\C,-1.8053021932,0.7248869974,0.0463510432\H,0.9024923521,1.52784
01429,0.2808117789\H,0.2346905034,1.7219781385,-1.358099239\H,2.504628
1451,0.8156473454,-1.1234052203\H,-1.6671860672,1.3780730335,0.9143958
101\H,-2.5883631758,0.0008208712,0.2847081789\H,-2.1462254539,1.336013
5099,-0.7985027716\C1,-0.0098515754,-1.0935673414,1.0507977614\H,-0.64
79001618,-0.6477560443,-1.1750031005\\Version=IA32L-G03RevC.02\State=1
-A\HF=-653.9440329\RMSD=7.568e-09\RMSF=3.881e-06\Dipole=-0.1204072,1.1
337382,-0.4086361\PG=C01 [X(C3H7C1101)]\@

n.CHClCH3-CH2Ph

1\1\GINC-LC113\FOpt\RB3LYP\Gen\C9H11Cl1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3
_2-CH2Ph.freq\0,1\C,-1.3627546287,-1.3424490975,-0.0322793563\C,0.151
162136,-1.3298667903,-0.2950855969\C,0.7696948417,0.0454234333,-0.4267
042641\C,0.6581659052,0.7591341894,-1.6279999338\C,1.4563958474,0.6372
272633,0.6402535825\C,1.2106768156,2.0331793124,-1.7589776395\C,2.0128
775497,1.9108165694,0.51319424\C,1.8908614441,2.6133076354,-0.68646756
91\H,2.3258046232,3.6041339861,-0.7869182452\H,1.1158361592,2.56950832
59,-2.6996140318\H,2.5426091817,2.3534627576,1.3526637499\H,0.13870781
55,0.3096018618,-2.4724983989\H,1.5507996078,0.0969735846,1.5785464848
\H,0.6477647454,-1.9025283003,0.4967112547\H,0.3035455982,-1.886846200
1,-1.2306842603\C,-1.9679137101,-2.7384846779,-0.1105312588\H,-1.49075
21307,-3.4126538461,0.6082636162\H,-1.8200166537,-3.1467344416,-1.1182
22296\H,-3.040869791,-2.7151851288,0.0981461662\C1,-1.7248381869,-0.63
14094652,1.6240295948\H,-1.8661771833,-0.6654987163,-0.7273103747\\Ver
sion=IA32L-G03RevC.02\State=1-A\HF=-809.7915585\RMSD=3.492e-09\RMSF=2.
642e-06\Dipole=0.2170693,-0.3678207,-0.7315216\PG=C01 [X(C9H11Cl1)]\@

n.CHClCH3-CH_CH2_2

1\1\GINC-LC3\FOpt\RB3LYP\Gen\C5H9Cl1\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-
CH_CH2_2.freq\0,1\C,-1.2407399211,1.2251482975,-1.0790530207\C,-1.312
9628164,1.3222463293,0.4277951779\C,0.0184329813,1.1464938593,-0.25756
45092\H,-1.6071679213,0.3114632326,-1.5366097583\H,-1.4063976531,2.123
5190846,-1.6674581842\H,-1.7257145103,0.470330609,0.9598423935\H,-1.53
09189828,2.2857782411,0.8800911174\H,0.6523666266,2.0337243959,-0.2867
045497\C,0.8786425217,-0.0969191745,-0.1208632579\C,1.7282150193,-0.08
63191102,1.145393783\H,1.0945807623,-0.0432647243,2.0362906361\H,2.361
8735462,-0.9754471758,1.2062424977\H,2.3754975342,0.799837807,1.140356
1372\C1,-0.1270426692,-1.6395312655,-0.1424880932\H,1.5160792659,-0.19
78111652,-1.0040017446\\Version=IA32L-G03RevC.02\State=1-A\HF=-656.122
9423\RMSD=5.712e-09\RMSF=4.560e-05\Dipole=0.4251232,0.7609732,0.054962
6\PG=C01 [X(C5H9Cl1)]\@

n.CHClCH3-CH2CH=CH2

1\1\GINC-LC32\FOpt\RB3LYP\Gen\C5H9Cl1\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl_CH3_2-
CH2CH=CH2.freq\0,1\C,0.3413973302,0.8571480098,-0.7441735006\C,0.363
5902146,0.5319413109,0.7586161761\H,1.3769269738,0.8443830121,-1.10949
51104\H,-0.0190019964,1.8908814285,-0.8421272452\C,-0.5079766243,-0.05
73627466,-1.5852035892\C,-1.0059415187,0.5297326506,1.4222457142\C,-1.
5486426317,0.3370244516,-2.3199406606\H,-0.2218208236,-1.1084097541,-1.
.5801603467\H,-2.1207440197,-0.3634477376,-2.9224553396\H,-1.865679287
4,1.3778210287,-2.3552763746\H,-0.9245148815,0.3099298812,2.490146191\H,
-1.6676007357,-0.20717423,0.9589774004\H,-1.464433517,1.5202005507,1.
.3064282713\C1,1.1778839833,-1.0995928782,1.0354360447\H,1.0282799503,
1.2379926924,1.2622849537\\Version=IA32L-G03RevC.02\State=1-A\HF=-656.
1328727\RMSD=8.760e-09\RMSF=7.460e-06\Dipole=-0.3921651,0.7561129,-0.1

499246\PG=C01 [X(C5H9C11)]\@

n.CHClCH3-CH2CH3

1\1\GINC-LC14\FOpt\RB3LYP\Gen\C4H9C11\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2
-CH2CH3.freq\0,1\C,0.7318202065,-0.1684705972,0.0569972943\C,0.778697
0868,-0.1543291896,1.5797143499\C,-0.1383245063,-1.2698725993,-0.55787
6136\C,-1.6088834799,-1.2829703548,-0.131353097\H,0.3343109823,-2.2250
677994,-0.2840947433\H,-0.0701569864,-1.1930373312,-1.6491063403\H,-0.
2076741964,0.0373562232,2.010910952\H,1.4655660172,0.6154559219,1.9418
605297\H,1.1310507219,-1.129104553,1.9411630731\Cl,0.1757537109,1.4869
64082,-0.5422330541\H,-2.1443178012,-2.085686918,-0.6496261942\H,-1.72
24279641,-1.4534962938,0.9447162408\H,-2.0991259622,-0.3363190966,-0.3
792873927\H,1.7451062609,-0.2546331017,-0.3434686728\Version=IA32L-G0
3RevC.02\State=1-A\HF=-618.0557526\RMSD=4.686e-09\RMSF=3.424e-05\Dipol
e=0.1957566,-0.8493336,0.312652\PG=C01 [X(C4H9C11)]\@

n.CHClCH3-CH_CH3_2

1\1\GINC-LC101\FOpt\RB3LYP\Gen\C5H11C11\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CH_CH3_2.freq\0,1\C,-0.0987338595,1.9993605013,0.4056754982\H,0.19
55139178,2.2702442597,1.4277632952\H,-1.1906650913,1.9912443925,0.3510
665014\H,0.2702241058,2.7724095578,-0.2739390033\C,0.4935062004,0.6404
689698,0.0512213517\Cl,0.017188911,0.2303010838,-1.6858639289\C,0.1273
731042,-0.5028143683,1.0167629311\C,0.9126310365,-1.7863458571,0.71218
64288\C,-1.3786959636,-0.7830094817,1.1157805428\H,-1.5663390716,-1.56
55956148,1.8593425187\H,-1.7761550377,-1.1284706025,0.1556982778\H,-1.
9462439077,0.1027837185,1.4194694742\H,1.9919768306,-1.5962872348,0.67
17989327\H,0.6101327694,-2.2135779923,-0.2494887889\H,0.7329542465,-2.
5385070141,1.4884705095\H,0.4665613866,-0.1324330911,1.9981795313\H,1.
5833452559,0.717112612,0.0015650262\Version=IA32L-G03RevC.02\State=1-
A\HF=-657.3693284\RMSD=3.016e-09\RMSF=2.091e-05\Dipole=0.1602536,0.155
1626,0.8811537\PG=C01 [X(C5H11C11)]\@

n.CHClCH3-C_CH3_3

1\1\GINC-LC142\FOpt\RB3LYP\Gen\C6H13C11\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-C_CH3_3.freq\0,1\C,-0.0584113933,-0.3888681948,2.1820790492\C,0.29
93894299,0.2291473801,0.8094548579\C,-0.2636226052,1.6599382454,0.7326
391145\C,-0.287737504,-0.6964122192,-0.2924576271\H,0.4493690767,0.165
6658539,2.9791901002\H,0.2646359159,-1.4353129796,2.2505228377\H,-1.13
27029683,-0.3489341873,2.3884628747\C,1.8362741822,0.2722546552,0.6909
707808\C,-1.7994546704,-0.9037853317,-0.2826949536\H,2.2608171893,0.85
87700668,1.5138705097\H,2.1552324602,0.7272100767,-0.250520769\H,2.266
6600252,-0.7357937977,0.7424421323\H,0.1795667833,2.2778076315,1.52218
74096\H,-1.3502239248,1.6805689436,0.8716020213\H,-0.033848256,2.12648
5426,-0.2301163417\H,-2.3371341232,0.0391494617,-0.4157555379\H,-2.115
9772032,-1.3555959689,0.6634747164\H,-2.0924477295,-1.577611044,-1.092
1914126\Cl,0.171380251,-0.1052871435,-1.9858420735\H,0.2139638535,-1.6
661752526,-0.2238006214\Version=IA32L-G03RevC.02\State=1-A\HF=-696.68
05371\RMSD=4.891e-09\RMSF=1.539e-05\Dipole=-0.2222464,-0.1962022,0.864
8582\PG=C01 [X(C6H13C11)]\@

n.CHClCH3-CCH

1\1\GINC-LC150\FOpt\RB3LYP\Gen\C4H5C11\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2-
CCH.freq\0,1\C,0.5619265838,-0.1186955553,0.0668228686\C,0.80864163
44,-0.0332780357,1.5737129295\C,-0.274707519,-1.2453758161,-0.31326468
73\C,-0.9516304177,-2.199195744,-0.611353156\H,-1.5557687823,-3.037615

0093,-0.8753789163\H,-0.1365619656,0.0673288485,2.1130718191\H,1.30783
11423,-0.9492996989,1.9088783337\H,1.4454606917,0.8244924592,1.8050432
676\C1,-0.2022545089,1.4607965242,-0.516140182\H,1.5119838753,-0.15917
66046,-0.4727391396\Version=IA32L-G03RevC.02\State=1-A\HF=-615.558908
4\RMSD=4.775e-09\RMSF=1.176e-04\Dipole=0.3667161,-0.6920818,0.3709468\
PG=C01 [X(C4H5C11)]\@

n.CHC1CH3-CH=C_CH3_2

1\1\GINC-LC139\FOpt\RB3LYP\Gen\C6H11C11\CYL509\26-Jun-2008\0\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CH=C_CH3_2.freq\0,1\H,3.4121464325,-0.0803518036,-0.6855031296\C,2
.7246306104,-0.9267779476,-0.5508044341\C,1.3854080666,-0.4545267081,-
0.0377467776\C,1.4384565961,0.2465914481,1.2967461361\C,0.2758482184,-
0.6567729923,-0.7670745466\C,-1.1557620589,-0.3174994574,-0.4432896631
\C,-1.7379982771,-1.0081905664,0.7884397768\H,0.3975781182,-1.14858873
53,-1.731793786\H,2.6391542615,-1.4520982176,-1.5068414678\H,3.2032331
637,-1.6038952012,0.170277476\H,2.2103902228,1.02735574,1.2802947107\H
,1.7265643297,-0.4573835812,2.0902991318\H,0.4962737837,0.7194470422,1
.5746345695\H,-1.6580279536,-2.0940112189,0.6557853297\H,-2.7930916898
, -0.7490978588,0.9168172719\H,-1.199274905,-0.7381083066,1.6995703676\
C1,-1.4263320651,1.5202977057,-0.2865464591\H,-1.7707995898,-0.5652715
136,-1.3098736183\Version=IA32L-G03RevC.02\State=1-A\HF=-695.4506281\
RMSD=9.476e-09\RMSF=2.766e-05\Dipole=0.4263179,-0.8853888,0.1180556\PG
=C01 [X(C6H11C11)]\@

n.CHC1CH3-CH=CH2

1\1\GINC-LC94\FOpt\RB3LYP\Gen\C4H7C11\CYL509\26-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2
-CH=CH2.freq\0,1\H,2.0757333033,0.7605289436,-0.4534988413\C,2.109869
1148,-0.0298854564,0.2892697289\H,3.0734088687,-0.2459091814,0.7416058
024\C,1.0251129323,-0.7168273257,0.6387344905\C,-0.3859595424,-0.55688
23702,0.1382286535\H,1.1085925964,-1.505878852,1.3887385824\C,-1.36639
5085,-0.2252896904,1.2650806294\H,-1.1068589716,0.7289579909,1.7324335
648\H,-1.3213827343,-1.0093496518,2.0310423263\H,-2.3910343452,-0.1687
288814,0.8877517314\C1,-0.5314687151,0.7115596592,-1.1741094559\H,-0.6
99255079,-1.4828255179,-0.35609343\Version=IA32L-G03RevC.02\State=1-A
\HF=-616.8164446\RMSD=3.016e-09\RMSF=2.647e-05\Dipole=0.038103,-0.5534
428,0.6497878\PG=C01 [X(C4H7C11)]\@

n.CHC1CH3-CH=CHCH3

1\1\GINC-LC107\FOpt\RB3LYP\Gen\C5H9C11\CYL509\26-Jun-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH=CHCH3.freq\0,1\H,1.5687253105,-0.2021272164,-0.8625914571\C,1.57
2808199,-0.1937831857,0.2256805469\C,2.9187910977,-0.2032236944,0.8914
274762\C,0.4088236188,-0.1791155789,0.875511447\C,-0.9859879791,-0.156
1065548,0.3090126339\H,0.4100110307,-0.1740132957,1.9682543747\C,-1.77
64126154,1.0746606512,0.7572553099\H,-1.297319342,1.9904833098,0.39917
83377\H,-1.8088366703,1.1077376541,1.8533847927\H,-2.8029212675,1.0403
052092,0.3817372331\C1,-1.013161223,-0.243395962,-1.5226402191\H,2.834
619655,-0.1958360725,1.9834123968\H,3.4962441488,-1.0907804604,0.60006
35813\H,3.5137009355,0.6692422601,0.5897001944\H,-1.5186169365,-1.0618
698575,0.6184197881\Version=IA32L-G03RevC.02\State=1-A\HF=-656.136168
7\RMSD=5.659e-09\RMSF=5.827e-06\Dipole=0.1658833,0.0915811,0.8245262\PG
G=C01 [X(C5H9C11)]\@

n.CHC1CH3-CHO

1\1\GINC-LC81\FOpt\RB3LYP\Gen\C3H5C11O1\CYL509\26-Jun-2008\0\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CHO.freq\0,1\O,0.5126599186,1.7206938147,-1.4933866366\C,0.6993707

478,0.8895845093,-0.6371607824\H,1.7157474466,0.6321764953,-0.27077793
\C,-0.4375897739,0.1477906808,0.05326238\C,-0.6856416959,0.6955076186,
1.4562647922\H,0.2195503346,0.6373748886,2.0691624999\H,-1.4776891413,
0.1286450855,1.9529896354\H,-0.996396674,1.7443337856,1.3845109174\C1,
0.0182959601,-1.6188293582,0.1263151401\H,-1.330358305,0.2147214653,-0
.5703477497\\Version=IA32L-G03RevC.02\State=1-A\HF=-652.7377152\RMSD=4
.292e-09\RMSF=1.298e-05\Dipole=-0.2280726,0.1457925,0.773602\PG=C01 [X
(C3H5C1101)]\@

n.CHClCH3-CN

1\1\GINC-LC77\FOpt\RB3LYP\Gen\C3H4Cl1N1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CN.freq\0,1\N,-0.6211939216,-0.0963590417,-2.3648366713\C,-0.52917
81826,0.0618745296,-1.218881924\C,-0.452075825,0.2532250778,0.23066337
74\C,-1.1663336416,-0.8578422905,1.00124296\H,-1.0969434828,-0.6650325
523,2.074534375\H,-2.2221622165,-0.8813801043,0.7104535835\H,-0.718334
8478,-1.8301395219,0.7826870107\C1,1.3027439143,0.3574699353,0.7312808
928\H,-0.8753226497,1.2305326694,0.4762600708\\Version=IA32L-G03RevC.0
2\State=1-A\HF=-631.6551463\RMSD=5.570e-09\RMSF=7.126e-05\Dipole=-0.65
3559,0.0258532,1.2166246\PG=C01 [X(C3H4Cl1N1)]\@

n.CHClCH3-COCH3

1\1\GINC-LC57\FOpt\RB3LYP\Gen\C4H7Cl1O1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-COCH3.freq\0,1\C,-0.9718251793,-0.3380338569,-1.837490918\C,-0.942
7049245,-0.4354996057,-0.325961398\C,0.4286955049,-0.4198944649,0.3769
906534\O,-1.9531104925,-0.5567121497,0.3362461698\H,-1.938170642,-0.69
5390745,-2.1989537696\H,-0.1570730093,-0.9078464605,-2.2970453093\H,-0
.8419432537,0.7064946228,-2.1423167329\C,0.3313076152,-0.4194669508,1.
8915959642\H,1.3283134719,-0.4216943376,2.3392708175\H,-0.2093168877,-
1.3134695716,2.2178713095\H,-0.2201958757,0.4548649731,2.2455948772\C1
,1.3873826641,1.0345767073,-0.2060482311\H,1.0049267499,-1.2796960383,
0.0176235674\\Version=IA32L-G03RevC.02\State=1-A\HF=-692.0634373\RMSD=
2.557e-09\RMSF=5.167e-06\Dipole=0.3494507,-0.504828,-0.3082377\PG=C01
[X(C4H7Cl1O1)]\@

n.CHClCH3-CON_CH2CH3_2

1\1\GINC-LC126\FOpt\RB3LYP\Gen\C7H14Cl1N1O1\CYL509\27-Jun-2008\0\#B3L
YP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1
_CH3_2-CON_CH2CH3_2.freq\0,1\H,2.3281079515,-0.9532158943,2.499069940
5\C,1.9013037418,-1.1754050105,1.5142690223\C,1.3439461234,0.108346480
8,0.8915345781\N,0.7816197982,-0.082491162,-0.4500637094\C,1.748152604
2,-0.2361261082,-1.5504569341\C,2.1014546831,1.0930064054,-2.223147924
\C,-0.5325212592,-0.0090511581,-0.8098504712\O,-0.8869211354,-0.072394
0321,-1.987209002\C,-1.6662617169,0.2395804037,0.2063676577\C,-1.78458
23734,1.6997032846,0.6389658844\H,2.1388290401,0.8625223448,0.81315967
42\H,0.5804266574,0.5247215558,1.5460424123\H,1.3156695677,-0.92078396
9,-2.2826711006\H,2.6449216886,-0.7068933143,-1.1364626784\H,1.1082719
042,-1.9171457554,1.6402595438\H,2.6938293062,-1.6160495604,0.90013711
51\H,1.2102114391,1.531792343,-2.6795800458\H,2.8474506657,0.931725892
, -3.0098429405\H,2.5191596813,1.8089757342,-1.5054824344\H,-0.93122584
49,2.0309644472,1.2367767678\H,-2.6955226608,1.8484174352,1.2253509826
\H,-1.8424538817,2.3245172462,-0.2598559001\C1,-1.6707065724,-0.874125
6089,1.6703231408\H,-2.5605841061,-0.0531485501,-0.3403676276\\Version
=IA32L-G03RevC.02\State=1-A\HF=-865.3649922\RMSD=3.898e-09\RMSF=5.737e
-06\Dipole=0.8704264,0.6434567,0.5170685\PG=C01 [X(C7H14Cl1N1O1)]\@

n.CHClCH3-CON_CH3_2

1\1\GINC-LC112\FOpt\RB3LYP\Gen\C5H10Cl1N1O1\CYL509\26-Jun-2008\0\#B3L

```
YP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_
_CH3_2-CON_CH3_2.freq\0,1\C,1.2104758095,0.2558482849,-0.0808313607\C
,-0.1754274725,0.8525603147,0.2402974838\N,-1.2757299665,0.0579824657,
0.4079330708\O,-0.2143806479,2.0722476198,0.3847848155\C,1.8661871697,
-0.4830979088,1.0829148879\C,-1.3265929359,-1.3958487603,0.3691559078\
C,-2.5419265906,0.6994485378,0.7441473951\H,-2.1050415821,-1.720117867
5,-0.332954185\H,-0.3848198296,-1.8235224752,0.0387361738\H,-1.5769277
985,-1.7955222436,1.3619399855\H,-3.3153180947,0.3975961088,0.02702901
17\H,-2.8679206704,0.402764105,1.7501282615\H,-2.4070166239,1.77893336
36,0.7116951299\H,2.898892213,-0.7410661216,0.832171215\H,1.3374378052
,-1.4001636862,1.3539941802\H,1.8771811069,0.1809764936,1.9554273146\C
1,1.2463659043,-0.7627567307,-1.6131938526\H,1.8041721686,1.1296657176
,-0.341787496\Version=IA32L-G03RevC.02\State=1-A\HF=-786.7336508\RMSD
=3.385e-09\RMSF=1.116e-05\Dipole=-0.3935793,-0.9663367,0.7252676\PG=C0
1 [X(C5H10Cl1N1O1)]\@
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n.CHClCH3-CONH2

```
1\1\GINC-LC84\FOpt\RB3LYP\Gen\C3H6Cl1N1O1\CYL509\26-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-CONH2.freq\0,1\C,0.5729067799,-0.2120505809,-0.2813584002\C,-0.8
346616978,0.2040768951,-0.7447897341\N,-1.8379237021,0.2144484705,0.16
43963784\O,-0.9694788507,0.5260719294,-1.9172169529\C,1.5682850459,0.9
295574809,-0.4650525477\H,-1.7072656617,-0.1063651721,1.1117956464\H,-
2.7618331984,0.4678927063,-0.1554194907\H,2.5848533631,0.5943861123,-0
.2443995929\H,1.3238393527,1.7702775458,0.1913182645\H,1.5150503573,1.
266002005,-1.5043790566\Cl,0.6451607569,-0.8329839619,1.4486234028\H,0
.8597388718,-1.0706833453,-0.891348552\Version=IA32L-G03RevC.02\State
=1-A\HF=-708.1230417\RMSD=3.668e-09\RMSF=8.952e-06\Dipole=-0.2442992,0
.0209417,0.5773673\PG=C01 [X(C3H6Cl1N1O1)]\@
```

n.CHClCH3-CONHCH3

```
1\1\GINC-LC133\FOpt\RB3LYP\Gen\C4H8Cl1N1O1\CYL509\26-Jun-2008\0\#B3LYP
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_
CH3_2-CONHCH3.freq\0,1\H,-2.6880173055,1.1183536084,-1.9224320825\C,-
2.5014405066,0.2334090211,-1.303163471\N,-1.2820122373,0.3877821061,-0
.5293939314\C,-0.2234750282,-0.4419240775,-0.6756564626\C,1.026698369,
-0.1993577474,0.1892483965\O,-0.1857242415,-1.3963698806,-1.4458263277
\C,1.3128088464,-1.3988243518,1.0874979694\H,-1.200699029,1.1568345347
,0.120766453\H,-2.3749306854,-0.6364575037,-1.9489995523\H,-3.36394762
36,0.0728478456,-0.6462598074\H,2.2633385774,-1.2712893123,1.611685567
1\H,1.3621633425,-2.2925501629,0.4591176861\H,0.517359558,-1.531051270
5,1.8273295453\Cl,0.9648022434,1.3360478598,1.2049962505\H,1.855424536
5,-0.0328341204,-0.5013345199\Version=IA32L-G03RevC.02\State=1-A\HF=-
747.4346902\RMSD=6.346e-09\RMSF=2.218e-05\Dipole=-0.4514605,0.3903596,
0.276185\PG=C01 [X(C4H8Cl1N1O1)]\@
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n.CHClCH3-COOC_CH3_3

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1\1\GINC-LC150\FOpt\RB3LYP\Gen\C7H13Cl1O2\CYL509\27-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-COOC_CH3_3.freq\0,1\H,-1.8449439955,-1.5955038188,-2.8608005598\
C,-1.6840263558,-1.2507399354,-1.8332452729\C,-0.2351902962,-0.7798488
451,-1.6758199341\C,0.0826449932,0.4412865821,-2.5434708393\O,0.035899
0766,-0.4646596312,-0.2539361822\C,-0.60365318,0.5188864117,0.38723998
75\O,-1.4917717636,1.2177241124,-0.0537498624\C,-0.1023328938,0.658215
533,1.8277022983\C,0.7464344233,-1.9198416413,-1.9535134209\C,-0.18779
46706,-0.6336522306,2.6298315196\H,0.6495772891,-2.2526733356,-2.99220
66429\H,0.5461566971,-2.7725711291,-1.2966743382\H,1.777120087,-1.5910
359058,-1.7878806236\H,-2.388118279,-0.4445654688,-1.6209567603\H,-1.8
888133173,-2.0896794721,-1.1590662728\H,0.0038879707,0.1655698176,-3.6
```

01003451\H,1.1051706471,0.7856932776,-2.3562146837\H,-0.6092952653,1.2
614233285,-2.3447706353\H,0.1457301256,-0.4666572021,3.6575918038\H,0.
4281423753,-1.4124650782,2.1750211184\H,-1.2291559031,-0.9780678991,2.
6548878468\Cl,1.6201634091,1.2766673919,1.8046267761\H,-0.6877470108,1
.4568361283,2.2825603329\\Version=IA32L-G03RevC.02\State=1-A\HF=-885.2
443448\RMSD=3.398e-09\RMSF=8.596e-07\Dipole=-0.2147846,-0.9441916,-0.2
430706\PG=C01 [X(C7H13Cl102)]\\@

n.CHClCH3-COOCH2CH3

1\1\GINC-LC27\FOpt\RB3LYP\Gen\C5H9Cl102\CYL509\26-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CCl_CH3
_2-COOCH2CH3.freq\\0,1\C,-1.463572167,0.0044500931,-0.2588024372\C,-0.
1334923222,-0.7277333299,-0.4241590704\O,-0.0527568839,-1.8928186028,-
0.7454022362\O,0.9151153833,0.0796902692,-0.2037168061\C,2.2238895736,
-0.5328489703,-0.3196257263\C,3.2544067203,0.5342906669,-0.0062624713\
C,-1.5789915142,1.2557802998,-1.1199345449\H,2.2749286228,-1.375240214
6,0.3770782216\H,2.3338717942,-0.9314578703,-1.3331577478\H,3.18082741
44,1.3695255758,-0.7100781314\H,4.2609874585,0.1087465573,-0.080791454
4\H,3.1177657823,0.923252505,1.0075280538\H,-0.8036808708,1.9791055035
, -0.8579166286\H,-2.5605480213,1.7186985756,-0.9876497152\H,-1.4635381
479,0.9829870502,-2.1762321405\Cl,-1.6944965734,0.4261186679,1.5067028
169\H,-2.2464820231,-0.718240927,-0.4870705055\\Version=IA32L-G03RevC.
02\State=1-A\HF=-806.6122284\RMSD=8.807e-09\RMSF=9.269e-06\Dipole=0.55
23989,0.5660461,-0.5872117\PG=C01 [X(C5H9Cl102)]\\@

n.CHClCH3-COOCH3

1\1\GINC-LC124\FOpt\RB3LYP\Gen\C4H7Cl102\CYL509\26-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CCl_CH
3_2-COOCH3.freq\\0,1\C,0.2670481952,-0.2231565527,-1.015206303\C,0.379
0585508,-0.5551699674,0.470509568\O,1.3294272074,-1.1258330568,0.95713
71643\O,-0.7094751217,-0.1674386816,1.1554680344\C,-0.6746184115,-0.43
03597868,2.5697249789\H,-1.6186075171,-0.0496297662,2.9592823474\C,-0.
9941277528,-0.7737239913,-1.6687370284\H,-0.5827813903,-1.5033653369,2
.7567653549\H,0.1701811894,0.0871955547,3.0310893235\H,-1.017030053,-1
.8646224818,-1.5553418405\H,-1.0024170715,-0.5367509345,-2.7359753045\
H,-1.8878129947,-0.3538992133,-1.2018715271\Cl,0.3496982576,1.59239280
86,-1.2237981547\H,1.1698172823,-0.6089698723,-1.4879686073\\Version=I
A32L-G03RevC.02\State=1-A\HF=-767.2929727\RMSD=9.886e-09\RMSF=6.835e-0
6\Dipole=-0.7658866,-0.4858429,0.1845002\PG=C01 [X(C4H7Cl102)]\\@

n.CHClCH3-COOH

1\1\GINC-LC118\FOpt\RB3LYP\Gen\C3H5Cl102\CYL509\26-Jun-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CCl_CH
3_2-COOH.freq\\0,1\C,-0.2434149775,0.0094922902,-0.653685019\C,-0.4969
709438,0.5833668577,0.7374394115\O,0.0710413805,1.542994202,1.20368889
62\O,-1.4525213952,-0.1120007038,1.3901501218\C,0.4073395393,1.0166539
156,-1.583791249\H,-1.5328331871,0.2915723118,2.2751654536\H,1.3352000
469,1.3954176368,-1.1500510987\H,-0.2713210843,1.8643725309,-1.7337114
391\H,0.6176365085,0.5594200233,-2.5537420207\Cl,0.8282822575,-1.46080
47152,-0.4430840072\H,-1.1793622525,-0.3821287107,-1.0557237776\\Versi
on=IA32L-G03RevC.02\State=1-A\HF=-727.9861408\RMSD=9.633e-09\RMSF=5.53
4e-05\Dipole=-0.7123123,0.2193289,-0.1755769\PG=C01 [X(C3H5Cl102)]\\@

n.CHClCH3-COPh

1\1\GINC-LC14\FOpt\RB3LYP\Gen\C9H9Cl101\CYL509\26-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CCl_CH3
_2-COPh.freq\\0,1\C,-3.0774132621,-0.4897119816,-0.4888341348\C,-3.213
8347333,-0.1668786183,0.8645283797\C,-2.0836775752,0.1392283541,1.6240
344592\C,-0.8180145851,0.122682157,1.0389483177\C,-0.6696224623,-0.204

```
7356555,-0.3192166322\C,-1.8165587047,-0.5081341586,-1.0746044571\C,0.
642337303,-0.2758754811,-1.0342246907\O,0.6927418811,-0.5464023881,-2.
2247305253\C,1.9989132795,-0.1076609693,-0.3210475461\C,2.322764361,-1
.2256925329,0.6668484526\H,-1.6894138831,-0.75828585,-2.1223660898\H,0
.0436720552,0.3873935128,1.6390467887\H,-2.1860302189,0.3974363319,2.6
743129809\H,-3.9548267479,-0.7268904924,-1.0841167022\H,-4.1984745857,
-0.1514928689,1.3242915774\H,3.3362653571,-1.1004363029,1.0581788424\H
,2.271463187,-2.1874060404,0.1420571371\H,1.6240189394,-1.2546172416,1
.505861556\C1,2.1627991019,1.5387173079,0.4733477164\H,2.7344443901,-0
.0920028613,-1.1249259571\\Version=IA32L-G03RevC.02\State=1-A\HF=-883.
7991525\RMSD=3.821e-09\RMSF=7.028e-06\Dipole=-0.5190777,-0.5828788,0.8
238685\PG=C01 [X(C9H9C1101)]\@
```

n.CC1_CH3_2-H

```
1\1\GINC-LC118\FOpt\RB3LYP\Gen\C3H7C11\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3_
2-H.freq\0,1\C,-0.2642908079,0.5163481481,0.0279960961\H,-0.583159544
9,1.1495423045,0.8598312719\C,0.7985234443,1.2266162271,-0.7995910308\
C,-1.4702482424,0.0645474145,-0.7847143771\H,1.649513375,1.5267061833,
-0.1820153603\H,0.3646815059,2.1273299675,-1.2521186453\H,1.1638239645
,0.579185418,-1.603382626\H,-1.1666652206,-0.6144950944,-1.5881013746\
H,-1.9523676175,0.9405334471,-1.2369252377\H,-2.2045750756,-0.44736487
6,-0.1567434837\C1,0.4908730735,-0.9474416522,0.8527830192\\Version=IA
32L-G03RevC.02\State=1-A\HF=-578.7436049\RMSD=6.291e-09\RMSF=2.321e-05
\Dipole=-0.3718307,0.7200024,-0.4642665\PG=C01 [X(C3H7C11)]\@
```

n.CC1_CH3_2-BH2

```
1\1\GINC-LC146\FOpt\RB3LYP\Gen\C3H8B1C11\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
3_2-BH2.freq\0,1\H,-1.732662069,1.0062342152,-1.2669009747\B,-1.34615
15582,-0.0133006919,-0.7809098445\C,-0.3533487938,0.0437549835,0.43120
17933\H,-1.801544827,-1.0654175487,-1.1135531076\C,-0.1385483634,-1.17
42632547,1.3028909216\C,-0.05465301,1.3600173328,1.1150601856\H,-0.900
058139,-1.1526214771,2.0950246064\H,0.8446569552,-1.1737490732,1.78690
61991\H,-0.2649930557,-2.1030288205,0.7421125341\H,-0.8131930554,1.506
2638305,1.8967435261\H,-0.120625927,2.2021049626,0.4225100804\H,0.9280
064197,1.3653827894,1.6001352879\C1,0.8159101466,-0.1115129287,-1.1384
321372\\Version=IA32L-G03RevC.02\State=1-A\HF=-604.1769697\RMSD=3.263e
-09\RMSF=2.319e-05\Dipole=0.0132455,0.0712199,0.9659024\PG=C01 [X(C3H8
B1C11)]\@
```

n.CC1_CH3_2-CH3

```
1\1\GINC-LC92\FOpt\RB3LYP\Gen\C4H9C11\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3_2
-CH3.freq\0,1\H,1.0680639153,-0.9591603655,-1.6962265327\C,1.02661294
49,-1.1673222102,-0.6231200909\H,2.0538268899,-1.283703071,-0.25420926
71\H,0.4980563476,-2.1132228796,-0.4731165244\C,0.3441127079,-0.028105
1412,0.1337352882\C,1.0327548522,1.3131940666,-0.1175219116\C,0.220508
6227,-0.3321042113,1.6266479186\H,2.0601943015,1.2709351358,0.26638061
63\H,0.5086627661,2.1274423588,0.3913267615\H,1.0741539524,1.541457206
3,-1.1865312636\H,1.2237609765,-0.4235141721,2.0624543776\H,-0.3146028
479,-1.2711607617,1.7952703278\H,-0.3101248967,0.468659838,2.149914422
9\C1,-1.3885838924,0.1134289228,-0.5396300085\\Version=IA32L-G03RevC.0
2\State=1-A\HF=-618.0595982\RMSD=3.263e-09\RMSF=3.743e-05\Dipole=0.893
3862,-0.0729853,0.3471937\PG=C01 [X(C4H9C11)]\@
```

n.CC1_CH3_2-NH2

```
1\1\GINC-LC101\FOpt\RB3LYP\Gen\C3H8C11N1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
```

```
3_2-NH2.freq\0,1\H,-1.5733884806,1.1592259833,-0.8903445623\N,-0.5634
983128,1.270095057,-0.8703344172\C,0.0555373471,0.4284889325,0.0739108
688\H,-0.198120604,1.1395421218,-1.8094970425\C,-0.5497200129,0.612568
9685,1.4593276744\C,1.5704542224,0.5821942199,0.0422948668\H,-0.104096
0094,-0.0831176557,2.1730893666\H,-1.6303781786,0.4411763635,1.4410874
891\H,-0.3636493784,1.6401318892,1.7930885083\H,1.8280174447,1.6087418
256,0.3282405555\H,1.963309262,0.3896485736,-0.960760562\H,2.045732400
4,-0.11389256,0.736263447\C1,-0.2635628004,-1.4595079215,-0.3630603964
\\Version=IA32L-G03RevC.02\State=1-A\HF=-634.0982757\RMSD=5.717e-09\RM
SF=3.296e-05\Dipole=0.0251664,0.9263142,0.0177847\PG=C01 [X(C3H8C11N1)
]\@
```

n.CC1_CH3_2-OH

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C3H7C11O1\CYL509\20-Aug-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CC1_CH3
_2-OH.freq\0,1\C,0.1564528167,-0.3549381386,0.0992646064\O,0.18010541
79,-0.5654413144,1.4682588615\C,1.5521247509,-0.3028044652,-0.51220972
5\C,-0.7529907293,-1.4077187301,-0.5109182384\H,0.785389891,0.07963662
02,1.8703090546\H,-0.865763367,-1.2488333191,-1.5853819646\H,-1.735841
0574,-1.37321253,-0.0358656279\H,-0.3130418892,-2.3965478735,-0.337427
6378\H,2.1499422777,0.4909457461,-0.0518222982\H,1.507344391,-0.114989
1342,-1.5875654822\H,2.0485595441,-1.2645575744,-0.3369242788\C1,-0.63
24090684,1.3378739167,-0.2434242656\\Version=IA64L-G03RevC.02\State=1-
A\HF=-653.9598664\RMSD=3.608e-09\RMSF=1.134e-05\Dipole=0.804194,-0.545
9475,-0.0418084\PG=C01 [X(C3H7C11O1)]\@
```

n.CC1_CH3_2-F

```
1\1\GINC-LC147\FOpt\RB3LYP\Gen\C3H6C11F1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-F.freq\0,1\C,0.1273984793,0.30775402,-1.6319906196\C,0.2791974782
,0.1967617915,-0.1263514897\C,1.5630248367,-0.4549267393,0.3526065301\
F,0.2059529274,1.4619558633,0.4128465877\H,0.9591651419,0.9016193533,-
2.0273808058\H,-0.8119241336,0.8081949609,-1.8784181844\H,0.1405915335
,-0.6797559759,-2.0994224393\H,2.413775349,0.1288534033,-0.0165404907\
H,1.6440882419,-1.478493017,-0.0210020277\H,1.5919006607,-0.4688441885
,1.4446079663\C1,-1.1534645825,-0.7451006906,0.5480558924\\Version=IA3
2L-G03RevC.02\State=1-A\HF=-677.9784235\RMSD=8.456e-09\RMSF=2.986e-05\
Dipole=-0.4637438,-0.8635674,0.0035956\PG=C01 [X(C3H6C11F1)]\@
```

n.CC1_CH3_2-SiH3

```
1\1\GINC-LC144\FOpt\RB3LYP\Gen\C3H9C11Si1\CYL509\26-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-SiH3.freq\0,1\H,-1.3791484382,-0.0314761315,-2.378950835\Si,-1.4
418874463,0.0002156677,-0.8890566692\C,0.3463098328,-0.0086906362,-0.2
032652268\H,-2.1432258104,1.2368277621,-0.4624597856\H,-2.1747214412,-
1.1991229313,-0.4119705517\C,1.10066605,-1.2918528902,-0.5571056837\C,
1.1333859578,1.2387866081,-0.6095575327\H,2.1292793532,1.235954995,-0.
1510407606\H,0.6224676749,2.1588963116,-0.3112807495\H,1.2615968152,1.
2535737608,-1.699649673\H,2.0965454763,-1.295766325,-0.0985665227\H,1.
2278679747,-1.3550969609,-1.6455804947\H,0.5662993548,-2.1853038807,-0.
2212397023\C1,0.1468995439,0.0322962124,1.6498295943\\Version=IA32L-G
03RevC.02\State=1-A\HF=-869.4294752\RMSD=2.595e-09\RMSF=1.473e-05\Dipo
le=0.3006837,-0.0202137,-0.7876825\PG=C01 [X(C3H9C11Si1)]\@
```

n.CC1_CH3_2-PH2

```
1\1\GINC-LC118\FOpt\RB3LYP\Gen\C3H8C11P1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-PH2.freq\0,1\H,-2.2298859135,-0.1392323202,-0.2270880963\P,-1.407
5524731,1.0070817179,-0.0526546472\H,-1.490799117,0.9770547562,1.36609
```

95824\C,0.261318622,0.1274428683,-0.2105212679\C,1.3770318047,1.056693
6133,0.2753169724\C,0.4772953923,-0.3022321085,-1.6641701646\H,1.44890
99761,-0.7950041684,-1.7744207906\H,0.4601865563,0.5785656501,-2.31719
68626\H,-0.29851742,-0.9972802652,-1.998171114\H,2.3512464926,0.567848
634,0.1706712318\H,1.243399843,1.331569689,1.3256120452\H,1.3837535531
,1.9734840538,-0.3263402203\C1,0.3265363629,-1.4055681236,0.8333470942
\\Version=IA32L-G03RevC.02\State=1-A\HF=-920.6793884\RMSD=4.749e-09\RM
SF=9.009e-06\Dipole=0.1790404,0.3919364,-0.3576728\PG=C01 [X(C3H8C11P1
)]\@

n.CC1_CH3_2-SH

1\1\GINC-LC47\FOpt\RB3LYP\Gen\C3H7C11S1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-SH.freq\0,1\C,0.1432729301,-0.2737833801,-0.1977972203\S,0.1163734
994,-0.073940743,1.653213863\C,1.5676928433,-0.2626281664,-0.744715422
6\C,-0.6521048766,-1.4972064124,-0.6436872755\H,0.771075057,-1.2306526
648,1.908395374\H,-0.6788315573,-1.5517312854,-1.7375544293\H,-1.67487
16302,-1.461311387,-0.2634978989\H,-0.1698920438,-2.4065000513,-0.2653
111708\H,2.1006707053,0.6385485718,-0.4353606972\H,1.5520477002,-0.311
0198022,-1.8390846269\H,2.1120421753,-1.1373516996,-0.3691408043\C1,-0
.7192577517,1.2261634094,-0.8195687085\\Version=IA32L-G03RevC.02\State
=1-A\HF=-976.9205237\RMSD=3.909e-09\RMSF=4.740e-05\Dipole=0.5514061,-1
.0134858,-0.2680765\PG=C01 [X(C3H7C11S1)]\@

n.CC1_CH3_2-C1

1\1\GINC-LC15\FOpt\RB3LYP\Gen\C3H6C12\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-C1.freq\0,1\C1,0.4557796979,0.725081096,-1.4080118623\C,0.151586239
3,0.1202672911,0.2906807779\C,1.4510774239,-0.4472575371,0.844523906\C
, -0.4261269669,1.2611275857,1.1166282596\H,2.2066542246,0.3438361428,0
.8849618443\H,1.8218222609,-1.2598126821,0.2165911233\H,1.2807355075,-
0.8292765899,1.8561509734\H,0.2972575284,2.0815184659,1.1617325305\H,-
0.6296549454,0.9093100996,2.1330656992\H,-1.3545627857,1.6309161299,0.
677014179\C1,-1.0841015785,-1.2239820138,0.2056286852\\Version=IA32L-G
03RevC.02\State=1-A\HF=-1038.334459\RMSD=5.697e-09\RMSF=7.090e-05\Dipo
le=0.4305726,0.3421934,0.8220189\PG=C01 [X(C3H6C12)]\@

n.CC1_CH3_2-Br

1\1\GINC-LC147\FOpt\RB3LYP\Gen\C3H6Br1C11\CYL509\26-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C
H3_2-Br.freq\0,1\Br,0.2678664751,-0.6096554932,-1.1751273218\C,-0.051
9055615,0.020359213,0.7054506789\C,1.2645021557,-0.0588149097,1.463913
2516\C,-1.164956118,-0.8242822116,1.3072501605\H,2.0313355803,0.559545
3187,0.9935791653\H,1.6125401692,-1.0960177079,1.4916416171\H,1.109602
7389,0.2909053756,2.4908681328\H,-0.8586550667,-1.8746353818,1.3322871
27\H,-2.0861928524,-0.7377946744,0.7280612353\H,-1.358847499,-0.486847
4116,2.3316906533\C1,-0.594761915,1.7564243643,0.6412731638\\Version=I
A32L-G03RevC.02\State=1-A'\HF=-3152.019208\RMSD=3.787e-09\RMSF=2.031e-
05\Dipole=0.1009758,-0.4938174,0.846942\PG=CS [SG(C1Br1C11),X(C2H6)]\@
@

n.CC1_CH3_2-N_CH3_2

1\1\GINC-LC133\FOpt\RB3LYP\Gen\C5H12C11N1\CYL509\26-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C
H3_2-N_CH3_2.freq\0,1\C,1.6589966018,0.1000102269,1.2759041796\H,2.72
8566138,0.3083552051,1.1919230444\H,1.5437257293,-0.7905190449,1.89534
1156\H,1.1689032046,0.9489093899,1.7754774544\N,1.1200401005,-0.124094
637,-0.0666355606\C,-0.2143970202,-0.519855655,-0.1671182248\C,1.60629
96677,0.8635457086,-1.0316366203\C,-0.6243848317,-1.6173927835,0.81006

22167\C,-0.6791382882,-0.8238560888,-1.588088756\H,2.6811571738,0.9952
810483,-0.8841017333\H,1.1076709164,1.8361496734,-0.9059163659\H,1.453
5190481,0.5164249723,-2.0544747885\H,-0.0552306868,-1.6251564525,-2.00
53775753\H,-0.6270508494,0.0463259453,-2.2426549206\H,-1.7169114978,-1
.1605549785,-1.5680977025\H,0.005203797,-2.500903576,0.6412432515\H,-1
.666585101,-1.8898842403,0.6359760654\H,-0.5335872547,-1.3084204401,1.
8515410285\Cl,-1.4361128292,1.0281145005,0.3729901906\Version=IA32L-G
03RevC.02\State=1-A\HF=-712.7103949\RMSD=2.909e-09\RMSF=4.086e-05\Dipo
le=1.1139467,-0.788911,-0.2864821\PG=C01 [X(C5H12Cl1N1)]\@

n.CCl₃CH₃-2-NHCH₃

1\1\GINC-LC129\FOpt\RB3LYP\Gen\C4H10Cl1N1\CYL509\26-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃
CH₃-2-NHCH₃.freq\0,1\C,2.0629261138,-0.4610290141,0.672745872\H,3.0952
788619,-0.4663045856,0.3130257335\H,1.9106682187,-1.3733533039,1.25582
93236\H,1.9159644723,0.4090225094,1.3284243546\N,1.1733822117,-0.44157
36645,-0.4850789966\C,-0.2082061935,-0.3275622427,-0.3118568501\C,-0.7
950300547,-1.3398041746,0.6625882844\C,-0.9278022777,-0.2933393549,-1.
6533303858\H,1.5069828877,0.1996691377,-1.1978404198\H,-0.5177536888,0
.4888972697,-2.2997327193\H,-1.992735432,-0.0977735523,-1.5158049333\H
, -0.801256116,-1.2623730417,-2.1512911958\H,-0.3695722109,-1.239664318
1,1.662891404\H,-0.5902353794,-2.3511664763,0.2890701908\H,-1.87514241
91,-1.2017867474,0.7398054532\Cl,-0.6639529532,1.4421327928,0.51472319
19\Version=IA32L-G03RevC.02\State=1-A\HF=-673.4055406\RMSD=4.968e-09\
RMSF=2.526e-05\Dipole=0.5909365,-0.937515,-0.464205\PG=C01 [X(C4H10Cl1
N1)]\@

n.CCl₃CH₃-2-NHCHO

1\1\GINC-LC127\FOpt\RB3LYP\Gen\C4H8Cl1N1O1\CYL509\26-Jun-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃
CH₃-2-NHCHO.freq\0,1\H,1.0017131936,-0.2363304246,-2.7975662208\C,1.1
005564083,-0.0462868317,-1.7102364227\O,2.0456521506,0.5475460509,-1.2
353926067\N,0.0414525991,-0.6016102593,-1.0233186793\C,-0.2868824817,-
0.4236239978,0.3635916444\H,-0.7304656312,-0.8963784351,-1.6104700495\
C,0.9222903399,-0.5101427033,1.2905531653\C,-1.380146275,-1.4208864244
,0.7431046062\H,-0.9890525113,-2.4408737444,0.6497813339\H,-2.25726956
08,-1.3157504165,0.095915016\H,-1.6982557409,-1.2568992483,1.774589943
6\H,1.6566798158,0.2568779293,1.0537271509\H,1.3908866977,-1.494153414
3,1.1693879001\H,0.591244391,-0.4008855526,2.3262851539\Cl,-1.04445729
42,1.2953492034,0.6036849071\Version=IA32L-G03RevC.02\State=1-A\HF=-7
47.4295251\RMSD=6.531e-09\RMSF=3.891e-05\Dipole=-0.7696477,-1.4369861,
-0.2863134\PG=C01 [X(C4H8Cl1N1O1)]\@

n.CCl₃CH₃-2-NHCOCH₃

1\1\GINC-LC97\FOpt\RB3LYP\Gen\C5H10Cl1N1O1\CYL509\26-Jun-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃
CH₃-2-NHCOCH₃.freq\0,1\H,-1.104712717,2.0352519571,-2.454852958\C,-0.
1226517332,2.2131658195,-2.0035206603\C,0.0329723113,1.5323317717,-0.6
50807014\H,0.0308939357,3.2854685408,-1.8736628612\H,0.6438921771,1.83
68870638,-2.6922473832\N,-0.6037281902,0.2985724782,-0.5741193774\O,0.
6578522596,2.033634085,0.2657920788\C,-0.4301331558,-0.6947369955,0.44
36783587\H,-0.9218531879,-0.071861717,-1.4616858549\C,-0.4781191088,-0
.1414549526,1.8646090738\C,-1.4526643513,-1.8083858183,0.2240914023\H,
-1.3732445029,-2.2296941685,-0.7836548394\H,-2.4628196068,-1.404820036
4,0.3622241134\H,-1.292791972,-2.6149266844,0.9423152632\H,0.311810244
,0.5874261869,2.0305030266\H,-0.3820773825,-0.9651057909,2.5765773267\
H,-1.44678425,0.3495338041,2.0179320363\Cl,1.2743848673,-1.516044596,0
.2329849517\Version=IA32L-G03RevC.02\State=1-A\HF=-786.7531917\RMSD=6
.470e-09\RMSF=2.907e-05\Dipole=-1.4308878,-0.2166797,-0.8550921\PG=C01

[X(C5H10Cl1N1O1)]\@

n.CC1_CH3_2-NO2

1\1\GINC-LC89\FOpt\RB3LYP\Gen\C3H6Cl1N1O2\CYL509\26-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-NO2.freq\0,1\O,-1.0901401466,-1.3632961084,-1.22403423\N,-0.9439
393913,-0.2941140335,-0.6356540105\C,0.4131735406,-0.1824313787,0.1293
754638\O,-1.7410808381,0.6247662508,-0.6140297352\C,1.5247447873,-0.29
29022625,-0.9102690939\C,0.4302289504,-1.2917312693,1.1771435181\H,2.4
930435652,-0.2342505004,-0.4068209309\H,1.459628475,0.5196417269,-1.63
88283036\H,1.4440185217,-1.2510294526,-1.4292741531\H,1.3759799088,-1.
2536559511,1.7235938745\H,0.3368033417,-2.2614477201,0.6823583055\H,-0
.3902267769,-1.1684920278,1.8891343016\Cl,0.4899537007,1.4246270872,0.
9386133748\Version=IA32L-G03RevC.02\State=1-A\HF=-783.2328945\RMSD=1.
914e-09\RMSF=5.988e-05\Dipole=1.1537271,-0.5308488,0.3510132\PG=C01 [X
(C3H6Cl1N1O2)]\@

n.CC1_CH3_2-OCF3

1\1\GINC-LC111\FOpt\RB3LYP\Gen\C4H6Cl1F3O1\CYL509\26-Jun-2008\0\#\B3LYP
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_
CH3_2-OCF3.freq\0,1\C,1.1063480013,0.1036870437,-0.1356692886\O,-0.07
73518769,-0.2882522892,-0.8396014528\C,-1.3453756667,-0.0407718468,-0.
4182441553\F,-1.5151252011,1.1897914536,0.1059090359\F,-1.7619832109,-
0.926975014,0.4976956084\F,-2.1383237779,-0.1502944869,-1.4895059215\C
,1.3099309186,1.6152477435,-0.1190610908\C,2.2236359077,-0.6387611423,
-0.8556242003\H,3.1820881655,-0.4325224473,-0.3743113718\H,2.264333148
, -0.301552984,-1.8968867367\H,2.0357124813,-1.7143083745,-0.8393323297
\H,2.2993151539,1.8402487702,0.287283793\H,0.5588808094,2.1223164045,0
.4843077501\H,1.2560713462,1.9890301394,-1.1474255642\Cl,1.0584746267,
-0.4968412681,1.6086988228\Version=IA32L-G03RevC.02\State=1-A\HF=-990
.9940134\RMSD=5.321e-09\RMSF=2.130e-06\Dipole=0.8471494,0.4516425,-0.4
951059\PG=C01 [X(C4H6Cl1F3O1)]\@

n.CC1_CH3_2-OCH2CH3

1\1\GINC-LC143\FOpt\RB3LYP\Gen\C5H11Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_C
H3_2-OCH2CH3.freq\0,1\H,-0.3690851097,-3.4250707885,1.6908501053\C,-0
.374064412,-2.8904617213,0.734698009\C,-0.4200035647,-1.3914814228,0.9
759601578\O,-0.449690534,-0.7532521958,-0.3084487889\C,-0.257827144,0.
6092971317,-0.3813732323\C,-0.4348119965,1.0024990933,-1.8400315076\C,
-1.1102389572,1.432752929,0.5798410438\H,-1.3139755105,-1.1174747274,1
.5518632693\H,0.4655224856,-1.0529744585,1.5271183144\H,0.5279642036,-
3.1622035008,0.1781137729\H,-1.2464609526,-3.2176180758,0.1597072796\H
,0.2153738162,0.3933435169,-2.4715678633\H,-0.1983189274,2.0579445015,
-1.9902888926\H,-1.4763969245,0.8219082076,-2.1306015669\H,-0.88209770
65,1.210127294,1.6242445215\H,-2.1679645213,1.2098231395,0.3915632286\
H,-0.9400148136,2.4989632589,0.4145475523\Cl,1.5626267458,1.0137419494
,0.0651455157\Version=IA32L-G03RevC.02\State=1-A\HF=-732.5844873\RMSD
=4.510e-09\RMSF=7.561e-06\Dipole=-0.9860269,-0.1798887,0.2225994\PG=C0
1 [X(C5H11Cl1O1)]\@

n.CC1_CH3_2-OCH3

1\1\GINC-LC102\FOpt\RB3LYP\Gen\C4H9Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-OCH3.freq\0,1\C,-1.3948660586,-0.3010057459,-1.603826632\O,-0.981
7340292,-0.7846261678,-0.3286165118\C,0.2283199662,-0.3555830022,0.177
1380684\H,-0.7731777711,-0.7001575256,-2.4143596538\H,-2.4199747043,-0
.652673129,-1.7348467029\H,-1.3778546794,0.7942160385,-1.6293475851\C,
0.4353417458,-1.0867766859,1.4945325819\C,1.4077389696,-0.4828574547,-

0.7827849254\H,1.3304831381,-0.7243522637,2.0041905525\H,0.546070351,-
2.1581681415,1.2903648579\H,-0.4324342382,-0.9414696755,2.1414401738\H
,2.3324220504,-0.1863480268,-0.2827135448\H,1.2863185256,0.1434952646,
-1.6690275094\H,1.4954599702,-1.5306502027,-1.0962380986\C1,0.10631481
49,1.5053208434,0.6064185322\\Version=IA32L-G03RevC.02\State=1-A\HF=-6
93.265286\RMSD=3.788e-09\RMSF=1.271e-05\Dipole=0.2431105,-0.7598907,-0
.6261186\PG=C01 [X(C4H9C1101)]\\@

n.CC1_CH3_2-OCHO

1\1\GINC-LC126\FOpt\RB3LYP\Gen\C4H7C1102\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
3_2-OCHO.freq\\0,1\C,-0.3570055295,-0.2350427667,-0.4826664513\O,-0.30
21646127,-0.8626391497,0.8054180655\C,0.768812013,-0.7397389194,1.6289
958649\H,0.5382322188,-1.2957752953,2.5505669694\O,1.7909901659,-0.143
3908344,1.4231761924\C,0.8307574218,-0.5851484501,-1.3710849287\C,-1.6
937222378,-0.6692880208,-1.0663732583\H,-1.6892405279,-1.7560940097,-1
.2050618547\H,-1.8573618275,-0.1868691462,-2.0327388236\H,-2.509252955
, -0.4032789307,-0.3901609357\H,1.7624557616,-0.2022127785,-0.958276078
2\H,0.673876932,-0.1628489598,-2.3671848387\H,0.8950797095,-1.67603148
62,-1.459870603\C1,-0.4127908084,1.5945093777,-0.2481914858\\Version=I
A32L-G03RevC.02\State=1-A\HF=-767.2918972\RMSD=5.777e-09\RMSF=2.248e-0
5\Dipole=-0.5439407,-0.985977,-0.4150138\PG=C01 [X(C4H7C1102)]\\@

n.CC1_CH3_2-OCOCH3

1\1\GINC-LC107\FOpt\RB3LYP\Gen\C5H9C1102\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH
3_2-OCOCH3.freq\\0,1\C,-0.8798668335,-0.1135691816,-0.2309785357\O,0.4
159777828,-0.6684936148,-0.4471673618\C,1.566341317,0.0611721568,-0.28
72029313\C,2.7603200667,-0.836537298,-0.5079786032\O,1.6092167064,1.23
15378072,-0.0028768092\C,-1.1507415341,1.1468493223,-1.0445893103\C,-1
.8450265443,-1.2476702494,-0.548771874\H,3.6703649834,-0.2360867854,-0
.4910604087\H,2.6724417139,-1.3655332202,-1.4619313533\H,2.8031178706,
-1.5926018285,0.2835376121\H,-1.7524018202,-1.5109259131,-1.6084147222
\H,-2.8728266789,-0.9374874013,-0.346895894\H,-1.6108245186,-2.1275274
073,0.0546823715\H,-0.4976776294,1.9629061243,-0.7419150994\H,-2.19424
46041,1.4453348707,-0.9128408666\H,-0.9825920795,0.9229035175,-2.10482
88445\C1,-1.0672395283,0.2866585884,1.5674793\\Version=IA32L-G03RevC.0
2\State=1-A\HF=-806.6179659\RMSD=6.519e-09\RMSF=2.541e-06\Dipole=-0.05
28274,-0.7965593,-0.9695362\PG=C01 [X(C5H9C1102)]\\@

n.CC1_CH3_2-Si_CH3_3

1\1\GINC-LC45\FOpt\RB3LYP\Gen\C6H15C11Si1\CYL509\26-Jun-2008\0\#B3LYP/
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C
H3_2-Si_CH3_3.freq\\0,1\H,2.0282784137,-1.1669177796,-1.550461104\C,1.
9861282582,-1.168941444,-0.4551052352\H,3.0177594747,-1.1057560687,-0.
087562342\H,1.5746350738,-2.1323199003,-0.1363995448\Si,0.9611400604,0
.2697805177,0.2169239836\C,-0.8684897976,0.1140406215,-0.3985125752\C,
1.0010830384,0.2807433808,2.1064819576\C,1.6586100568,1.9078014081,-0.
4418763656\C,-0.9833847896,0.0303492998,-1.9222907614\C,-1.7832796537,
1.2075495627,0.1578171695\H,2.6979113036,2.034632671,-0.1139963217\H,1
.0943728659,2.7734186427,-0.0753188349\H,1.6566780931,1.9458775592,-1.
5375805698\H,2.0361679996,0.3388460032,2.4650434523\H,0.5538301594,-0.
6300076641,2.5181801528\H,0.4615420794,1.1388379916,2.5238000616\H,-1.
4556072539,2.1865063022,-0.2156927321\H,-1.7698873951,1.2369702094,1.2
511082734\H,-2.8197454301,1.0539257806,-0.1656968543\H,-0.3912497169,-
0.7919622447,-2.3340068562\H,-0.6271581638,0.9672829653,-2.3700552547\H,
-2.0260775872,-0.1141102106,-2.2296115686\C1,-1.5030243178,-1.514200
5017,0.2789546497\\Version=IA32L-G03RevC.02\State=1-A\HF=-987.4112896\
RMSD=9.812e-09\RMSF=1.037e-05\Dipole=0.4649346,0.7694093,-0.2566454\PG

=C01 [X(C6H15Cl1Si1)]\@

n.CC1_CH3_2-P_CH3_2

1\1\GINC-LC82\FOpt\RB3LYP\Gen\C5H12Cl1P1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-P_CH3_2.freq\0,1\C,-0.9525734203,0.9402575684,1.828488824\H,-0.28
43500962,1.7555033223,2.1217743094\H,-1.5131967668,0.6384284426,2.7200
318326\H,-1.6544302981,1.3048023072,1.0716745265\H,0.0326523061,-0.526
6647355,1.2423985957\C,-1.3618891778,-1.6530704214,0.7399080243\C,0.69
29610699,0.0722978841,-0.4327932506\H,-0.9679969371,-2.5759219334,0.30
36071919\H,-2.0469480662,-1.1821009677,0.0277662183\H,-1.9182874018,-1
.9281257796,1.6426891993\C,1.7001308026,1.2059144266,-0.2178628293\C,1
.3367190176,-1.0966204812,-1.1843769249\H,2.138406343,-1.528577327,-0.
5733198561\H,1.7704973913,-0.7494684424,-2.1280785345\H,0.6129554663,-
1.8833399801,-1.4129006099\H,2.5146769379,0.8554283663,0.4273922544\H,
1.2383555048,2.0791216124,0.2503861809\H,2.1287876074,1.5206188206,-1.
1751848436\C1,-0.6470790604,0.7518193372,-1.547764698\Version=IA32L-G
03RevC.02\State=1-A\HF=-999.3206828\RMSD=2.845e-09\RMSF=1.919e-05\Dipo
le=0.200327,-0.1678679,0.3245936\PG=C01 [X(C5H12Cl1P1)]\@

n.CC1_CH3_2-SC_CH3_2CN

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C7H12Cl1N1S1\CYL509\04-Sep-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1
CH3_2-SC_CH3_2CN.freq\0,1\N,-1.4399539234,-1.6332381661,-2.37459028
43\C,-0.9101005799,-1.6022388468,-1.3410221528\C,-0.2312432193,-1.5978
216014,-0.0357252598\H,-0.7036867849,-0.0688992583,0.93865349\C,0.0108
132247,1.4315107671,0.1427963784\C,-0.1764524004,1.518444283,-1.368989
8023\C1,1.8384739205,1.5773808444,0.4855384134\C,1.2872279818,-1.77163
37448,-0.2191714453\C,-0.8060795411,-2.7533596061,0.8182782977\H,1.723
4809613,-0.9811360134,-0.8315199959\H,1.7768092287,-1.7566741834,0.758
0549653\H,1.4845862257,-2.7350075896,-0.7034503681\H,-0.311037943,-2.7
716698571,1.7935401834\H,-0.6212570241,-3.7057288037,0.3110087112\H,-1
.8839168913,-2.64468667,0.9673815982\H,-1.2397041867,1.4378406865,-1.6
154749337\H,0.3576665486,0.7307849859,-1.9025465504\H,0.1993738628,2.4
840982467,-1.7223687247\C,-0.6612591425,2.603453843,0.8672773974\H,-0.
2253233631,3.5431656057,0.5157000898\H,-0.5191803175,2.5411231391,1.94
96283499\H,-1.7343256679,2.60734083,0.648909318\Version=IA64L-G03RevC
.02\State=1-A\HF=-1187.0966429\RMSD=7.617e-09\RMSF=1.758e-05\Dipole=0.
1218008,-0.0184922,0.6805267\PG=C01 [X(C7H12Cl1N1S1)]\@

n.CC1_CH3_2-SCH2COOCH3

1\1\GINC-LC152\FOpt\RB3LYP\Gen\C6H11Cl1O2S1\CYL509\26-Jun-2008\0\#B3LY
YP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1
CH3_2-SCH2COOCH3.freq\0,1\S,1.1496054678,0.4701000332,0.3898193186\C
,0.4102386091,-0.8246817993,1.4752577825\C,1.5787580564,-1.4216257168,
2.2614065523\C,-0.3833070665,-1.8855692823,0.7181224144\C,-0.310445602
3,1.2652810587,-0.4023034725\C,-0.6504146535,0.6668618186,-1.752051604
8\O,-1.4596513356,-0.2163166244,-1.9437336307\O,0.0811734996,1.2393192
88,-2.7283638762\C,-0.1240403625,0.7054585516,-4.048026804\H,-0.045428
1364,2.3189580465,-0.5139385792\H,-1.1647573948,1.1773869818,0.2717214
283\H,-1.1660243518,0.8303422019,-4.3536753698\H,0.130263564,-0.357347
74,-4.0730982472\H,0.5391577559,1.2751369225,-4.6990868633\H,1.2048543
934,-2.1846508329,2.9504501247\H,2.284911201,-1.8945635496,1.569404439
4\H,2.1052642463,-0.6570390569,2.8379589506\H,-0.7871812423,-2.6178902
939,1.4251913867\H,-1.2059078707,-1.4554787913,0.1440506941\H,0.285127
3621,-2.4005868985,0.0193042447\C1,-0.745345777,-0.0455433302,2.708644
6788\Version=IA32L-G03RevC.02\State=1-A\HF=-1244.1082374\RMSD=7.570e-
09\RMSF=3.871e-06\Dipole=0.4713476,-0.1128009,-0.725873\PG=C01 [X(C6H1
1Cl1O2S1)]\@

n.CCl₄_CH₃_2-SCH₂Ph

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H13Cl1S1\CYL509\03-Sep-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₄_CH₃_2-SCH₂Ph.freq\0,1\C,-1.5360140793,-1.0720642182,-0.9382406467\S,
-1.4578928837,-1.0499043148,0.8972560677\C,0.3346942208,-1.0956126856,
1.340364288\C,-2.9967365242,-1.3689576845,-1.2885210359\C,1.1521755455
,0.1478483977,1.0733404253\H,0.7984809176,-1.9734242929,0.8823730725\H
,0.2824576226,-1.29674573,2.4174924018\C,2.3259686882,0.0644508608,0.3
162212515\C,0.7871063461,1.388025363,1.6148016814\C,3.1198798518,1.193
0209572,0.0999586238\C,1.576841468,2.5151336049,1.4011880818\C,2.74680
07371,2.4219444271,0.6418760674\H,3.3607325682,3.3027936746,0.47432153
23\H,1.2788029602,3.469928898,1.8261739553\H,4.0268764897,1.109143824
8,-0.4929112044\H,-0.1292941866,1.4693421245,2.1936110136\H,2.62712495
37,-0.8930328475,-0.1040158313\H,-3.2637922415,-2.3742573629,-0.945043
5921\H,-3.1326716231,-1.316886357,-2.3728842001\H,-3.67127952,-0.64631
10499,-0.8212618951\C1,-1.1412534961,0.5987322258,-1.6605179457\C,-0.5
788069332,-2.071112293,-1.583022477\H,0.4650841244,-1.8054100382,-1.40
33654886\H,-0.7388231338,-2.0873157823,-2.6659297955\H,-0.7675592819,-
3.0739282308,-1.1836495311\Version=IA64L-G03RevC.02\State=1-A\HF=-124
7.2845659\RMSD=4.551e-09\RMSF=3.388e-06\Dipole=0.3379363,-0.7087472,0.
0427732\PG=C01 [X(C10H13Cl1S1)]\@

n.CCl₄_CH₃_2-SCH₃

1\1\GINC-LC105\FOpt\RB3LYP\Gen\C4H9Cl1S1\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₄_CH₃_2-SCH₃.freq\0,1\S,0.4878365644,-0.122967365,-1.3766065872\C,0.20759
97536,-0.3922516284,0.4161209233\C,1.5317499056,-0.8888158195,0.997208
956\C,-0.9468268752,-1.3462187085,0.7151344495\C,-1.1312391457,0.48665
6841,-1.957340646\H,-0.97889546,0.7999162354,-2.9935751323\H,-1.445431
5126,1.3512558746,-1.3671244297\H,-1.8998506332,-0.289782048,-1.933432
4279\H,1.4347176037,-1.0268060389,2.0781134725\H,1.7944695609,-1.85128
45326,0.5436169902\H,2.3391142495,-0.1772193165,0.8069899115\H,-1.0474
118763,-1.4846381294,1.7965807582\H,-1.8976329303,-0.9669616932,0.3334
864962\H,-0.7437694727,-2.3175047306,0.2509721546\C1,-0.1957880229,1.2
220163595,1.2637256179\Version=IA32L-G03RevC.02\State=1-A\HF=-1016.23
8754\RMSD=3.179e-09\RMSF=9.421e-06\Dipole=-0.3550256,-0.6728734,-0.155
873\PG=C01 [X(C4H9Cl1S1)]\@

n.CCl₄_CH₃_2-SO₂CH₃

1\1\GINC-LC43\FOpt\RB3LYP\Gen\C4H9Cl1O2S1\CYL509\26-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₄_CH₃_2-SO₂CH₃.freq\0,1\C,-0.2878360868,-0.0776874448,-0.8374623387\S,-0
.2067439921,0.0251344582,1.0400413142\C,1.299496488,-0.850317331,1.531
6942722\O,-0.0491933521,1.4363615707,1.4149495509\O,-1.3622825281,-0.7
528954754,1.520995608\H,1.2521085675,-1.8888817731,1.2010412955\H,1.30
25486964,-0.8054808681,2.6234775138\H,2.1711784062,-0.3385583076,1.124
8613548\C,-0.5074075689,-1.5186264391,-1.2827639688\C,-1.4097258596,0.
8639046864,-1.2641165017\H,-1.4955996506,0.8520411536,-2.354554475\H,-
1.2141391477,1.883795605,-0.9278471714\H,-2.354728838,0.5212864194,-0.
8296705114\H,0.3262426227,-2.1677503764,-1.0016876682\H,-0.606240429,-
1.5471297663,-2.3722086541\H,-1.4255162382,-1.9034186525,-0.8302644198
\C1,1.2986291229,0.5306220967,-1.5085575495\Version=IA32L-G03RevC.02\
State=1-A\HF=-1166.6230701\RMSD=5.528e-09\RMSF=5.507e-06\Dipole=0.4574
855,-1.0097111,-0.7766609\PG=C01 [X(C4H9Cl1O2S1)]\@

n.CCl₄_CH₃_2-SOCH₃

1\1\GINC-LC25\FOpt\RB3LYP\Gen\C4H9Cl1O1S1\CYL509\26-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₄_C

H3_2-SOCH3.freq\0,1\C,-0.6387326955,-0.1039732637,-0.6395868678\S,-0.5998524149,0.4051708114,1.1158629598\O,0.5623862481,-0.6109653781,1.7836837687\C,1.8750435269,-0.0307667599,1.9067292022\C,-0.6584337561,-1.6204854128,-0.7960368762\H,2.4733477276,-0.7891435493,2.4194682785\H,1.8465975989,0.8828096792,2.5108679035\H,2.3089682337,0.1878589391,0.9272759243\C,-1.8608478812,0.5856836253,-1.2490413763\H,-1.9001183582,0.3745146965,-2.3215679371\H,-1.8181519187,1.6709113615,-1.1164278763\H,-2.7758978177,0.2046342847,-0.7827549001\H,0.2028514301,-2.0737315398,-0.301564229\H,-0.6438460848,-1.8884989669,-1.8569671436\H,-1.5702787963,-2.0193652613,-0.3384291072\Cl,0.8631118514,0.5218971333,-1.5644448771\Version=IA32L-G03RevC.02\State=1-A\HF=-1091.4246978\RMSD=4.525e-09\RMSF=7.088e-06\Dipole=-0.2557232,-0.138638,-0.0168332\PG=C01 [X(C4H9Cl1O1S1)]\@

n.CC1_CH3_2-Ph

1\1\GINC-LC92\FOpt\RB3LYP\Gen\C9H11Cl1\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2-Ph.freq\0,1\H,-3.9414644159,-1.4999655141,-0.1796828412\C,-2.9141525347,-1.1488080923,-0.1349983297\C,-1.8559574484,-2.0587224863,-0.1576183676\C,-0.5397495019,-1.6048063033,-0.1001515\C,-0.2457532504,-0.231975555,-0.0186775486\C,-1.3162428501,0.6684528848,0.003122502\C,-2.6361949217,0.2139767443,-0.0544683655\H,-2.0524345489,-3.1258474562,-0.2201467958\C,1.2307193674,0.1781755779,0.0404402841\C,1.9132810929,-0.3741148028,1.2993544585\C,1.9767488296,-0.2373027132,-1.2349412029\H,-1.1214595591,1.7320795495,0.0654196345\H,0.2649092466,-2.3346743659,-0.1194013626\H,-3.4479140949,0.9364566351,-0.0357942076\H,2.9595294834,-0.0572386096,1.3394052292\H,1.8838473824,-1.469483235,1.2891682228\H,1.4041332638,-0.0267926481,2.2022343893\H,3.022834655,0.0792230046,-1.1883987669\H,1.5123646344,0.2065126506,-2.1194928425\H,1.9497948049,-1.3273258151,-1.3441438813\Cl,1.4052744972,2.0269296635,0.1446153919\Version=IA32L-G03RevC.02\State=1-A\HF=-809.7876684\RMSD=6.720e-09\RMSF=1.116e-05\Dipole=-0.105439,-0.8510249,-0.0485826\PG=C01 [X(C9H11Cl1)]\@

n.CC1_CH3_2-C6H4CN

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C10H10Cl1N1\CYL509\03-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2-C6H4CN.freq\0,1\N,-4.9812866061,-0.6947974489,0.2936632168\C,-3.8354588004,-0.5000892518,0.24309078\C,-2.4232270449,-0.2598050764,0.1832976241\C,-1.5146297598,-1.3058308709,0.4219621256\C,-0.1492540277,-1.0641812546,0.3640039184\C,0.354390205,0.2142452782,0.0685794069\C,-0.5616745593,1.2465778216,-0.1722158047\C,-1.9354735088,1.0189877582,-0.1161544304\H,-1.8868673177,-2.3000852584,0.6465873497\C,1.8616491022,0.4619557462,0.0702371852\C,2.4613465082,0.1922100107,1.4561447977\H,-0.2148856447,2.245991175,-0.4072786937\H,0.5394804257,-1.886591044,0.5277695953\H,-2.6313448201,1.8297671081,-0.3059681112\H,3.5468842332,0.3250125116,1.4356568123\H,2.2414986987,-0.8205205797,1.8021810142\H,2.0340294253,0.9002969478,2.1765903644\Cl,2.638654143,-0.7697172788,-1.1034507141\C,2.2776659654,1.8432555546,-0.4367167866\H,3.3677949757,1.909844516,-0.4698932378\H,1.9123399143,2.6212623045,0.2440393705\H,1.8909514415,2.0398439059,-1.4400377382\Version=IA64L-G03RevC.02\State=1-A\HF=-902.0315787\RMSD=3.678e-09\RMSF=1.224e-05\Dipole=1.4673861,0.8734191,0.5160582\PG=C01 [X(C10H10Cl1N1)]\@

n.CC1_CH3_2-C6H4NO2

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C9H10Cl1N1O2\CYL509\03-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2-C6H4NO2.freq\0,1\O,-2.9830782071,2.8671665013,-0.9475943067\N,-2.1968843542,2.1950198329,-1.6147298155\C,-1.3221475429,1.2549150392,-0.8971490165\O,-2.0910079589,2.2516014046,-2.8395195059\C,-1.4159071

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07,1.1636586126,0.4864839977\C,-0.5841399756,0.2696344208,1.1594973186
\C,0.3343270633,-0.5297547201,0.4647353428\C,0.4022803748,-0.406248476
,-0.9344543526\C,-0.4175573464,0.479210789,-1.6214485385\H,-0.36641845
33,0.5814670713,-2.6983388026\C,1.2079365726,-1.5562318079,1.184463082
2\C,0.8710758784,-2.9804615244,0.7244017055\H,-0.6639710556,0.20601553
82,2.2381143497\H,1.1239005895,-0.9956326193,-1.4902625473\H,-2.126654
1078,1.7843991365,1.01786689\H,1.532335331,-3.7044808524,1.2090749628\
H,0.9692516613,-3.0899830947,-0.3581914512\H,-0.1651363851,-3.21176892
26,0.999547836\C1,2.9811742448,-1.2320749028,0.6906750231\C,1.17311686
29,-1.4604438226,2.7101186618\H,1.8773774176,-2.1771849796,3.139335615
1\H,0.171609909,-1.7074858841,3.0817170477\H,1.4447140579,-0.461025186
2,3.05979071\\Version=IA64L-G03RevC.02\State=1-A\HF=-1014.2897003\RMSD
=8.951e-09\RMSF=2.809e-05\Dipole=0.2866842,-1.4019759,1.1308685\PG=C01
[X(C9H10C11N1O2)]\\@
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n.CC1_CH3_2-C6H4OCH3

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1\1\GINC-AC24\FOpt\RB3LYP\Gen\C10H13C11O1\CYL509\04-Sep-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC1
_CH3_2-C6H4OCH3.freq\\0,1\C,-1.9454986442,-0.4032086368,-0.1407337396\
C,-1.9669676919,-0.0102232333,1.2073585393\C,-0.7928484127,0.459796691
6,1.7994835311\C,0.3834819106,0.5344211794,1.0447683729\C,0.4222555499
,0.1554566476,-0.2989205154\C,-0.77308091,-0.3188303407,-0.8729354907\
C,1.6819965717,0.2836543016,-1.1429702435\O,-3.1687277231,-0.128961738
2,1.8406867055\C,-3.2448421843,0.2384214512,3.2090678696\C,1.46387271,
1.2024675856,-2.3507593618\H,-0.7758557233,-0.6519877491,-1.9063978721
\H,1.2766821125,0.9030174059,1.5371297862\H,-0.7729986494,0.7672728249
,2.8387479184\H,-2.8616235944,-0.777324071,-0.5869533519\H,-2.57715613
39,-0.3744289856,3.8289249968\H,-4.2791566793,0.0616744679,3.509476118
\H,-3.0006977801,1.2988701235,3.356462578\H,2.3609319974,1.2397794966,
-2.9759997389\H,1.2417477857,2.2151811379,-1.9922045299\H,0.6253919899
,0.8692523367,-2.966866899\C1,2.0853707004,-1.417831569,-1.8451030612
\C,2.9275418886,0.7098563589,-0.3655135834\H,3.7948708904,0.7185241657
,-1.0303651562\H,3.137925003,0.0308049477,0.4646506542\H,2.7929939336,
1.723322447,0.0314014132\\Version=IA64L-G03RevC.02\State=1-A\HF=-924.3
119119\RMSD=5.821e-09\RMSF=1.293e-05\Dipole=-0.2955928,1.0000393,0.898
8047\PG=C01 [X(C10H13C11O1)]\\@
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n.CC1_CH3_2-C6H4OH

```
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C9H11C11O1\CYL509\03-Sep-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC1
_CH3_2-C6H4OH.freq\\0,1\C,-1.9795246051,-1.3163878142,0.4201522017\C,-2
.397910772,-0.2680360822,1.2413666824\C,-1.6108173677,0.8856049813,1.3
398597112\C,-0.425946444,0.9819022575,0.618619841\C,0.013228676,-0.058
1295243,-0.2151355957\C,-0.7873173447,-1.2066784573,-0.2928481637\C,1.
2898119892,0.0973909909,-1.0300379917\O,-3.5721100807,-0.4233280893,1.
9224165399\C,1.2156223765,1.3028741626,-1.9743825496\H,-0.4903088052,-
2.0401250688,-0.9196832145\H,0.1817562641,1.8749356246,0.7287090545\H,
-1.9222449047,1.7047241789,1.9859083747\H,-2.5921306053,-2.2097040438,
0.3517400563\H,-3.7342446115,0.3693321175,2.4572617695\H,2.1591597762,
1.4319707013,-2.5129906697\H,0.9951049384,2.2266240128,-1.4342658651\H
,0.4135398876,1.1351024619,-2.7037435803\C1,2.7030096038,0.4541944198,
0.1642631831\C,1.7102042642,-1.1570210754,-1.7963266922\H,2.663364295,
-0.9811083841,-2.3011484402\H,0.9608205947,-1.3988459056,-2.5596223963
\H,1.8267959178,-2.0167027506,-1.1315761822\\Version=IA64L-G03RevC.02\
State=1-A\HF=-885.0052681\RMSD=6.130e-09\RMSF=1.910e-05\Dipole=-0.7554
211,0.3308946,-0.3155862\PG=C01 [X(C9H11C11O1)]\\@
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n.CC1_CH3_2-CF2CF3

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H6C11F5\CYL509\03-Sep-2008\0\\#B3LYP/G
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EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC1_C
H3_2-CF2CF3.freq\\0,1\\F,-0.6828501088,1.30732088,-1.2218378767\\C,-0.13
52600024,0.6511151896,-0.1490334017\\C,1.3356494159,0.3721746355,-0.561
9007327\\C,-1.0899728916,-0.5210905495,0.198914306\\F,-0.0790758022,1.53
0605897,0.8852720557\\F,1.382007888,-0.3817441634,-1.6765626456\\F,2.026
5619415,-0.2467314313,0.399975043\\F,1.9342172372,1.5424328975,-0.82743
77538\\C,-2.4699787392,0.0624203073,0.5276927393\\H,-2.8873215212,0.5497
957772,-0.3586303502\\H,-2.407237319,0.793082118,1.3362608593\\H,-3.1388
768587,-0.7454223101,0.8335369836\\C1,-0.4675883467,-1.3483966286,1.715
5076169\\C,-1.1758752665,-1.5623733394,-0.9190912321\\H,-0.2277122543,-2
.0774991854,-1.0768433098\\H,-1.4698774707,-1.0735578528,-1.8536989685\\
H,-1.9350981812,-2.3040900383,-0.6584241781\\Version=IA64L-G03RevC.02\\
State=1-A\\HF=-1153.5516045\\RMSD=8.208e-09\\RMSF=6.473e-06\\Dipole=-0.775
0409,-0.2607689,-0.4353367\\PG=C01 [X(C5H6C11F5)]\\@
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n.CC1_CH3_2-CF2H

```
1\\1\\GINC-LC93\\FOpt\\RB3LYP\\Gen\\C4H7C11F2\\CYL509\\26-Jun-2008\\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-CF2H.freq\\0,1\\C,0.5512399364,-0.0349617491,-1.0465923037\\C,0.34924
93633,0.0302800656,0.4716448825\\C,0.9123654792,1.3425405573,1.01726656
7\\H,1.6235603783,-0.0199291286,-1.2852485286\\F,-0.0343589445,1.0259709
999,-1.6671882262\\F,0.0191467897,-1.1757061898,-1.5654590065\\C,0.97408
85735,-1.1972668711,1.1346191783\\H,2.0553371536,-1.2131615105,0.946138
017\\H,0.5376490131,-2.1178367162,0.7416139888\\H,0.8159945528,-1.162763
9917,2.2154800648\\H,1.9919920655,1.3933891718,0.8257016043\\H,0.7537092
756,1.400173642,2.0970587072\\H,0.4326980874,2.200731546,0.5420730994\\C
1,-1.4585700734,0.0013800988,0.7970222469\\Version=IA32L-G03RevC.02\\St
ate=1-A\\HF=-816.5248515\\RMSD=5.437e-09\\RMSF=1.037e-04\\Dipole=1.2340922
,0.0513044,0.4612711\\PG=C01 [X(C4H7C11F2)]\\@
```

n.CC1_CH3_2-CF3

```
1\\1\\GINC-LC95\\FOpt\\RB3LYP\\Gen\\C4H6C11F3\\CYL509\\26-Jun-2008\\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-CF3.freq\\0,1\\F,0.2749454564,0.9755173046,-1.5478664497\\C,0.2544554
283,0.9037350513,-0.2061316862\\F,1.516583189,1.0329660409,0.23675954\\C
,-0.4151477131,-0.3872219962,0.3013005327\\F,-0.4452177443,1.9735532172
,0.2462201053\\C,-1.8329250839,-0.5005845579,-0.2592231235\\C,-0.3801301
737,-0.4333387809,1.8289651105\\H,-1.825858331,-0.4894347029,-1.3512827
654\\H,-2.437254526,0.3397391383,0.0983626985\\H,-2.2909369497,-1.432422
0121,0.0811813388\\H,0.645198971,-0.3750199917,2.2005386138\\H,-0.830384
2188,-1.3648293917,2.1804854602\\H,-0.9509520725,0.4085199529,2.2347548
17\\C1,0.5774043689,-1.7894364914,-0.3440896426\\Version=IA32L-G03RevC.
02\\State=1-A\\HF=-915.7761734\\RMSD=7.401e-09\\RMSF=1.018e-04\\Dipole=-0.7
769825,-0.032633,0.5416187\\PG=C01 [X(C4H6C11F3)]\\@
```

n.CC1_CH3_2-CC12H

```
1\\1\\GINC-LC153\\FOpt\\RB3LYP\\Gen\\C4H7C13\\CYL509\\26-Jun-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3
_2-CC12H.freq\\0,1\\C,0.2025188533,0.1670081656,-0.7152605695\\C,0.272869
558,-0.0696656088,0.8140129648\\H,1.084286384,-0.2475326107,-1.19942818
21\\C1,0.2113078063,1.9414174253,-1.0960784186\\C1,-1.2194642478,-0.6005
13326,-1.5056832668\\C,1.5332353019,0.5768080567,1.4005634646\\C,-0.9880
055254,0.3476212741,1.5647195007\\H,2.4293316922,0.2851183475,0.8445554
824\\H,1.6534248861,0.2560258065,2.4383782995\\H,1.4453257313,1.66644048
34,1.3791810362\\H,-0.8693502799,0.1345062454,2.6302332777\\H,-1.8673481
489,-0.1837996823,1.1961296987\\H,-1.1488397674,1.4238773518,1.44004644
94\\C1,0.4875364636,-1.8976845267,1.0068612016\\Version=IA32L-G03RevC.0
2\\State=1-A\\HF=-1537.2354217\\RMSD=3.729e-09\\RMSF=4.310e-05\\Dipole=0.38
29716,0.4450879,0.5433585\\PG=C01 [X(C4H7C13)]\\@
```

n.CC1_CH3_2-CC13

1\1\GINC-LC116\FOpt\RB3LYP\Gen\C4H6Cl4\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CC13.freq\0,1\C,0.2017677327,-0.0188648757,-0.5163264615\C,0.066193
1412,-0.0028057943,1.0514422754\Cl,1.9594430421,-0.171920972,-0.954354
7227\Cl,-0.4185339815,1.497578067,-1.2626589989\Cl,-0.6697609301,-1.41
05471213,-1.2545977691\C,0.7741990921,1.2060881444,1.6741778958\C,0.55
66507527,-1.3117763995,1.6811597349\H,1.8504285386,1.1530851699,1.4871
480852\H,0.6085320988,1.1883725574,2.7541814823\H,0.3899854809,2.14790
16195,1.279785709\H,1.6259328758,-1.4451859706,1.4943512254\H,0.016401
7764,-2.1758883118,1.2917769813\H,0.3969930429,-1.2599623128,2.7609707
604\Cl,-1.722979785,0.1528800733,1.4474388489\Version=IA32L-G03RevC.0
2\State=1-A\HF=-1996.8113257\RMSD=4.583e-09\RMSF=7.319e-06\Dipole=0.64
69482,-0.0540284,0.6745208\PG=C01 [X(C4H6Cl4)]\@

n.CC1_CH3_2-CH2Cl

1\1\GINC-LC119\FOpt\RB3LYP\Gen\C4H8Cl2\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH2Cl.freq\0,1\C,-0.2271821068,0.0597914494,-0.4495724989\C,0.10268
3762,-0.0165038216,1.0474127455\Cl,1.8301956493,-0.5096419247,1.351777
2887\C,0.5608194058,1.1450641256,-1.1783421032\C,-0.1407561704,-1.2946
417849,-1.1480745109\H,-0.521785417,-0.7580226142,1.5460071946\H,-0.02
91455037,0.9546710781,1.5247469045\H,0.8989634391,-1.6386729592,-1.150
2027816\H,-0.4826508446,-1.2123051945,-2.1833664434\H,-0.7534082906,-2
.0436950961,-0.6378288541\H,1.6244445374,0.8841649823,-1.1815330982\H,
0.442971598,2.116580213,-0.6894226785\H,0.2205657883,1.2332170321,-2.2
13695905\Cl,-2.0168629817,0.574453851,-0.4484388259\Version=IA32L-G03
RevC.02\State=1-A\HF=-1077.6521835\RMSD=5.063e-09\RMSF=2.938e-05\Dipol
e=0.1284089,-0.0402902,-0.2756311\PG=C01 [X(C4H8Cl2)]\@

n.CC1_CH3_2-CH2F

1\1\GINC-LC25\FOpt\RB3LYP\Gen\C4H8Cl1F1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH2F.freq\0,1\C,-0.414652345,0.1283724618,-0.1209305561\C,0.694272
5569,1.1489206945,-0.3680515539\F,1.8280099246,0.5444953551,-0.8824104
881\C,-0.6762364819,-0.7223833924,-1.3620419068\C,-1.6726754502,0.8351
806586,0.38288402\H,0.9611481859,1.6653001842,0.5600595927\H,0.3364160
239,1.8852393128,-1.1015326057\H,-1.4683308884,1.4233194808,1.28292740
01\H,-2.4508766799,0.1050511948,0.6204886251\H,-2.058757686,1.50738389
78,-0.3937775182\H,0.2409671076,-1.2143321207,-1.6915212565\H,-1.03742
65168,-0.0797522416,-2.1753546639\H,-1.435773562,-1.481977436,-1.15875
48805\Cl,0.1691938244,-1.0030137061,1.2239999812\Version=IA32L-G03Rev
C.02\State=1-A\HF=-717.2833972\RMSD=8.551e-09\RMSF=1.380e-05\Dipole=-0
.8367554,0.7414078,-0.4273614\PG=C01 [X(C4H8Cl1F1)]\@

n.CC1_CH3_2-CH2OH

1\1\GINC-LC79\FOpt\RB3LYP\Gen\C4H9Cl1O1\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH2OH.freq\0,1\C,-0.4550530191,0.111377562,-0.1405117478\C,0.61418
31087,1.1649257317,-0.4757814455\O,1.8276360443,0.6243280307,-0.951060
473\C,-0.7192015619,-0.8293927686,-1.3113855795\C,-1.7256145172,0.7678
830884,0.3897838508\H,0.7688523121,1.8109116972,0.401711262\H,0.222566
7093,1.7903135025,-1.2875237179\H,2.1926942233,0.0801955637,-0.2329308
193\H,-1.5160153602,1.404423911,1.254710118\H,-2.4613325702,0.01435318
6,0.6845746479\H,-2.1694873122,1.3892100811,-0.3986606437\H,0.21381525
92,-1.2636238359,-1.6762436638\H,-1.174908233,-0.2594195879,-2.1313730
77\H,-1.4053355991,-1.6315839793,-1.0261442794\Cl,0.2601281267,-0.9187
156744,1.2498666759\Version=IA32L-G03RevC.02\State=1-A\HF=-693.266422

2\RMSD=3.912e-09\RMSF=1.887e-05\Dipole=-0.6241045,0.3541039,-0.1376112
\PG=C01 [X(C4H9C11O1)]\@

n.CC1_CH3_2-CH2Ph

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C10H13Cl1\CYL509\03-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC1_C
H3_2-CH2Ph.freq\\0,1\C,-1.2367110908,-1.2895773163,0.0499251717\C,0.26
84757752,-1.2385811191,-0.3125845627\C,0.924084395,0.1243369024,-0.398
6288026\C,0.9943116278,0.8075888789,-1.6209791608\C,1.498221821,0.7237
949661,0.7312344629\C,1.6047122234,2.0593048366,-1.7124242735\C,2.1100
423062,1.9744917709,0.6443418195\C,2.1635874334,2.6480267893,-0.577369
372\H,2.6434795684,3.6207281741,-0.6455256112\H,1.6492975835,2.5696171
309,-2.6711021946\H,2.5494005928,2.4212892059,1.5324104594\H,0.5730063
499,0.3505375754,-2.5139535943\H,1.4621237445,0.2057390807,1.685053960
9\H,0.805509245,-1.8672685957,0.4065357898\H,0.3559129783,-1.736824397
1,-1.2883677279\C,-1.7307949401,-2.7374367449,0.0225612957\H,-1.131586
3455,-3.3735467174,0.6808972584\H,-1.65660258,-3.1304338872,-0.9994694
096\H,-2.7758038408,-2.7992405483,0.3392648812\C1,-1.4410724002,-0.697
5686346,1.8040189704\C,-2.1001557994,-0.3875052253,-0.8293095156\H,-1.
7830985095,0.6556594033,-0.7654952581\H,-3.1512182166,-0.453876626,-0.
5338138896\H,-2.0168322771,-0.7103754421,-1.8753595365\\Version=IA64L-
G03RevC.02\State=1-A\HF=-849.1062256\RMSD=3.944e-09\RMSF=6.434e-06\Dip
ole=0.11639,-0.2765594,-0.8013206\PG=C01 [X(C10H13Cl1)]\@

n.CC1_CH3_2-CH_CH2_2

1\1\GINC-LC96\FOpt\RB3LYP\Gen\C6H11Cl1\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3_
2-CH_CH2_2.freq\\0,1\C,-1.4737754463,1.2589065297,-0.8875610043\C,-1.5
279837785,1.3506197899,0.6209428356\C,-0.2061508046,1.1726590078,-0.07
87502686\H,-1.8500471283,0.3474617277,-1.3417467163\H,-1.6442585787,2.
1591417008,-1.4718045364\H,-1.9397352006,0.4991851735,1.1539724836\H,-
1.7358899911,2.3141704551,1.0782956281\H,0.4256508503,2.061508169,-0.1
101096825\C,0.6683332374,-0.0721711567,0.0283963548\C,1.4771072247,-0.
056696077,1.3270597095\C,1.5678868427,-0.2105485141,-1.2014553876\H,2.
227351014,0.6643605865,-1.2679716685\H,0.97278919,-0.2615042581,-2.117
189098\H,2.19161259,-1.1069020087,-1.1356991762\H,0.8178870218,0.00101
28082,2.1973494858\H,2.1000481104,-0.9516870795,1.4150609262\H,2.13391
85213,0.8226971176,1.3340927897\C1,-0.395990003,-1.6003565806,0.083173
8899\\Version=IA32L-G03RevC.02\State=1-A\HF=-695.4389179\RMSD=5.525e-0
9\RMSF=4.770e-05\Dipole=0.4836792,0.7557222,-0.028614\PG=C01 [X(C6H11C
11)]\@

n.CC1_CH3_2-CH2CH=CH2

1\1\GINC-LC104\FOpt\RB3LYP\Gen\C6H11Cl1\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH3_
2-CH2CH=CH2.freq\\0,1\C,0.1881508886,0.6584180779,-0.9279613202\C,0.2
276606536,0.3467002497,0.5844202184\H,1.2188125945,0.6134564302,-1.305
5456279\H,-0.1426377133,1.7017005434,-1.0294200516\C,-0.695617031,-0.2
298656765,-1.760723094\C,1.1749859616,1.304493501,1.3068694141\C,-1.16
14999696,0.340330235,1.218843336\C,-1.7267179328,0.1980345108,-2.49042
22489\H,-0.4423869608,-1.2890749111,-1.7575205303\H,-2.3236275015,-0.4
836780312,-3.0904071938\H,-2.0111125425,1.2483059086,-2.5237604789\H,2.
.1778806114,1.2743689385,0.8706893345\H,1.2511426897,1.0530135966,2.36
86223552\H,0.7915742146,2.3294014927,1.2222659977\H,-1.1027453482,0.09
48002633,2.2830652079\H,-1.8216366091,-0.3773050102,0.7261758893\H,-1.
6080493543,1.3381304465,1.118395554\C1,0.9394712057,-1.3653991208,0.79
59577478\\Version=IA32L-G03RevC.02\State=1-A\HF=-695.4488552\RMSD=7.37
8e-09\RMSF=7.191e-06\Dipole=-0.3043338,0.8320854,-0.0832647\PG=C01 [X(
C6H11Cl1)]\@

n.CC1_CH3_2-CH2CH3

1\1\GINC-LC134\FOpt\RB3LYP\Gen\C5H11Cl1\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-CH2CH3.freq\0,1\C,0.4560005632,-0.1246122373,0.1103050686\C,0.4649
560795,-0.1194819845,1.6390128337\C,1.875466099,-0.2188874473,-0.45174
80675\C,-0.4373828916,-1.2250174197,-0.4898365788\C,-1.8963752062,-1.2
6196527,-0.0274564979\H,0.0463118243,-2.1822594952,-0.2438779485\H,-0.
4005413322,-1.133119996,-1.5818464701\H,2.5012440723,0.5976380408,-0.0
801426487\H,1.8709636088,-0.1820450815,-1.5451666771\H,2.3282045879,-1
.1691141433,-0.1404323364\H,-0.5326959875,0.0494985538,2.0509481996\H,
1.1292063877,0.6615752284,2.0201684969\H,0.8298194668,-1.089008638,2.0
028054426\C1,-0.2193183017,1.5283514889,-0.4362789261\H,-2.4352686878,
-2.0566199463,-0.5549455066\H,-1.9829730189,-1.4641456751,1.0454695205
\H,-2.401847656,-0.3145880056,-0.2378988764\Version=IA32L-G03RevC.02\
State=1-A\HF=-657.3715007\RMSD=6.281e-09\RMSF=9.251e-06\Dipole=0.30523
06,-0.8508913,0.2688651\PG=C01 [X(C5H11Cl1)]\@

n.CC1_CH3_2-CH_CH3_2

1\1\GINC-LC83\FOpt\RB3LYP\Gen\C6H13Cl1\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH_CH3_2.freq\0,1\C,-0.432113292,1.863181237,0.3978807981\H,-0.1806
300386,2.1505012414,1.4273108239\H,-1.5174187328,1.7786380301,0.318027
0559\H,-0.1043453113,2.6646830576,-0.2702039349\C,0.277855398,0.551636
2238,0.0482235174\C,1.7909294561,0.7800080519,-0.0219021313\C1,-0.2663
153257,0.1063145576,-1.6844565681\C,-0.1024412809,-0.6042673574,1.0167
904156\C,0.6146174242,-1.9309483857,0.7180038822\C,-1.6160352844,-0.84
43318429,1.138987123\H,2.3222446269,-0.0922528223,-0.4069720084\H,2.17
2645187,1.0039235277,0.9829249379\H,2.0191099649,1.6299999768,-0.67122
62873\H,-1.8058925494,-1.6448107838,1.8625793508\H,-2.0431228561,-1.15
13125585,0.1785875698\H,-2.1559285572,0.0421202835,1.4846382462\H,1.70
39709369,-1.8381307665,0.7561212019\H,0.3387908328,-2.311657215,-0.270
9285912\H,0.3250044352,-2.6827992699,1.4604611497\H,0.2560580724,-0.24
79177411,1.9965405144\Version=IA32L-G03RevC.02\State=1-A\HF=-696.6819
61\RMSD=5.465e-09\RMSF=4.145e-05\Dipole=0.2522146,0.1788418,0.8741676\
PG=C01 [X(C6H13Cl1)]\@

n.CC1_CH3_2-C_CH3_3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C7H15Cl1\CYL509\03-Sep-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH
3_2-C_CH3_3.freq\0,1\C,-0.081620677,-0.1284922714,2.2416550185\C,0.26
25819041,0.4377370051,0.8410351475\C,-0.344140575,1.8543994514,0.74178
72778\C,-0.3125619688,-0.5194188242,-0.2711758023\H,0.322308043,0.5432
403585,3.0074494472\H,0.3587225259,-1.1160799543,2.4127282055\H,-1.161
0560954,-0.1990134701,2.4099463831\C,1.7989227438,0.5619013412,0.74577
72045\C,-1.8420222116,-0.6301578177,-0.2653513825\H,2.1560346671,1.260
3646478,1.5111078528\H,2.1128640011,0.9419641912,-0.2300984355\H,2.303
2386554,-0.3941280507,0.9200099337\H,0.1047766839,2.4972602468,1.50750
19044\H,-1.4255368199,1.8546876028,0.9128526194\H,-0.1515682139,2.3079
656895,-0.234184041\H,-2.3276384078,0.3411823537,-0.3771737796\H,-2.18
49261793,-1.0861098371,0.6702743263\H,-2.1720801987,-1.2687473613,-1.0
893084806\C1,0.1181220224,0.1914349671,-1.9567528513\C,0.3041664692,-1
.923459891,-0.262298444\H,1.389948942,-1.899048863,-0.3731492423\H,-0.
1054733492,-2.5149224339,-1.0856988005\H,0.0603572564,-2.4380635211,0.
6739664621\Version=IA64L-G03RevC.02\State=1-A\HF=-735.9904563\RMSD=3.
480e-09\RMSF=7.203e-06\Dipole=-0.188575,-0.3109366,0.861905\PG=C01 [X(
C7H15Cl1)]\@

n.CC1_CH3_2-CCH

```
1\1\GINC-LC152\FOpt\RB3LYP\Gen\C5H7C11\CYL509\26-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CCH.freq\0,1\C,0.3007747729,-0.0912892995,0.156337345\C,0.498724044
3,-0.0079471487,1.6750642321\C,1.6351856022,-0.1556462117,-0.597235379
4\C,-0.5666520983,-1.2078645069,-0.2048601142\C,-1.2506999233,-2.16228
0598,-0.4850269387\H,-1.8687961141,-2.9935334073,-0.7390061667\H,-0.46
11134446,0.0769548777,2.1895308271\H,1.0028635019,-0.9169877324,2.0226
643601\H,1.11666987,0.8587602188,1.9264189021\H,1.4728089215,-0.174403
7744,-1.6772599717\H,2.2520312566,0.7112100515,-0.3437073119\H,2.16833
30966,-1.0684509674,-0.30761767\C1,-0.5521642044,1.4856833719,-0.37274
69317\Version=IA32L-G03RevC.02\State=1-A\HF=-654.8753908\RMSD=7.168e-
09\RMSF=2.009e-05\Dipole=0.4953616,-0.7024241,0.2938406\PG=C01 [X(C5H7
C11)]\@
```

n.CC1_CH3_2-CH=C_CH3_2

```
1\1\GINC-AC22\FOpt\RB3LYP\Gen\C7H13C11\CYL509\20-Aug-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\CC1_CH3_
2-CH=C_CH3_2.freq\0,1\H,-2.3116802367,-1.351356085,-2.5095158799\C,-2
.5270660552,-0.8932677486,-1.534298085\C,-1.2750875065,-0.8049294754,-
0.6937039685\C,-0.6379077683,-2.1378475572,-0.3878838909\C,-0.81704310
16,0.3961089293,-0.3031992478\C,0.3653530809,0.7559531142,0.5700876851
\C,0.5026596186,2.2781823015,0.6659677676\C,0.3119404009,0.1344483194,
1.9699589722\H,-1.3776596428,1.2670614107,-0.642862797\H,-2.9773988172
,0.0882908929,-1.7104543574\H,-3.2786460337,-1.5323956315,-1.050267175
3\H,-0.5586571034,-2.7339380221,-1.3064901048\H,-1.2671164807,-2.71640
66753,0.303393451\H,0.361848265,-2.0516370508,0.0373872742\H,-0.590095
6533,0.4928630182,2.4810452997\H,1.1862575802,0.4309162594,2.557734392
2\H,0.2695921464,-0.9554404081,1.9354461481\H,0.597360628,2.7274590004
,-0.3268107162\H,1.3774502174,2.5558141801,1.2598982295\H,-0.391813484
6,2.6922233896,1.1489392724\C1,1.9660862708,0.1596857895,-0.2293540255
\Version=IA64L-G03RevC.02\State=1-A\HF=-734.7656665\RMSD=2.895e-09\RM
SF=5.647e-05\Dipole=-0.9248381,0.0377974,0.3132699\PG=C01 [X(C7H13C11)
]\@
```

n.CC1_CH3_2-CH=CH2

```
1\1\GINC-LC91\FOpt\RB3LYP\Gen\C5H9C11\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_2
-CH=CH2.freq\0,1\H,2.1933991482,1.0548354673,-0.3471848306\C,2.223322
3056,0.2585877938,0.3891517669\H,3.1823499992,0.0461694998,0.853173481
3\C,1.140355134,-0.4391465463,0.722311656\C,-0.2741507453,-0.308361277
7,0.2047610841\H,1.2274867123,-1.2303095003,1.4701004135\C,-0.71278425
02,-1.6076191237,-0.4845579344\C,-1.2281341678,0.0667728393,1.34704830
75\H,-0.0581199648,-1.8417439666,-1.3280138945\H,-1.7421064335,-1.5261
04051,-0.8462492022\H,-0.6628722887,-2.4366140767,0.2326023558\H,-0.93
83667088,1.0182175015,1.800485704\H,-1.1943078062,-0.7099754091,2.1213
613985\H,-2.2567384223,0.1459614922,0.9828062243\C1,-0.3907278761,1.03
87153488,-1.0594924077\Version=IA32L-G03RevC.02\State=1-A\HF=-656.132
2134\RMSD=2.881e-09\RMSF=2.137e-05\Dipole=0.0131274,-0.6477005,0.59579
97\PG=C01 [X(C5H9C11)]\@
```

n.CC1_CH3_2-CH=CHCH3

```
1\1\GINC-LC135\FOpt\RB3LYP\Gen\C6H11C11\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3_
2-CH=CHCH3.freq\0,1\H,1.7932487993,0.0003080638,-0.958349261\C,1.791
5441515,0.0001770674,0.1296508183\C,3.1346423732,0.0002398749,0.802191
4416\C,0.6255079923,-0.000025676,0.7758921955\C,-0.7796677615,-0.00011
10418,0.2179270075\H,0.6287539691,-0.0001561019,1.8688999672\C,-1.5298
832928,-1.2668742615,0.6516118605\C,-1.5301619362,1.2663796415,0.65192
53874\H,-1.018293789,-2.1641821933,0.2939045427\H,-2.5539499966,-1.264
```

440962,0.2661897743\H,-1.5727489468,-1.3075673831,1.7473593737\H,-1.01
87696293,2.1638887158,0.2944407319\H,-1.5730371075,1.3067917582,1.7476
829309\H,-2.5542278652,1.2638167293,0.2665021404\Cl,-0.7584111419,0.00
01207923,-1.636030404\H,3.0453577563,0.0001067494,1.8938197204\H,3.722
4744147,-0.8797037256,0.5083376766\H,3.722292648,0.8803712546,0.508537
0054\Version=IA32L-G03RevC.02\State=1-A\HF=-695.4518346\RMSD=7.713e-0
9\RMSF=2.321e-05\Dipole=0.1188932,-0.0000938,0.8532152\PG=C01 [X(C6H11
Cl1)]\@

n.CCl₃CH₃-2-CHO

1\1\GINC-LC99\FOpt\RB3LYP\Gen\C4H7Cl1O1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃CH₃
_2-CHO.freq\0,1\O,0.8624209089,1.5585374315,-1.4500214669\C,0.9553647
296,0.8541847485,-0.473293026\H,1.9256591761,0.6855490339,0.0394692533
\C,-0.2335992708,0.1437116119,0.1791295496\C,-1.5011592201,0.255484135
5,-0.6542718906\C,-0.4036935583,0.64039872,1.6161228918\H,-1.341841727
6,-0.1263834135,-1.6650124139\H,-1.787572784,1.3095994369,-0.733174137
9\H,-2.3178114476,-0.299922731,-0.1852747392\H,0.5299683138,0.56028719
28,2.1813608923\H,-1.1706570712,0.0550370041,2.1314113737\H,-0.7168157
505,1.691516297,1.6036638672\Cl,0.2987192904,-1.6298033863,0.248329558
3\Version=IA32L-G03RevC.02\State=1-A\HF=-692.0560821\RMSD=5.642e-09\R
MSF=1.150e-05\Dipole=-0.4090094,0.255635,0.7654174\PG=C01 [X(C4H7Cl1O1
)]\@

n.CCl₃CH₃-2-CN

1\1\GINC-LC144\FOpt\RB3LYP\Gen\C4H6Cl1N1\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃CH₃
_2-CN.freq\0,1\N,-0.4485430282,-0.3819140365,-2.4427339078\C,-0.3600
063864,-0.1986166461,-1.2999593762\C,-0.3053043056,0.0358993154,0.1501
82196\C,-0.9943764297,-1.1092846239,0.9025487909\C,-0.9006424397,1.407
3946792,0.4920634138\H,-0.9149684454,-0.9384916731,1.9795718128\H,-2.0
536193497,-1.1421509285,0.6244750025\H,-0.5369627964,-2.070806002,0.65
9268213\H,-0.3775490983,2.2062310156,-0.0381926653\H,-1.9578846548,1.4
270489511,0.2052625011\H,-0.8212676549,1.5818436778,1.5685025145\Cl,1.
4802370921,0.0469039333,0.6253670487\Version=IA32L-G03RevC.02\State=1
-A\HF=-670.9724383\RMSD=5.196e-09\RMSF=3.947e-06\Dipole=-0.7429095,0.2
318994,1.2514258\PG=C01 [X(C4H6Cl1N1)]\@

n.CCl₃CH₃-2-COCH₃

1\1\GINC-LC80\FOpt\RB3LYP\Gen\C5H9Cl1O1\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃CH₃
_2-COCH₃.freq\0,1\C,-1.1805037552,0.0711474384,-1.7975608546\C,-1.100
9735284,-0.2294789876,-0.3144224468\C,0.2736602491,-0.2079147727,0.400
6509432\O,-2.085915451,-0.5333515886,0.3288610577\H,-2.1111133055,-0.3
445609177,-2.1894349206\H,-0.3214957812,-0.3195933472,-2.3505704822\H,
-1.1858415523,1.1567780842,-1.9479972293\C,1.0210112321,-1.5110729497,
0.0884326956\C,0.1141502615,0.0109390095,1.9023233978\H,1.0934210528,0.
0168548037,2.3886095121\H,-0.4929098691,-0.7960670014,2.3217341555\H,
-0.3907685029,0.9574344925,2.1106243972\H,2.0014121863,-1.5068083712,0.
5735296472\H,1.1689205978,-1.6504111916,-0.9860190666\H,0.4426228986,
-2.358209868,0.475570056\Cl,1.2775887723,1.1946869175,-0.2766751142\Ver
sion=IA32L-G03RevC.02\State=1-A\HF=-731.3791488\RMSD=4.215e-09\RMSF=
8.367e-06\Dipole=0.3519534,-0.4383668,-0.2380373\PG=C01 [X(C5H9Cl1O1)]
\@

n.CCl₃CH₃-2-CON₂CH₃-2

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H16Cl1N1O1\CYL509\03-Sep-2008\0\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCl₃CH₃
_2-CON₂CH₃-2.freq\0,1\H,2.5766330646,-0.9102403315,2.57581687

84\C,2.1597969663,-1.1335936872,1.5869303544\C,1.5804395218,0.14469460
13,0.9720571316\N,1.0290500839,-0.0454485818,-0.3752821322\C,2.0232864
137,-0.1849149226,-1.4552901697\C,2.3363983271,1.1430743379,-2.1495302
381\C,-0.2796617084,-0.0224510124,-0.7755957674\O,-0.5712717039,-0.135
5000672,-1.966232188\C,-1.4613977846,0.2370682216,0.207182735\C,-1.478
5782639,1.6965195742,0.678882256\H,2.3628028109,0.912706197,0.90063010
24\H,0.810921934,0.5394845456,1.6302419444\H,1.6371937726,-0.903306606
9,-2.1806842541\H,2.9302866172,-0.606681154,-1.0125629434\H,1.38037519
96,-1.8910188855,1.7032285845\H,2.9640944387,-1.554987796,0.9747262337
\H,1.4386952919,1.5361968151,-2.6338961651\H,3.1050688916,0.9961210334
, -2.9170796983\H,2.7093599605,1.8897353468,-1.4384601022\H,-0.58570070
11,1.9776180285,1.24092095\H,-2.3544583501,1.8770794933,1.3088596712\H
, -1.5456131899,2.3451597433,-0.2026888784\Cl,-1.3738972654,-0.87152076
15,1.7005689286\C,-2.7800712065,-0.1141156654,-0.4858620276\H,-2.78159
39369,-1.1515521945,-0.825043699\H,-2.9170782627,0.5260154451,-1.36042
99189\H,-3.6091845784,0.0379751913,0.2109362927\\Version=IA64L-G03RevC
.02\State=1-A\HF=-904.6784924\RMSD=5.382e-09\RMSF=3.101e-06\Dipole=0.7
102357,0.6647818,0.4428593\PG=C01 [X(C8H16Cl1N1O1)]\\@

n.CC1_CH3_2-CON_CH3_2

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C6H12Cl1N1O1\CYL509\03-Sep-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.CC
1_CH3_2-CON_CH3_2.freq\\0,1\C,1.0244243798,0.1417048482,-0.0815241766\
C,-0.3867262166,0.7344010098,0.2148587954\N,-1.4470785131,-0.072210657
6,0.5416657766\O,-0.4941020852,1.9581321491,0.2045900115\C,1.613100873
6,-0.6000168627,1.1236255334\C,1.9613502779,1.2677229302,-0.520693073\
C,-1.4983104789,-1.526302098,0.6076629225\C,-2.7115695298,0.5731250851
,0.8840195744\H,-2.3619049898,-1.882958618,0.0321841857\H,-0.611364181
7,-1.9855666818,0.1841677753\H,-1.6241183771,-1.8607251696,1.647228887
9\H,-3.4937482897,0.2733050506,0.1746729767\H,-3.0262866138,0.27240391
57,1.8918844555\H,-2.5791273559,1.6522230932,0.8478468887\H,2.93941960
26,0.8496835912,-0.7751405975\H,2.0765461296,1.9871388401,0.2945405427
\H,1.559161821,1.8006608704,-1.3831198959\H,2.624846926,-0.9453257372,
0.891719939\H,1.0197767847,-1.4599031442,1.4374843035\H,1.6732000061,0
.0991665763,1.9666254811\Cl,0.9336675868,-1.0296173324,-1.5297748781\\
Version=IA64L-G03RevC.02\State=1-A\HF=-826.0474627\RMSD=8.607e-09\RMSF
=7.566e-06\Dipole=-0.2488647,-0.7872117,0.8406746\PG=C01 [X(C6H12Cl1N1
O1)]\\@

n.CC1_CH3_2-CONH2

1\1\GINC-LC131\FOpt\RB3LYP\Gen\C4H8Cl1N1O1\CYL509\26-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_
CH3_2-CONH2.freq\\0,1\C,0.457037537,-0.0623264816,-0.1575371733\C,-0.9
554108358,0.3950356373,-0.5979611107\N,-1.9633964469,0.3710009495,0.30
52260483\O,-1.0959333053,0.7600934988,-1.7584277359\C,0.8707216119,-1.
2764087546,-0.9924221581\C,1.4315671963,1.107133399,-0.3146725417\H,-1
.8267652978,0.0688087878,1.2575126476\H,-2.8766580267,0.6739842854,-0.
0018703802\H,2.4486118044,0.7911973266,-0.0666092779\H,1.1548957551,1.
9431724934,0.3340792775\H,1.400062005,1.4467779647,-1.3540893845\H,1.8
902242697,-1.5817741372,-0.7412211605\H,0.8242765778,-1.0012302914,-2.
050207363\H,0.1981961741,-2.1220214129,-0.8220196285\Cl,0.4985238384,-
0.5810160267,1.6324013365\\Version=IA32L-G03RevC.02\State=1-A\HF=-747.
4394654\RMSD=6.131e-09\RMSF=5.333e-05\Dipole=-0.2045315,-0.0811875,0.4
508155\PG=C01 [X(C4H8Cl1N1O1)]\\@

n.CC1_CH3_2-CONHCH3

1\1\GINC-LC88\FOpt\RB3LYP\Gen\C5H10Cl1N1O1\CYL509\26-Jun-2008\0\\#B3LY
P/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_
CH3_2-CONHCH3.freq\\0,1\H,-2.9473067316,1.0933826165,-1.8396259325\C,-

2.7496990679,0.2196369538,-1.2080278849\N,-1.5193382193,0.391281269,-0.4552512803\C,-0.4680551531,-0.4494635842,-0.58846389\C,0.8078135091,-0.1935667883,0.2534347682\O,-0.450294851,-1.4192142983,-1.3419285635\C,1.9850984568,0.0643270687,-0.6898592239\C,1.0522233163,-1.3962538399,1.1678314596\H,-1.4362402049,1.161979569,0.1923273304\H,-2.6307001056,-0.6612574713,-1.8400977838\H,-3.6021809418,0.0693276304,-0.5356703144\H,2.9107872658,0.1858510408,-0.1205029302\H,1.8210856514,0.9636547134,-1.2905097644\H,2.0822293237,-0.7921915729,-1.3632130027\H,1.9827262298,-1.267204264,1.7276036572\H,1.1231930546,-2.2937217235,0.5465590581\H,0.2302112731,-1.5271401592,1.8775048523\Cl,0.6435079507,1.3067050743,1.3504894662\\Version=IA32L-G03RevC.02\State=1-A\HF=-786.7509894\RMSD=4.195e-09\RMSF=7.351e-05\Dipole=-0.3250687,0.3874589,0.1413627\PG=C01 [X(C5H10Cl1N1O1)]\\@

n.CC1_CH3_2-COOC_CH3_3

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H15Cl1O2\CYL509\03-Sep-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC1_CH3_2-COOC_CH3_3.freq\\0,1\H,-1.7481005396,-1.7421467001,-3.0893217642\C,-1.610716252,-1.3867693016,-2.0619217375\C,-0.1502424176,-0.9728065685,-1.8579759552\C,0.2498285547,0.2193999811,-2.7319255595\O,0.0836893417,-0.6473006839,-0.4322628111\C,-0.5332387031,0.3747090953,0.1709992383\O,-1.3775015629,1.0940145501,-0.3204393009\C,-0.0495860888,0.5346333943,1.629258521\C,0.7919857602,-2.1569492058,-2.0836348987\C,0.0135990093,-0.8019409011,2.3675113292\H,0.7180496718,-2.5022091773,-3.1201609815\H,0.5329498156,-2.9900940377,-1.4221644773\H,1.829070052,-1.8683749027,-1.8859535821\H,-2.2882260922,-0.5492901144,-1.8883379887\H,-1.8743877156,-2.205210412,-1.3829870619\H,0.1992446448,-0.071221942,-3.7872221304\H,1.2779092575,0.5251300541,-2.5111859253\H,-0.4143906311,1.0704146554,-2.5726615376\H,0.3821468386,-0.6503020192,3.3861065579\H,0.6643110849,-1.5091327498,1.8517841619\H,-0.9943543075,-1.2320149292,2.4254711916\Cl,1.6784195134,1.201937584,1.507681235\C,-0.8980603622,1.5679807993,2.3610197631\H,-0.5035589989,1.7303230409,3.3676953599\H,-1.9280575163,1.2022536072,2.4390408298\H,-0.9166565245,2.5156820118,1.820949044\\Version=IA64L-G03RevC.02\State=1-A\HF=-924.5611097\RMSD=8.022e-09\RMSF=9.502e-06\Dipole=-0.2973498,-0.9000583,-0.163327\PG=C01 [X(C8H15Cl1O2)]\\@

n.CC1_CH3_2-COOCH2CH3

1\1\GINC-LC113\FOpt\RB3LYP\Gen\C6H11Cl1O2\CYL509\26-Jun-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_C H3_2-COOCH2CH3.freq\\0,1\C,-1.2270195874,0.082121297,-0.1769374612\C,0.1168703404,-0.6568785015,-0.3107867421\O,0.2152680912,-1.8533323649,-0.4733408148\O,1.1610463021,0.1840061979,-0.2412984548\C,2.4732133478,-0.4266731314,-0.3125643894\C,3.4981825388,0.6844332436,-0.1932039374\C,-1.2733033728,1.3529970328,-1.0247727988\C,-2.3844902948,-0.8643586955,-0.4726944866\H,2.5594402835,-1.1580860678,0.49696703\H,2.5559149396,-0.9677539722,-1.2605025674\H,3.3898876008,1.4074114947,-1.0080914304\H,4.5078405585,0.2621506072,-0.2395111806\H,3.3890988615,1.2156867206,0.7573991077\H,-2.3357212798,-1.1808816718,-1.5206928322\H,-3.3366940544,-0.3552602036,-0.3013940173\H,-2.3321132802,-1.7570297932,0.1523765659\H,-0.4613196695,2.033337004,-0.7645604428\H,-2.2298629486,1.8634265435,-0.8811482626\H,-1.1798218074,1.0857925531,-2.084937527\Cl,-1.3386989519,0.5809393324,1.6068805063\\Version=IA32L-G03RevC.02\State=1-A\HF=-845.9292036\RMSD=4.965e-09\RMSF=7.982e-06\Dipole=0.4430693,0.4554047,-0.7176712\PG=C01 [X(C6H11Cl1O2)]\\@

n.CC1_CH3_2-COOCH3

1\1\GINC-LC132\FOpt\RB3LYP\Gen\C5H9Cl1O2\CYL509\26-Jun-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CC1_CH

3_2-COOCH3.freq\0,1\C,0.1318295677,-0.1397808408,-0.8416965415\C,0.23
81014076,-0.4513138655,0.661211589\O,1.2420233974,-0.862639253,1.19895
07477\O,-0.9208635283,-0.2266245183,1.3037225362\C,-0.8925333934,-0.45
4430388,2.723704862\H,-1.8982905295,-0.2237512658,3.074814038\C,-1.153
5139054,-0.692465283,-1.4570430933\C,1.3837877226,-0.6139753582,-1.570
3885858\H,-0.6358427815,-1.4947817893,2.9394314958\H,-0.1582179848,0.2
011659756,3.1985909157\H,2.2844088542,-0.1972150057,-1.1170488621\H,1.
3369317406,-0.321067916,-2.622605619\H,1.4474701783,-1.7062918282,-1.5
095384867\H,-1.154944354,-1.786579626,-1.3739302052\H,-1.2036544558,-0
.427303208,-2.5169085319\H,-2.0366858844,-0.303750778,-0.9483226807\C1
,0.0707951688,1.7109105897,-0.9553292775\Version=IA32L-G03RevC.02\Sta
te=1-A\HF=-806.6099792\RMSD=7.515e-09\RMSF=1.039e-05\Dipole=-0.636031,
-0.6379755,0.1032274\PG=C01 [X(C5H9C11O2)]\@

n.CC1_CH3_2-COOH

1\1\GINC-LC81\FOpt\RB3LYP\Gen\C4H7C11O2\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC1_CH3
_2-COOH.freq\0,1\C,-0.065590965,0.0813292258,-0.5096698086\C,-0.28080
96768,0.6532496366,0.8989625221\O,0.2216308311,1.6748897412,1.30756537
96\O,-1.117758256,-0.103334463,1.6409768573\C,0.7080521951,1.072043251
, -1.3716003923\C,-1.3790062615,-0.3630798717,-1.1539382291\H,-1.170712
6772,0.3281346862,2.5144702007\H,1.6433508854,1.3644632963,-0.89182490
05\H,0.1045520259,1.9747951022,-1.5184450721\H,0.9232918925,0.62857272
08,-2.3473038639\H,-1.1823346715,-0.7888143582,-2.1418727293\H,-2.0369
611963,0.5062968456,-1.2764612196\H,-1.8926545944,-1.1048872937,-0.540
6031884\C1,0.9932127049,-1.4201327456,-0.2687542162\Version=IA32L-G03
RevC.02\State=1-A\HF=-767.3025529\RMSD=9.467e-09\RMSF=2.000e-05\Dipole
=-0.7765976,0.1814612,-0.1922883\PG=C01 [X(C4H7C11O2)]\@

n.CC1_CH3_2-COPh

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C10H11C11O1\CYL509\03-Sep-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\n.CC1
_CH3_2-COPh.freq\0,1\C,-3.3187509209,-0.5995181404,-0.2986622683\C,-3
.4508512987,-0.2630576483,1.0511565553\C,-2.3272262817,0.1274740358,1.
780547084\C,-1.0730904986,0.1756674915,1.1723244447\C,-0.9268515409,-0
.165144194,-0.1833535786\C,-2.0703426592,-0.5464855829,-0.9092489889\C
,0.3663360472,-0.1604205697,-0.9493574015\O,0.3486814856,-0.2730393498
, -2.1647929549\C,1.7593549984,-0.1130339762,-0.2568253778\C,1.93196151
36,-1.2343345404,0.7722465145\H,-1.952127104,-0.7993955571,-1.95720704
16\H,-0.221742944,0.5104042337,1.7509051099\H,-2.4249505803,0.40245535
18,2.8270727924\H,-4.1895188116,-0.9018810021,-0.8739129951\H,-4.42548
92279,-0.3012897565,1.5304773083\H,2.9250101416,-1.1733077397,1.227094
0251\H,1.8479378115,-2.2007192432,0.2594863326\H,1.181265046,-1.204268
6972,1.5628441335\C1,1.9087772599,1.5262169737,0.6119080901\C,2.872854
4005,-0.1517050338,-1.3010171232\H,3.8439516706,-0.0592054113,-0.80690
43093\H,2.7600537867,0.6522738438,-2.0297865101\H,2.8365823497,-1.1030
908263,-1.8410218989\Version=IA64L-G03RevC.02\State=1-A\HF=-923.11408
03\RMSD=5.841e-09\RMSF=2.240e-05\Dipole=-0.3831507,-0.7168689,0.702418
2\PG=C01 [X(C10H11C11O1)]\@

n.C_CH3_3-H

1\1\GINC-AC13\FOpt\RB3LYP\Gen\C4H10\CYL509\29-Sep-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\n.C_CH3_3-H
.freq\0,1\C,0.0063830854,0.0152106332,0.3726497867\H,0.0253133966,0.0
601177036,1.4721322164\C,1.4591279253,0.047813066,-0.1230070116\C,-0.7
777424063,1.2344792707,-0.1330015261\H,2.0323251476,-0.8037904495,0.26
28939348\H,1.9687220061,0.966171896,0.1926184388\H,1.4988322803,0.0057
290925,-1.2196035733\H,-0.8279769714,1.2391720815,-1.2299571764\H,-0.3
047367477,2.1725317225,0.1816753703\H,-1.8066516337,1.2334980157,0.246

5084993\C,-0.686328514,-1.2940329969,-0.0313357544\H,-1.7138816534,-1.3365313518,0.3494633319\H,-0.7324975825,-1.390513374,-1.1242126724\H,-0.1480887839,-2.1672051738,0.356648663\\Version=IA64L-G03RevC.02\State=1-A\HF=-158.4588104\RMSE=2.930e-09\RMSE=6.095e-06\Dipole=0.0005697,0.0013688,0.0335115\PG=C01 [X(C4H10)]\\@

n.C_CH3_3-BH2

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H11B1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-BH2.freq\\0,1\H,-1.4862942218,0.6544294458,-1.8689714431\B,-1.391098062,-0.0007490537,-0.8691161045\C,-0.0413930162,-0.0572344829,-0.0735983622\H,-2.3772702464,-0.5321510944,-0.4412116063\C,0.1160075601,-1.3167273644,0.8002119083\C,-0.2103785801,1.1868069495,0.8582554636\H,-0.7548220177,-1.467784825,1.4485630436\H,1.0056434599,-1.2448264395,1.4416267891\H,0.229274995,-2.2174161266,0.1841909769\H,-1.0774192014,1.0942902576,1.5235711057\H,-0.3104128538,2.120958228,0.2922464186\H,0.6816648733,1.2816595874,1.4928996069\C,1.2093632401,0.1434435457,-0.9510353841\H,2.1148080262,0.2348419127,-0.3347125817\H,1.3603228715,-0.7052201086,-1.6296591364\H,1.1283994016,1.0472325441,-1.5659644049\\Version=IA64L-G03RevC.02\State=1-A\HF=-183.8820887\RMSE=6.301e-09\RMSE=2.023e-06\Dipole=0.1870236,0.0513103,0.1596832\PG=C01 [X(C4H11B1)]\\@

n.C_CH3_3-CH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C5H12\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-CH3.freq\\0,1\H,0.8032803202,-1.212418433,-1.6370948177\C,0.7910349383,-1.2061679829,-0.5400787124\H,1.8319490952,-1.1837032858,-0.1941852169\H,0.3477933131,-2.1522573094,-0.205281864\C,-0.0000871037,-0.000017162,-0.0000249344\C,0.6534978016,1.3048489459,-0.4924988548\C,0.0077477207,-0.0287819265,1.5399360696\H,1.6914203865,1.3830520007,-0.1457300396\H,0.1103956286,2.1835564614,-0.1229649219\H,0.6625482579,1.3539241028,-1.5884709275\H,1.0314407715,0.0198862395,1.931522841\H,-0.4525994001,-0.9488475591,1.9209756183\H,-0.5495395666,0.8204285714,1.9545551189\C,-1.4519228545,-0.0698802765,-0.5072340986\H,-2.0423220466,0.778327446,-0.1383848725\H,-1.490442962,-0.0512479023,-1.6037020142\H,-1.945546812,-0.9907099203,-0.1718357201\\Version=IA64L-G03RevC.02\State=1-A\HF=-197.7729783\RMSE=2.415e-09\RMSE=1.019e-04\Dipole=-0.0000435,-0.000066,-0.0000139\PG=C01 [X(C5H12)]\\@

n.C_CH3_3-NH2

1\1\GINC-AC21\FOpt\RB3LYP\Gen\C4H11N1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-NH2.freq\\0,1\H,-1.4176008455,-0.0299580547,-1.50299916\N,-1.4138826382,-0.031575588,-0.4819357992\C,-0.0152979127,-0.0055193505,-0.0017688754\H,-1.879418274,0.8338882373,-0.2047428824\C,0.653210103,-1.305344411,-0.4759598972\C,-0.061675175,0.0318128329,1.5337314996\H,1.6858800883,-1.3720511076,-0.1152117863\H,0.6798884434,-1.3548303708,-1.5723686019\H,0.0962657443,-2.1745652469,-0.1120417932\H,-0.6259958212,-0.8235902235,1.9184333158\H,-0.5513212662,0.9480402187,1.8887620055\H,0.9478850149,0.0083557831,1.9594479919\C,0.7680172573,1.2130875394,-0.5339335917\H,1.8040634027,1.2233799585,-0.1722858404\H,0.7978893163,1.2078905658,-1.6311218388\H,0.2941170284,2.150249691,-0.2147356272\\Version=IA64L-G03RevC.02\State=1-A\HF=-213.803109\RMSE=5.696e-09\RMSE=2.042e-05\Dipole=0.2104756,0.4111022,-0.1986749\PG=C01 [X(C4H11N1)]\\@

n.C_CH3_3-OH

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4H10O1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-OH.freq\\0,1\C,-0.0023387412,0.0046050106,0.0139643451\O,0.0180871281

```
, -0.0360828335, 1.451817302\C, 1.4368581678, -0.0351360072, -0.5222939886\
C, -0.8209274649, -1.1796460328, -0.5226004165\H, 0.4412153031, -0.87057035
57, 1.7106696804\H, -0.8963187964, -1.1545311143, -1.6159835332\H, -1.83233
50174, -1.1615455349, -0.1034539968\H, -0.3534407057, -2.1337526618, -0.244
6556564\H, 2.0200547818, 0.7912728068, -0.1029051683\H, 1.461401973, 0.0406
74937, -1.6156605309\H, 1.9299969343, -0.9762512828, -0.2443831234\C, -0.67
65663443, 1.3347536546, -0.3299090567\H, -0.7450062234, 1.4698687214, -1.41
4721281\H, -1.6869539146, 1.3671891243, 0.0907567772\H, -0.1054650641, 2.16
88482763, 0.0908331165\\Version=IA64L-G03RevC.02\State=1-A\HF=-233.6709
544\RMSD=8.470e-09\RMSF=2.933e-05\Dipole=0.2113698, -0.41669, -0.3674224
\PG=C01 [X(C4H10O1)]\\@
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n.C_CH3_3-F

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1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4H9F1\CYL509\29-Sep-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
F.freq\\0,1\C, 0.0181634023, 0.0393406872, -1.5268775994\C, 0.0007416112, -
0.0016359379, -0.0004996215\C, 1.4065667743, 0.0284969419, 0.5949659963\F,
-0.6422962407, 1.1852869446, 0.4263126991\H, 0.5618465959, 0.9229337042, -1
.8770231248\H, -1.0035646282, 0.0869771189, -1.9176831969\H, 0.5048736215,
-0.8520499117, -1.9377673486\H, 1.9502056638, 0.9108537411, 0.2416273823\H
, 1.9730419959, -0.8646334658, 0.3091027368\H, 1.3555013734, 0.0708431995, 1
.6878978598\C, -0.8310764447, -1.1632594416, 0.5378794871\H, -0.8791125929
, -1.1219239882, 1.6309952464\H, -1.8524823996, -1.1126329268, 0.1466541745
\H, -0.3960155224, -2.1256034709, 0.2465724043\\Version=IA64L-G03RevC.02\
State=1-A\HF=-257.6976136\RMSD=8.648e-09\RMSF=3.254e-05\Dipole=0.30084
67, -0.5553826, -0.1996803\PG=C01 [X(C4H9F1)]\\@
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n.C_CH3_3-SiH3

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1\1\GINC-AC22\FOpt\RB3LYP\Gen\C4H12Si1\CYL509\29-Sep-2008\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-SiH3.freq\\0,1\H, -1.3667677909, -0.000013785, -2.0793331797\Si, -1.4147
61572, -0.0000038751, -0.5891483005\C, 0.3496148164, -0.0000022008, 0.14537
02472\H, -2.169918578, 1.2076136362, -0.1483543098\H, -2.1699246891, -1.207
6130829, -0.1483478656\C, 1.1032007399, -1.2601753115, -0.3287702377\C, 1.1
03179192, 1.2601787941, -0.328783061\H, 2.1211235612, 1.2752199958, 0.08695
68835\H, 0.6036331524, 2.1813967519, -0.0049202993\H, 1.195135924, 1.294688
3252, -1.4212184248\H, 2.121053552, -1.2753093397, 0.0871910814\H, 1.195380
2435, -1.2945888409, -1.4211893892\H, 0.6035392951, -2.1813914368, -0.00508
7752\C, 0.2637199996, 0.0000014025, 1.6863943242\H, 1.2723365491, 0.0000317
04, 2.1243672861\H, -0.2586224889, 0.8863899625, 2.0663499823\H, -0.2585952
101, -0.8863857445, 2.0663945573\\Version=IA64L-G03RevC.02\State=1-A\HF=
-449.1448162\RMSD=3.328e-09\RMSF=4.527e-05\Dipole=0.3050921, 0.0000024,
0.127042\PG=C01 [X(C4H12Si1)]\\@
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n.C_CH3_3-PH2

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1\1\GINC-AC12\FOpt\RB3LYP\Gen\C4H11P1\CYL509\29-Sep-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-PH2.freq\\0,1\H, 0.1471568127, -1.5741795372, -1.5644050222\P, 0.14646775
17, -1.5319017707, -0.1380709096\H, 1.5703576951, -1.5741834123, -0.0546046
292\C, -0.0512596453, 0.3518475972, 0.0483205024\C, 0.2183586775, 0.6982861
006, 1.5252636051\C, -1.5097204394, 0.6982916555, -0.3079703581\H, -1.68789
95559, 1.7727065714, -0.1669106845\H, -2.2210752836, 0.1554331744, 0.324797
8447\H, -1.7372232876, 0.4607603862, -1.354125779\H, 0.0670352803, 1.772700
978, 1.6948128234\H, 1.2492674689, 0.4607505111, 1.8140952098\H, -0.4552807
332, 0.1554277283, 2.1980424538\C, 0.9102704054, 1.1369410916, -0.858053542
3\H, 0.7662063865, 2.2185012526, -0.7222511598\H, 1.9570324434, 0.909203891
6, -0.6271310758\H, 0.7415125116, 0.9092063472, -1.9166175769\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-500.3968035\RMSD=6.329e-09\RMSF=2.197e-05\
Dipole=0.1283181, 0.5039212, -0.1209568\PG=C01 [X(C4H11P1)]\\@
```

n.C_CH3_3-SH

```
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C4H10S1\CYL509\29-Sep-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3_3
-SH.freq\0,1\C,-0.0125962372,0.0251211532,-0.354184934\S,0.0295576162
,-0.0584319526,1.5160428405\C,1.4167697456,-0.0148134073,-0.9123997977
\C,-0.8460025648,-1.1372504082,-0.9115189122\H,0.6290017492,-1.2663422
756,1.6070627587\H,-0.9045843436,-1.0656739513,-2.0060227871\H,-1.8637
142587,-1.1232736857,-0.509945794\H,-0.3952404293,-2.1052038343,-0.664
703897\H,2.0216925226,0.8040025289,-0.5114081929\H,1.3945557936,0.0748
614295,-2.0069164969\H,1.9148155494,-0.9593316226,-0.6656685587\C,-0.6
793576236,1.3690300133,-0.6833256733\H,-0.7414159526,1.4927689332,-1.7
71614758\H,-1.6961061502,1.4206526374,-0.278962531\H,-0.1048062595,2.2
09926976,-0.2799292872\Version=IA64L-G03RevC.02\State=1-A\HF=-556.643
0088\RMSD=3.374e-09\RMSF=1.125e-04\Dipole=0.1141639,-0.2305551,-0.6762
245\PG=C01 [X(C4H10S1)]\@
```

n.C_CH3_3-Cl

```
1\1\GINC-AC12\FOpt\RB3LYP\Gen\C4H9Cl1\CYL509\29-Sep-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3_3
-Cl.freq\0,1\Cl,0.0337617049,0.0847267047,-1.4912397176\C,-0.00834671
1,-0.0209898577,0.3697987367\C,1.4414794545,0.0112477869,0.8522869124\
C,-0.8000413176,1.1874581431,0.8685553953\H,1.9377008016,0.9382150605,
0.5503889555\H,2.0098659051,-0.8331585946,0.4516126895\H,1.4606870902,
-0.0490733996,1.9481493884\H,-0.3217046865,2.1242836186,0.568233841\H,
-0.8496082106,1.1614808595,1.9648078651\H,-1.8218360319,1.1787318479,0
.4780170673\C,-0.6968543933,-1.3378471779,0.7273635861\H,-1.7154534813
,-1.3714170374,0.3299749553\H,-0.1417091616,-2.1936928261,0.3323902637
\H,-0.7493134038,-1.4349368751,1.8194723914\Version=IA64L-G03RevC.02\
State=1-A\HF=-618.0595976\RMSD=1.935e-09\RMSF=3.457e-05\Dipole=-0.0219
984,-0.0544173,0.9598649\PG=C01 [X(C4H9Cl1)]\@
```

n.C_CH3_3-Br

```
1\1\GINC-AC21\FOpt\RB3LYP\Gen\C4H9Br1\CYL509\29-Sep-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3_3
-Br.freq\0,1\Br,0.0158178465,-0.0388078696,-1.181019657\C,-0.01157368
26,0.0283410737,0.8590713009\C,1.4441224858,0.0101535462,1.3188761371\
C,-0.7768161172,-1.2062570411,1.3291291984\H,1.9957481563,0.8732989677
,0.9358515461\H,1.9552941473,-0.9006944888,0.9947047449\H,1.4710175639
,0.045941059,2.4168045148\H,-0.2874078554,-2.1287034291,1.0041788317\H
,-1.8041813866,-1.2072628481,0.9542407201\H,-0.8127424403,-1.205922724
4,2.4273842936\C,-0.7194207153,1.3239998913,1.2469890347\H,-1.74584011
99,1.3480067689,0.8703096198\H,-0.7548946095,1.3957575174,2.3429135879
\H,-0.1884899089,2.2004297915,0.8649061108\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-2731.7451444\RMSD=3.860e-09\RMSF=4.876e-05\Dipole=-0.0139
305,0.0341166,1.0364173\PG=C01 [X(C4H9Br1)]\@
```

n.C_CH3_3-N_CH3_2

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H15N1\CYL509\29-Sep-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3_3
-N_CH3_2.freq\0,1\C,0.8821298687,-1.0285210674,1.4455934849\H,0.98087
77861,-0.8967869224,2.5290679772\H,1.8917461643,-1.0746227953,1.032002
073\H,0.396254244,-2.0091438522,1.2782824275\N,0.1443875044,0.10830446
28,0.9050630368\C,0.0565474397,0.1651760535,-0.5836007749\C,-1.1238041
89,0.2487059716,1.6127231723\C,1.4852344512,0.1658083244,-1.1661455113
\C,-0.6061424031,1.4973483626,-0.9918411686\H,-0.9182815209,0.31246708
94,2.687300692\H,-1.8255568327,-0.5944645936,1.463406346\H,-1.63424245
36,1.1704532634,1.3257636121\H,-0.1184602585,2.3370089369,-0.484680320
1\H,-1.674746648,1.5246903346,-0.7568397427\H,-0.5116362291,1.64458413
```

43,-2.073027526\H,2.099224052,0.9250293085,-0.6694802935\H,1.451052931
5,0.3950246918,-2.2365964759\H,1.9822754519,-0.8036881684,-1.061678785
6\C,-0.7424352419,-1.0093990092,-1.1973097176\H,-0.7770042439,-0.92074
07015,-2.2894125043\H,-0.2847000761,-1.9762933262,-0.9602046345\H,-1.7
766944517,-1.0263604516,-0.8358610121\Version=IA64L-G03RevC.02\State=
1-A\HF=-292.4111143\RMSD=2.422e-09\RMSF=2.958e-05\Dipole=-0.1010927,-0
.1476094,-0.0852576\PG=C01 [X(C6H15N1)]\@

n.C_CH3_3-NHCH3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C5H13N1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.C_CH3_3
-NHCH3.freq\ \0,1\C,0.8780928644,-0.904530112,1.6900275061\H,0.87178055
62,-0.8249775784,2.7824672052\H,1.9141159412,-0.767677316,1.3635365363
\H,0.5771223535,-1.934424377,1.427632509\N,0.0358563917,0.1575447582,1
.1469457078\C,-0.1732503241,0.1902223067,-0.3183352742\C,1.1772783561,
0.430303091,-1.0151726835\C,-1.1002254975,1.3878485314,-0.5878426085\H
, -0.8789956205,0.1075516039,1.5930643455\H,-2.0708607238,1.2516427472,
-0.0925819237\H,-1.2899296269,1.5059553621,-1.660562568\H,-0.652113726
1,2.3104930384,-0.2052413109\H,1.8521853828,-0.4259669945,-0.906923743
4\H,1.6711429649,1.3116700612,-0.5924439092\H,1.028400535,0.5953749771
, -2.0881294626\C,-0.827952883,-1.0968467323,-0.8701828831\H,-1.0028703
242,-1.0192437376,-1.950012992\H,-0.1975297046,-1.9770686256,-0.702624
3705\H,-1.7970978454,-1.2781249767,-0.3877646107\Version=IA64L-G03Rev
C.02\State=1-A\HF=-253.1074575\RMSD=4.505e-09\RMSF=3.796e-06\Dipole=-0
.1920298,-0.2787322,-0.0544474\PG=C01 [X(C5H13N1)]\@

n.C_CH3_3-NHCHO

1\1\GINC-AC2\FOpt\RB3LYP\Gen\C5H11N1O1\CYL509\29-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.C_CH3_
3-NHCHO.freq\ \0,1\H,0.8482056673,0.0061421654,-2.7144068899\C,0.902739
9078,-0.1898277572,-1.6230462008\O,1.8651378569,-0.740154905,-1.109624
6625\N,-0.2095338632,0.2546293349,-0.9808755095\C,-0.475266315,0.15882
03775,0.4748587518\H,-0.9184399453,0.6905290256,-1.5557042865\C,-0.495
2872097,-1.320462961,0.9026581733\C,-1.8528454437,0.7957881594,0.71124
83677\H,-2.6366607958,0.2638451681,0.1577719669\H,-1.861561742,1.84887
41944,0.4036493042\H,-2.1083995306,0.7558219981,1.7746564467\H,0.46848
60119,-1.7899895881,0.6937696763\H,-1.2753392453,-1.8681826084,0.36180
8979\H,-0.7008435585,-1.4003195923,1.9763283707\C,0.6063155705,0.93208
65758,1.2519531432\H,0.4115703165,0.8744662728,2.329055682\H,1.5937703
403,0.510934132,1.0505338423\H,0.6109076092,1.9882863619,0.9596293631\
\Version=IA64L-G03RevC.02\State=1-A\HF=-327.1469338\RMSD=6.898e-09\RMS
F=1.034e-05\Dipole=-1.3086642,0.6447161,-0.0298483\PG=C01 [X(C5H11N1O1
)]\@

n.C_CH3_3-NHCOCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H13N1O1\CYL509\29-Sep-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.C_CH3_
3-NHCOCH3.freq\ \0,1\H,-2.7282169224,0.4929622984,-1.5143700478\C,-2.7
963671047,0.1029828817,-0.4935270538\C,-1.4476097511,-0.1147841486,0.1
861523193\H,-3.3362538853,-0.8487525411,-0.5132612467\H,-3.3856707938,
0.7980652855,0.112498608\N,-0.3576746495,0.2065231308,-0.5706120469\O,
-1.3794646019,-0.5489913525,1.3322209857\C,1.0577954523,0.0886606323,-
0.1485889571\H,-0.5255310925,0.5558800273,-1.5030591363\C,1.3889535601
, -1.3801740634,0.1758232226\C,1.9062416939,0.567260026,-1.3368315068\H
, 1.6814012648,1.6107654219,-1.5908178727\H,1.7320354535,-0.0532091654,
-2.2248914524\H,2.9705414344,0.5053168123,-1.089336448\H,0.7579437383,
-1.7403714078,0.9909026337\H,2.439579307,-1.4736965361,0.4743461527\H,
1.2240627527,-2.0153725109,-0.7021159498\C,1.3171236364,0.9847738936,1
.0770396456\H,2.3670822618,0.9114278931,1.3834172654\H,1.1013168659,2.

0330767651,0.8405226625\H,0.6843240553,0.6778612325,1.9122752554\\Version=IA64L-G03RevC.02\State=1-A\HF=-366.4694952\RMSD=3.353e-09\RMSF=6.131e-06\Dipole=0.2821909,0.4862748,-1.2555462\PG=C01 [X(C6H13N1O1)]\@

n.C_CH3_3-NO2

1\1\GINC-AC15\FOpt\RB3LYP\Gen\C4H9N1O2\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-NO2.freq\\0,1\O,-0.7684965045,-0.0000214459,-1.7173174016\N,-0.8552708274,0.0000118125,-0.4917548617\C,0.4779239254,0.0000066307,0.2987908076\O,-1.9100003272,-0.0000098228,0.1343601137\C,1.2268361064,1.2684771131,-0.1315462712\C,1.2268210288,-1.2684755042,-0.1315385484\H,2.1968012051,1.3018908537,0.3752374351\H,0.6671867513,2.1686243647,0.1445575519\H,1.392618656,1.2743398744,-1.2111359571\H,2.1967856723,-1.3018979633,0.3752454529\H,1.3926036555,-1.2743465057,-1.2111281984\H,0.6671607248,-2.1686143325,0.1445705071\C,0.1676865013,0.0000129944,1.7933918808\H,1.1136985029,0.0000102535,2.3458022185\H,-0.4037907345,0.8849667738,2.0841001026\H,-0.4037993609,-0.8849332602,2.0841060098\\Version=IA64L-G03RevC.02\State=1-A\HF=-362.9615247\RMSD=7.477e-09\RMSF=2.594e-05\Dipole=1.2535969,0.000019,0.7306086\PG=C01 [X(C4H9N1O2)]\@

n.C_CH3_3-OCF3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C5H9F3O1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-OCF3.freq\\0,1\C,-0.5952642849,-0.1173893644,-1.0788487297\O,-0.5910555533,-0.2637594484,0.3964339619\C,0.4650582179,0.0630490566,1.1484851377\F,1.0050781319,1.2728711366,0.8465728255\F,1.4812351355,-0.831754519,1.0627045398\F,0.072920574,0.0988985021,2.4283721732\C,-0.9566455736,1.3327804175,-1.4165003106\C,-1.7147326789,-1.0722351826,-1.496896711\H,-1.863034041,-1.0257329387,-2.5807400604\H,-2.6539864446,-0.8003066221,-1.005518208\H,-1.4661359884,-2.1017274291,-1.2216322531\H,-1.108384026,1.4350475437,-2.4967616467\H,-0.1667696449,2.022991222,-1.1129092077\H,-1.8837409092,1.6194855441,-0.9102413107\C,0.740010861,-0.536045215,-1.7010362244\H,0.6490033529,-0.4908196116,-2.7914929629\H,1.5544844661,0.1291213182,-1.4031702321\H,1.0033438395,-1.559077788,-1.4190706312\\Version=IA64L-G03RevC.02\State=1-A\HF=-570.7173876\RMSD=3.355e-09\RMSF=2.635e-05\Dipole=-0.2860668,-0.0081397,-1.0466315\PG=C01 [X(C5H9F3O1)]\@

n.C_CH3_3-OCH2CH3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H14O1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-OCH2CH3.freq\\0,1\H,-2.2320361387,-0.402658208,-2.9513184052\C,-2.1609693101,-0.2007842315,-1.8765416089\C,-0.7079177044,-0.2230656085,-1.4236988266\O,-0.6951764752,0.0439917002,-0.0300782528\C,0.5723361474,0.0838590028,0.6550489046\C,0.1786560772,0.387092952,2.1055229528\C,1.2886545619,-1.2748647393,0.5752412473\H,-0.26125497,-1.2045354614,-1.6452932972\H,-0.1305176788,0.5317308741,-1.9793790015\H,-2.6096553803,0.7772735829,-1.6745449797\H,-2.7405296819,-0.9589175529,-1.3398224087\H,-0.3587666005,1.3394664628,2.1598093435\H,1.0636526013,0.4470084884,2.7482104049\H,-0.480913665,-0.397763217,2.4899124587\H,1.621226327,-1.5058955293,-0.4424952193\H,0.6203919131,-2.0758041455,0.9098732046\H,2.1761780648,-1.2767316917,1.217914763\C,1.4647593716,1.2087851455,0.1038621331\H,2.3612251745,1.3231870431,0.723545409\H,1.7982686077,1.0057965191,-0.9195305505\H,0.9210283675,2.1597741081,0.1071354874\\Version=IA64L-G03RevC.02\State=1-A\HF=-312.2936952\RMSD=1.721e-09\RMSF=5.131e-07\Dipole=0.3763719,-0.0626682,-0.1836395\PG=C01 [X(C6H14O1)]\@

n.C_CH3_3-OCH3

1\1\GINC-AC12\FOpt\RB3LYP\Gen\C5H12O1\CYL509\29-Sep-2008\0\#B3LYP/GEN

```
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-OCH3.freq\\0,1\\C,-1.212605941,-0.1522518985,-1.6406365535\\O,-1.090421
132,0.106166591,-0.257281843\\C,0.2243504046,0.0333923103,0.330020283\\H
,-0.8999546442,-1.1705972405,-1.9144144134\\H,-2.2756334536,-0.04615767
85,-1.8759227813\\H,-0.650485266,0.5619699406,-2.2600224405\\C,-0.030849
3562,0.3664360873,1.8043774454\\C,0.8096512176,-1.382768908,0.200652819
7\\H,0.901677725,0.3452996683,2.3785666176\\H,-0.727020424,-0.3576666217
,2.2399960845\\H,-0.4756333045,1.3627670618,1.8950931979\\H,1.742571792,
-1.4635718168,0.7695894768\\H,1.0379589209,-1.640727379,-0.8391941883\\H
,0.1028721082,-2.122396169,0.5923339165\\C,1.1663640267,1.0770570812,-0
.2931435409\\H,2.1149337368,1.1099103758,0.2542751445\\H,1.4002567134,0.
8484902015,-1.3385874368\\H,0.7103630423,2.072158896,-0.2510811561\\Ver
sion=IA64L-G03RevC.02\\State=1-A\\HF=-272.9747731\\RMSD=1.784e-09\\RMSF=1.
113e-05\\Dipole=0.3888994,-0.1022902,-0.2312134\\PG=C01 [X(C5H12O1)]\\@
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n.C_CH3_3-OCHO

```
1\\1\\GINC-AC27\\FOpt\\RB3LYP\\Gen\\C5H10O2\\CYL509\\29-Sep-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-OCHO.freq\\0,1\\C,-0.4021669876,0.130139509,-0.5292275694\\O,-0.4104258
369,0.2299197497,0.9481102757\\C,0.6398471541,-0.1521788822,1.683443996
6\\H,0.3937412249,0.017799692,2.7450114933\\O,1.6931355603,-0.6081773966
,1.3038081176\\C,-0.2535699129,-1.3360231269,-0.9475947419\\C,-1.7825271
108,0.6706883042,-0.9076056234\\H,-2.5732630802,0.0631460545,-0.4558492
257\\H,-1.9082456362,0.6509998916,-1.9952722451\\H,-1.9017188315,1.70296
25296,-0.5631435039\\H,0.72482689,-1.7305678043,-0.6682793601\\H,-0.3681
783964,-1.4187693707,-2.0342426017\\H,-1.0307257194,-1.9479358221,-0.47
68900331\\C,0.7094110396,1.0156736396,-1.1010264788\\H,0.6357008954,1.03
35215091,-2.1942123452\\H,0.6039127577,2.0434605339,-0.7370413113\\H,1.6
963070144,0.6416472988,-0.8233655129\\Version=IA64L-G03RevC.02\\State=1
-A\\HF=-347.0142025\\RMSD=8.919e-09\\RMSF=3.857e-06\\Dipole=-0.6835729,0.2
536374,-0.4017595\\PG=C01 [X(C5H10O2)]\\@
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n.C_CH3_3-OCOCH3

```
1\\1\\GINC-AC27\\FOpt\\RB3LYP\\Gen\\C6H12O2\\CYL509\\29-Sep-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-OCOCH3.freq\\0,1\\C,-0.4686196645,0.1189629642,-0.9254354131\\O,-0.4383
895606,0.2031290674,0.5473972584\\C,0.6473212575,-0.1657225246,1.258715
2708\\C,0.3881948748,0.0298870305,2.7384410524\\O,1.6844628623,-0.592692
9472,0.7957802203\\C,-0.3042973929,-1.3380939781,-1.3707385601\\C,-1.870
8267608,0.6342630712,-1.2594241521\\H,1.2712552587,-0.2705404121,3.3035
442125\\H,-0.4756197624,-0.5653952002,3.0521873933\\H,0.1524348175,1.079
0645149,2.9448396495\\H,-2.6354842165,0.0058925879,-0.7912515177\\H,-2.0
28477276,0.6231528577,-2.3431297238\\H,-2.0016060747,1.6602930055,-0.90
04254239\\H,0.6890538788,-1.7165198311,-1.1249051191\\H,-0.4494311298,-1
.4085474884,-2.4547305112\\H,-1.0557858107,-1.9714938496,-0.8864765452\\
C,0.604202111,1.0345050387,-1.5250285128\\H,0.4953130228,1.0613801413,-
2.6152056682\\H,0.4870040839,2.0563479337,-1.1475322612\\H,1.6069102442,
0.6800671685,-1.2815124253\\Version=IA64L-G03RevC.02\\State=1-A\\HF=-386
.3389759\\RMSD=1.348e-09\\RMSF=1.837e-05\\Dipole=-0.6942649,0.2614854,-0.
0641197\\PG=C01 [X(C6H12O2)]\\@
```

n.C_CH3_3-Si_CH3_3

```
1\\1\\GINC-AC27\\FOpt\\RB3LYP\\Gen\\C7H18Si1\\CYL509\\29-Sep-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-Si_CH3_3.freq\\0,1\\H,1.7228665749,-1.4382040395,-1.5957116155\\C,1.75
94012625,-1.4135297527,-0.5001587366\\H,2.8153906465,-1.3473655847,-0.2
101154718\\H,1.3800859673,-2.3747671482,-0.1337430084\\Si,0.7844710522,0
.0531277344,0.2098306021\\C,-1.0759285719,-0.0730119254,-0.2876467733\\C
,0.9652279177,0.0420466143,2.1000173564\\C,1.5410436462,1.6610168714,-0
```

.4596548803\C,-1.2181851029,-0.0611805532,-1.8249593712\C,-1.864274782
 ,1.1204440883,0.293377812\H,2.5987165584,1.7328188689,-0.1771340297\H,
 1.0362308166,2.5493422405,-0.062073675\H,1.4915575544,1.7128818228,-1.
 5536834496\H,2.0231440492,0.1047241591,2.3837927335\H,0.5615928541,-0.
 874701857,2.545749246\H,0.4517288058,0.891515962,2.5655984311\H,-1.491
 6991093,2.0813344965,-0.0820442286\H,-1.8187115595,1.1495267017,1.3889
 053647\H,-2.9261472222,1.0519577583,0.0140594169\H,-0.697379397,-0.905
 5260033,-2.29291028\H,-0.8234108236,0.8614588724,-2.2675552961\H,-2.27
 73910174,-0.1325654989,-2.1134829374\C,-1.6852984318,-1.3827485286,0.2
 57113124\H,-2.7461783061,-1.4590495228,-0.0238662861\H,-1.1795271717,-
 2.2697622932,-0.1434995226\H,-1.635379578,-1.4356281003,1.3515549942\\
 Version=IA64L-G03RevC.02\State=1-A\HF=-567.12298\RMSD=2.633e-09\RMSF=1
 .635e-05\Dipole=0.0631331,0.0042776,0.0168957\PG=C01 [X(C7H18Si1)]\\@

n.C_CH3_3-P_CH3_2

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C6H15P1\CYL509\29-Sep-2008\0\#\B3LYP/GEN
 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
 -P_CH3_2.freq\\0,1\C,1.9075455849,-0.9480678584,0.599811327\H,1.823094
 0795,-1.0022191565,1.6897863383\H,2.9682490226,-0.8102561589,0.3621433
 377\H,1.5813062499,-1.9027095598,0.1715152254\H,0.9694897598,0.5327573
 289,-0.0495529254\C,1.1516426669,0.1968932291,-1.8794385868\C,-0.85338
 58877,0.0645500273,0.2900004096\H,0.5587127185,0.9129399421,-2.4572110
 713\H,0.86596287,-0.8191891988,-2.1746911557\H,2.2020358871,0.35031828
 22,-2.1509247897\C,-1.0582962706,0.1328696561,1.8168479286\C,-1.727173
 6721,1.1460221342,-0.3769570541\H,-1.4500909424,2.1515916367,-0.039753
 7435\H,-2.7840588815,0.9866630203,-0.1237779187\H,-1.6464079215,1.1215
 237682,-1.4698058435\H,-0.7612764933,1.1082378856,2.2194481731\H,-0.48
 41356307,-0.6389721999,2.3422444891\H,-2.1172992252,-0.0232835638,2.06
 30801081\C,-1.2725186524,-1.3225435551,-0.2228021207\H,-2.3296254258,-
 1.5077569768,0.0139658396\H,-1.1643629935,-1.4100424572,-1.3094818338\H,
 -0.6913323241,-2.1265469966,0.241985305\\Version=IA64L-G03RevC.02\St
 ate=1-A\HF=-579.0329591\RMSD=6.095e-09\RMSF=1.504e-05\Dipole=-0.158040
 3,-0.4472829,-0.1583778\PG=C01 [X(C6H15P1)]\\@

n.C_CH3_3-SC_CH3_2CN

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C8H15N1S1\CYL509\29-Sep-2008\0\#\B3LYP/G
 EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3
 _3-SC_CH3_2CN.freq\\0,1\N,-0.3308866566,-1.4703156406,-2.3703223917\C,
 -0.2419009486,-1.4544946517,-1.2114958185\C,-0.1030913073,-1.469428652
 6,0.2495643256\S,-0.5154877468,0.1991311573,1.0048694273\C,0.187285937
 ,1.6084072574,-0.0355328856\C,-0.7415221782,1.9169334215,-1.219926368\
 C,0.1733955348,2.7840977345,0.9588868324\C,1.6199803355,1.3449867622,-
 0.5130922207\C,1.3136005296,-1.945338238,0.6345394003\C,-1.1619998195,
 -2.4293359176,0.8409957695\H,2.0865944616,-1.2874752678,0.2347249381\H
 ,1.4008418286,-1.9620023011,1.7246132707\H,1.487888271,-2.957268121,0.
 2495569187\H,-1.1051720069,-2.4082732433,1.9341301253\H,-0.9646298903,
 -3.4524265587,0.5033323823\H,-2.1711680598,-2.1430252202,0.5364771461\
 H,-1.756864032,2.1339210024,-0.8737332396\H,-0.7889691221,1.0879507667
 ,-1.929521508\H,-0.3673106434,2.7992922386,-1.7565241601\H,-0.83067636
 82,2.9612974301,1.3604560295\H,0.4895031463,3.6970281784,0.4389766333\
 H,0.8553598664,2.6107735516,1.7972917858\H,1.9998556037,2.2445028469,-
 1.0149159869\H,2.2880457506,1.1195082982,0.3242771909\H,1.6662232399,0
 .5273410717,-1.2384298319\\Version=IA64L-G03RevC.02\State=1-A\HF=-766.
 8155045\RMSD=5.196e-09\RMSF=2.125e-05\Dipole=0.4700547,0.1463657,0.909
 0209\PG=C01 [X(C8H15N1S1)]\\@

n.C_CH3_3-SCH2COOCH3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C7H14O2S1\CYL509\29-Sep-2008\0\#\B3LYP/G
 EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3

```
_3-SCH2COOCH3.freq\0,1\S,1.1407748956,0.5756067513,-0.4120343407\C,1.1982494615,0.5177568947,1.4645402579\C,2.6887111499,0.2728126564,1.7577595066\C,0.3503224321,-0.63561517,2.016990676\C,-0.6197478979,0.9324614138,-0.8304329593\C,-1.4479332836,-0.3190836746,-1.0343754987\O,-2.1732953012,-0.8228242888,-0.2018570981\O,-1.2711533817,-0.8187918794,-2.2740369403\C,-1.964842246,-2.0470156872,-2.548700154\H,-0.5869376628,1.5099575239,-1.7575657895\H,-1.0798797508,1.5389795242,-0.0490646625\H,-3.0442645753,-1.9109253106,-2.4415428455\H,-1.635361205,-2.8328658331,-1.8638875733\H,-1.7096352236,-2.3025645938,-3.5773676971\H,2.840224169,0.2143396727,2.8425421164\H,3.0327612105,-0.6693963756,1.3179013785\H,3.3147532112,1.084374203,1.3713175792\H,0.4486752935,-0.6717024955,3.1105045468\H,-0.7093063574,-0.519740394,1.7739099668\H,0.6846334705,-1.5965035608,1.6127543128\C,0.7611975027,1.8597695876,2.0669725373\H,0.8878753805,1.8316935642,3.1571828132\H,1.359385024,2.6870569281,1.6725202244\H,-0.2954745622,2.0740023475,1.8739711939\Version=IA64L-G03RevC.02\State=1-A\HF=-823.8258954\RMSD=3.964e-09\RMSF=5.281e-06\Dipole=-0.0244373,0.0664805,-0.0330379\PG=C01 [X(C7H14O2S1)]\@
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n.C_CH3_3-SCH2Ph

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C11H16S1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C_CH3_3-SCH2Ph.freq\0,1\C,-1.7344607477,-0.9612373528,-0.9900861999\S,-1.5962366928,-0.7546415901,0.8691962779\C,0.1967713771,-0.9184955768,1.277059584\C,-1.0098523449,-2.228834599,-1.4606933636\C,-3.2489189752,-1.1058231539,-1.2213628227\C,1.1129288014,0.2213210478,0.8879962574\H,0.5745385428,-1.8662726975,0.882593343\H,0.1709347887,-1.0251238904,2.3683697474\C,2.2605346422,-0.0258104515,0.1244749201\C,0.8617221546,1.5338378522,1.3133838678\C,3.1364307006,1.0099349359,-0.2111045426\C,1.7347085073,2.5683271742,0.9832343101\C,2.875863517,2.3107726822,0.2178094233\H,3.5545834143,3.1190270507,-0.0410747819\H,1.5247530387,3.5793794653,1.3227491361\H,4.020490187,0.7972792411,-0.8066807587\H,-0.0321369291,1.7414117349,1.8958992785\H,2.4742768154,-1.0397841355,-0.2076216587\H,-3.6477771758,-1.9952431127,-0.7226273261\H,-3.4482315155,-1.1962128898,-2.2965355865\H,-3.7944766925,-0.2303791006,-0.8517670019\H,-1.1962464589,-2.3840207144,-2.5315761526\H,-1.3622468417,-3.113726473,-0.9206931338\H,0.0746738417,-2.1510949061,-1.3299835329\C,-1.2081503317,0.275801372,-1.7335874035\H,-1.3788015196,0.1589331166,-2.8128325325\H,-1.7240124041,1.1822636278,-1.4021310836\H,-0.1359978103,0.4190655449,-1.5759725859\Version=IA64L-G03RevC.02\State=1-A\HF=-827.0044307\RMSD=8.437e-09\RMSF=1.935e-06\Dipole=0.4000259,-0.0686834,-0.4403244\PG=C01 [X(C11H16S1)]\@
```

n.C_CH3_3-SCH3

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H12S1\CYL509\29-Sep-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C_CH3_3-SCH3.freq\0,1\S,0.2883625865,-0.0072932525,-1.2358904639\C,0.2624702567,-0.026872923,0.6349554857\C,1.7438667072,-0.1426203497,1.0302205558\C,-0.5178611703,-1.2414729404,1.1575688699\C,-1.4754824491,0.1295081735,-1.692468251\H,-1.5005856673,0.1448587495,-2.7856557768\H,-1.9258023217,1.0557402817,-1.3245830377\H,-2.058620549,-0.7285240095,-1.3464401898\H,1.834402444,-0.161904178,2.1233969034\H,2.1906389386,-1.0620561215,0.6367120389\H,2.3235451257,0.7084947899,0.6568811427\H,-0.4712800082,-1.2724811184,2.2544294579\H,-1.5760283222,-1.1974590463,0.8779319622\H,-0.0997309555,-2.1757352674,0.7698891438\C,-0.3286961629,1.2783387896,1.1865073536\H,-0.2805543329,1.2766997153,2.2837330418\H,0.2253404302,2.14822849,0.8200490371\H,-1.3809092561,1.3995452547,0.9071996143\Version=IA64L-G03RevC.02\State=1-A\HF=-595.9558923\RMSD=2.892e-09\RMSF=6.796e-06\Dipole=-0.4712942,0.0297771,0.4659475\PG=C01 [X(C5H12S1)]\@
```

n.C_CH3_3-SO2CH3

```
1\1\GINC-AC14\FOpt\RB3LYP\Gen\C5H12O2S1\CYL509\29-Sep-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3
_3-SO2CH3.freq\0,1\C,-0.0681820292,0.017275387,-1.0173034083\S,-0.098
7734778,-0.0026854853,0.8501690543\C,1.6268241644,-0.1393648478,1.3973
533624\O,-0.5904988879,1.3113575041,1.3059831025\O,-0.7828040046,-1.23
85514205,1.2756030117\H,2.062840948,-1.0732169159,1.0396903853\H,1.573
8119215,-0.1476000077,2.4886108374\H,2.1989949743,0.726032058,1.059958
0997\C,0.5350141396,-1.2988001886,-1.5237214739\C,-1.5477712068,0.1340
722337,-1.4216457061\H,-1.6154960416,0.1522427239,-2.515332462\H,-1.99
15216778,1.0535965027,-1.0299618246\H,-2.1256013997,-0.7172229458,-1.0
51132691\H,1.5992886269,-1.3876279166,-1.2791178367\H,0.4473099618,-1.
3336527922,-2.615982981\H,0.0061372572,-2.1609712954,-1.1084587361\C,0
.7271105871,1.2391775783,-1.4935500287\H,0.647610697,1.3126232237,-2.5
845261802\H,0.3332390688,2.1610601844,-1.0570969908\H,1.7922105182,1.1
610953008,-1.248839874\#Version=IA64L-G03RevC.02\State=1-A\HF=-746.346
6439\RMSD=1.864e-09\RMSF=3.894e-06\Dipole=1.3263888,-0.0854358,-1.2222
603\PG=C01 [X(C5H12O2S1)]\@
```

n.C_CH3_3-SOCH3

```
1\1\GINC-AC15\FOpt\RB3LYP\Gen\C5H12O1S1\CYL509\29-Sep-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.C_CH3
_3-SOCH3.freq\0,1\C,-0.5163972835,-0.1989590747,-0.8622609648\S,-0.45
44352166,-0.1614191295,0.9969171355\O,1.2210139799,-0.1508041434,1.283
8602495\C,1.7282669953,1.1024907884,1.75237587\C,0.188186779,-1.464869
5034,-1.3690562694\H,2.8034449746,0.950029239,1.890156177\H,1.27904100
96,1.3836466816,2.7127038216\H,1.5617846537,1.9104116333,1.0303145377\
C,-2.0210803063,-0.2395747213,-1.1755334661\H,-2.1635460934,-0.2972537
134,-2.2614790976\H,-2.5338850263,0.6600863143,-0.8169431625\H,-2.5033
110566,-1.116256352,-0.7285186067\H,1.2317915287,-1.482758397,-1.04058
53052\H,0.1727161687,-1.492264836,-2.4668264083\H,-0.3040714719,-2.367
5564705,-0.9936798807\C,0.1319738229,1.0565757432,-1.4598593439\H,0.05
80553942,1.0312362742,-2.5552713194\H,-0.3592236232,1.9680205635,-1.10
39751821\H,1.1943551241,1.1078188899,-1.2014466919\#Version=IA64L-G03R
evC.02\State=1-A\HF=-671.1425628\RMSD=4.990e-09\RMSF=2.685e-05\Dipole=
0.0193522,0.4978831,-0.4977765\PG=C01 [X(C5H12O1S1)]\@
```

n.C_CH3_3-Ph

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H14\CYL509\30-Sep-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\#n.C_CH3_3-
Ph.freq\0,1\H,0.1300764159,0.0003538242,-3.9955372506\C,0.1026929396,
0.000248957,-2.9091169607\C,1.2847085029,0.0008633436,-2.1721579671\C,
1.2477841667,0.0007345032,-0.774703427\C,0.0323732306,-0.0000345764,-0
.0763766214\C,-1.1488348356,-0.0005968838,-0.8392154755\C,-1.118759552
4,-0.0004712965,-2.2322709637\H,2.2453912529,0.0014565961,-2.681225687
5\C,-0.0482605538,-0.000132248,1.4617451251\C,-0.8068224868,1.26144205
95,1.9383239832\C,-0.8053231691,-1.2626284671,1.9382740657\H,-2.113565
9596,-0.0011400793,-0.3388360749\H,2.1873960918,0.0012515599,-0.233144
5121\H,-2.0519882808,-0.0009327303,-2.7900360524\H,-0.8788982287,1.273
2039989,3.03292121\H,-1.8249540593,1.3011041745,1.5372635479\H,-0.2877
824198,2.1733862958,1.6218307527\H,-0.8773912447,-1.2745120415,3.03287
03251\H,-0.2851927065,-2.1739425884,1.6217559577\H,-1.8234045236,-1.30
34965752,1.537212082\C,1.3432336483,0.0006772133,2.1226339891\H,1.2337
292155,0.0007816295,3.2130562313\H,1.9253714325,-0.8868686042,1.849659
9312\H,1.9244616721,0.8887389101,1.8493950534\#Version=IA64L-G03RevC.0
2\State=1-A\HF=-389.5035789\RMSD=2.223e-09\RMSF=2.015e-06\Dipole=-0.00
9388,0.0000154,0.1191215\PG=C01 [X(C10H14)]\@
```

n.C_CH3_3-C6H4CN

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C11H13N1\CYL509\29-Sep-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-C6H4CN.freq\\0,1\N,0.0789403735,0.000356855,-4.8007052211\C,0.052819
3311,0.0002388961,-3.6373921791\C,0.0217631857,0.0000986366,-2.2043706
898\C,-1.2010715247,-0.0054079608,-1.5197657402\C,-1.2228354145,-0.005
506366,-0.1264789705\C,-0.0403248118,-0.0001817633,0.6278109368\C,1.17
66076794,0.005298263,-0.0792041111\C,1.2181310514,0.0054856432,-1.4672
374314\H,-2.1305958699,-0.0095934276,-2.0803497823\C,-0.031744286,-0.0
001435703,2.1662762193\C,0.6990363279,1.2662675723,2.6737178733\C,0.71
04117092,-1.2599224031,2.6737171429\H,2.1165311927,0.0095305619,0.4644
202054\H,-2.186385936,-0.0098453575,0.3695184471\H,2.1701213782,0.0097
725868,-1.9887001155\H,0.7299751082,-1.2709447105,3.7699903568\H,1.746
9971659,-1.2941230322,2.3226431396\H,0.2110561001,-2.1741337427,2.3335
795867\H,0.718499672,1.2774649823,3.7699910937\H,0.1914677856,2.175944
95,2.3335808445\H,1.735271744,1.309802274,2.3226438925\C,-1.4528445603
, -0.0065429273,2.7608471943\H,-1.3927047689,-0.0062724354,3.8546366855
\H,-2.025254122,0.8791909982,2.4627306203\H,-2.0172541886,-0.897395753
8,2.4627301066\\Version=IA64L-G03RevC.02\State=1-A'\HF=-481.7481928\RM
SD=3.488e-09\RMSF=3.221e-05\Dipole=-0.0353158,-0.0001596,2.0870149\PG=
CS [SG(C9H5N1),X(C2H8)]\\@

n.C_CH3_3-C6H4NO2

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H13N1O2\CYL509\29-Sep-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH
3_3-C6H4NO2.freq\\0,1\O,-2.8083162303,0.0000052652,-2.8099171083\N,-2.
8450337138,-0.0000707482,-1.5788545388\C,-1.5659816772,-0.0000540023,-
0.857448013\O,-3.8800658035,0.0003438027,-0.9115558956\C,-0.3745824386
, -0.0002374331,-1.581347704\C,0.828626062,-0.0002228389,-0.8868109861\
C,0.8747511861,-0.0000268832,0.520756332\C,-0.3487462695,0.000155669,1
.2089078258\C,-1.5678348924,0.0001448221,0.5331439505\H,-2.510363942,0
.0002856042,1.0668750984\C,2.2340966101,-0.0000208113,1.2406639503\C,3
.0289409583,-1.2635534953,0.8311402277\C,3.0291180628,1.2632853892,0.8
307853443\H,1.7520109727,-0.0003681558,-1.4576000787\H,-0.3656156466,0
.0003100604,2.292244252\H,-0.4062203889,-0.000388728,-2.6639798401\H,4
.0032420925,1.2749787708,1.3338081519\H,2.4907685726,2.175356032,1.112
0390878\H,3.2117120602,1.3011561896,-0.2480895107\H,4.0030636324,-1.27
52417647,1.334165765\H,3.2115289145,-1.3017532249,-0.2477240782\H,2.49
04639541,-2.1754696509,1.1126507303\C,2.0867102769,0.0002048846,2.7740
567309\H,3.0793791321,0.0002003626,3.2372340592\H,1.5559300683,0.88867
56982,3.1344033519\H,1.5558055746,-0.8880903036,3.1346528641\\Version=
IA64L-G03RevC.02\State=1-A'\HF=-594.006674\RMSD=4.070e-09\RMSF=1.427e-0
5\Dipole=1.8626701,-0.0002273,1.0388973\PG=C01 [X(C10H13N1O2)]\\@

n.C_CH3_3-C6H4OCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C11H16O1\CYL509\29-Sep-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-C6H4OCH3.freq\\0,1\C,-1.8562953224,0.,-0.4163759676\C,-1.8244183425,
0.,0.9821903631\C,-0.5856891039,0.,1.6328593695\C,0.5896189391,0.,0.87
92785717\C,0.5856982384,0.,-0.5223107703\C,-0.6720551727,0.,-1.1473439
003\C,1.9136467893,0.,-1.3014902436\O,-3.0385971025,0.,1.6114890562\C,
-3.0558406031,0.,3.02861032\C,2.7306619491,-1.26143696,-0.9339161059\C
,2.7306619491,1.26143696,-0.9339161059\H,-0.7436460791,0.,-2.229519225
5\H,1.5346936997,0.,1.4161230462\H,-0.5213823426,0.,2.7153085822\H,-2.
821204461,0.,-0.9143963545\H,-2.568758212,-0.8943818999,3.440277388\H,
-4.1090220986,0.,3.316354036\H,-2.568758212,0.8943818999,3.440277388\H
,3.684044612,-1.2734299954,-1.4768386336\H,2.1801777015,-2.1731663163,
-1.19261514\H,2.9571069534,-1.3016338942,0.1369020174\H,3.684044612,1.
2734299954,-1.4768386336\H,2.9571069534,1.3016338942,0.1369020174\H,2.

1801777015,2.1731663163,-1.19261514\C,1.6953520612,0.,-2.8264214337\H,
2.6643643151,0.,-3.3384326666\H,1.1458916938,-0.8877811704,-3.15989285
65\H,1.1458916938,0.8877811704,-3.1598928565\\Version=IA64L-G03RevC.02
\State=1-A'\HF=-504.0257884\RMSD=5.749e-09\RMSF=1.175e-05\Dipole=0.159
0394,0.,0.4559783\PG=CS [SG(C9H6O1),X(C2H10)]\\@

n.C_CH3_3-C6H4OH

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C10H14O1\CYL509\29-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-C6H4OH.freq\\0,1\C,-2.1290106934,-0.0000156151,-0.1998869208\C,-2.17
77745968,-0.0000205291,1.1980679354\C,-0.9857064682,-0.0000137608,1.92
20119553\C,0.2412659131,-0.0000023484,1.2527459733\C,0.3204212099,0.00
00024176,-0.1447498334\C,-0.8990099796,-0.0000043281,-0.8473110061\C,1
.654526169,0.0000155157,-0.9126821478\O,-3.4124421714,-0.0000316915,1.
7907620482\C,1.7392752822,-1.2615302168,-1.8044766729\C,1.7392542053,1
.2615679199,-1.8044692387\H,-0.8942687353,-0.0000004834,-1.9340355387\
H,1.1450125392,0.0000027557,1.8521751369\H,-1.0085588729,-0.0000173177
,3.0109080867\H,-3.0593501996,-0.0000207206,-0.7595602445\H,-3.2960807
02,-0.0000339737,2.7535089028\H,2.6825385614,1.273067006,-2.3646547854
\H,1.6923257706,2.1732852849,-1.1980196642\H,0.9207036782,1.302345674,
-2.5308905598\H,2.6825603722,-1.2730107233,-2.3646613917\H,0.920726226
2,-1.302316983,-2.5308990802\H,1.692361115,-2.17325195,-1.1980325581\C
,2.8713252174,0.000022755,0.0317893316\H,3.7960173754,0.0000315654,-0.
5564265476\H,2.8890693584,0.8879891804,0.6741300457\H,2.8890833311,-0.
8879466421,0.6741255577\\Version=IA64L-G03RevC.02\State=1-A'\HF=-464.71
94905\RMSD=2.454e-09\RMSF=1.210e-05\Dipole=0.3156751,0.0000012,0.41923
76\PG=C01 [X(C10H14O1)]\\@

n.C_CH3_3-CF2CF3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H9F5\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CF2CF3.freq\\0,1\F,-0.2573804033,0.3529806868,-1.6977799118\C,-0.21180
00756,0.3855973573,-0.3278502867\C,1.2984250607,0.4444539305,0.0173113
124\C,-1.092502184,-0.7459730653,0.2492822985\F,-0.7085092571,1.602276
1223,0.063308201\F,1.9422177108,-0.6615833281,-0.3978841192\F,1.496385
1492,0.5745758934,1.3417443526\F,1.8567695122,1.5007592116,-0.59026021
94\C,-2.5232175484,-0.5068203984,-0.287023542\C,-0.5976523257,-2.12593
02697,-0.2293861059\H,-0.5124905905,-2.1615731804,-1.3196731769\H,-1.3
195254869,-2.8894633668,0.0793639785\H,0.3724503721,-2.3898229474,0.19
90668758\H,-2.5512694195,-0.5425312351,-1.379690025\H,-2.9138193311,0.
4622904948,0.0357871086\H,-3.1861884812,-1.2883578427,0.0979137348\C,-
1.1153149645,-0.6928011803,1.7904474932\H,-1.8526144133,-1.4131999307,
2.1603409106\H,-0.1474857639,-0.9496905503,2.2282594728\H,-1.402029066
,0.3001130387,2.1497893743\\Version=IA64L-G03RevC.02\State=1-A'\HF=-733
.2754183\RMSD=3.153e-09\RMSF=1.234e-05\Dipole=-0.5194906,-0.6221257,0.
3081053\PG=C01 [X(C6H9F5)]\\@

n.C_CH3_3-CF2H

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C5H10F2\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CF2H.freq\\0,1\C,0.105547363,-0.2016105776,-0.9504100741\C,0.07124048
41,-0.1360795263,0.5771220807\C,1.5212410919,-0.1840248948,1.093390748
2\H,0.5835081368,-1.1145840994,-1.3277189516\F,0.7898060619,0.86945456
37,-1.4684714067\F,-1.164528708,-0.1536806496,-1.4684714067\C,-0.71552
06421,-1.3550165432,1.0933907482\H,-0.2474221298,-2.2967740918,0.77980
55749\H,-1.7450229874,-1.3476554483,0.7226182587\H,-0.7454381852,-1.34
82270089,2.1884590204\H,2.028475948,-1.1052937472,0.7798055749\H,1.532
7074489,-0.1555700214,2.1884590204\H,2.1017684641,0.666220502,0.722618
2587\C,-0.6128969826,1.1707210034,1.017236575\H,-0.644566649,1.2312146

013,2.1107028428\H,-0.0695574668,2.0433631034,0.6416776266\H,-1.639616
6505,1.2214042136,0.6416776266\\Version=IA64L-G03RevC.02\State=1-A'\HF
=-396.246391\RMSE=4.518e-09\RMSE=3.253e-05\Dipole=0.2115788,-0.4041458
,0.5808209\PG=CS [SG(C3H2),X(C2H8F2)]\\@

n.C_CH3_3-CF3

1\1\GINC-AC13\FOpt\RB3LYP\Gen\C5H9F3\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CF3.freq\0,1\F,0.3672447,0.6717887214,-1.6253953104\C,0.366378044,0.6
296956996,-0.271428219\F,1.6613773026,0.672802198,0.1236996355\C,-0.35
51004293,-0.6107326032,0.2630845706\F,-0.2128145087,1.7770597134,0.156
4440572\C,-1.8145229488,-0.5818369013,-0.2299124337\C,-0.3107122622,-0
.5805705365,1.8028581393\H,-1.8644793939,-0.5912082689,-1.3231861445\H
, -2.3371642609,0.3099225564,0.1296965394\H,-2.3466508173,-1.4631157153
,0.1433825143\H,0.7200999609,-0.5890138073,2.1705216156\H,-0.822817617
6,-1.4618536501,2.2031643179\H,-0.8080689245,0.3111957985,2.1966911693
\C,0.3637792221,-1.8655085829,-0.2679620174\H,-0.1396756343,-2.7637175
434,0.1049223279\H,0.3513657754,-1.8970606395,-1.3619020819\H,1.406193
7113,-1.8962868799,0.0641340632\\Version=IA64L-G03RevC.02\State=1-A'\HF
=-495.4995758\RMSE=8.311e-09\RMSE=2.870e-05\Dipole=-0.3852156,-0.66246
57,0.2853819\PG=C01 [X(C5H9F3)]\\@

n.C_CH3_3-CCl2H

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C5H10Cl2\CYL509\29-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CCl2H.freq\0,1\C,0.3207567265,0.0014257664,-0.5635296189\C,0.340649
8023,-0.0633628652,0.9826696623\H,1.3334370279,-0.050919825,-0.9614936
854\C1,-0.3647959618,1.5528328936,-1.20947325\C1,-0.5638969118,-1.3857
137809,-1.3300261817\C,1.1964222358,1.1138725622,1.5009170664\C,-1.072
2123416,0.0077508816,1.5846946263\H,2.2010992306,1.1055821592,1.060635
9069\H,1.3089593138,1.0288459392,2.5872002024\H,0.7354490339,2.0802897
67,1.281798894\H,-1.0083665314,-0.0417207952,2.6772808207\H,-1.6939064
18,-0.8256769232,1.2438360661\H,-1.5738726506,0.942603632,1.3169481481
\C,1.0268183909,-1.3836393389,1.3984691246\H,1.1442128002,-1.403167859
8,2.4873758776\H,0.4405289726,-2.2577691651,1.1042178845\H,2.025629188
, -1.4753738813,0.9543650606\\Version=IA64L-G03RevC.02\State=1-A'\HF=-11
16.9556593\RMSE=1.986e-09\RMSE=1.138e-05\Dipole=0.5752525,-0.0713905,0
.7920093\PG=C01 [X(C5H10Cl2)]\\@

n.C_CH3_3-CCl3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H9Cl3\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CCl3.freq\0,1\C,0.0212660928,-0.0000028955,-0.3679592796\C,-0.069105
9476,-0.0000114511,1.1981271596\C1,1.7431112078,-0.0003527694,-0.94032
4022\C1,-0.7814578829,1.460508588,-1.0859070134\C1,-0.7820866531,-1.46
01339995,-1.0859812084\C,0.6248582168,1.2568932662,1.7670285364\C,0.62
49582044,-1.2568582113,1.7670394275\H,1.685781606,1.2901062158,1.50590
08153\H,0.5470763116,1.2321833305,2.8590119457\H,0.1513515346,2.177659
9468,1.4165950182\H,1.6858787362,-1.2900055079,1.505897295\H,0.1515072
363,-2.1776642336,1.4166309369\H,0.5471923456,-1.2321355788,2.85902349
99\C,-1.5484786382,-0.0000668273,1.6413136606\H,-1.5830185797,-0.00004
44104,2.7357862245\H,-2.079734303,0.8873579541,1.287713515\H,-2.079655
8783,-0.8875519266,1.2877518688\\Version=IA64L-G03RevC.02\State=1-A'\HF
=-1576.5349695\RMSE=5.601e-09\RMSE=7.591e-06\Dipole=-0.0557678,-0.0000
067,0.9699653\PG=C01 [X(C5H9Cl3)]\\@

n.C_CH3_3-CH2Cl

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C5H11Cl1\CYL509\29-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-

3-CH2Cl.freq\0,1\C,-0.4730457469,-0.0001343218,-0.6265361562\C,-0.417
7011257,-0.0001400342,0.9108173594\C,1.267801116,0.0003509959,1.61212
89726\C,0.1941945345,1.2624827807,-1.1996673888\C,0.1947782625,-1.2624
230885,-1.1997123769\H,-0.9029426715,-0.8894837903,1.3198052521\H,-0.9
03452448,0.888916235,1.3198250745\H,1.2593039527,-1.2976663585,-0.9489
002354\H,0.1019456727,-1.280232816,-2.2917886958\H,-0.275661321,-2.172
9570979,-0.8083982453\H,1.2586973581,1.2982240246,-0.9488252492\H,-0.2
766876419,2.172784865,-0.8083459743\H,0.1013831151,1.280271462,-2.2917
457411\C,-1.9734519706,-0.0004751597,-0.9947236979\H,-2.0948484759,-0.
0004707877,-2.08396027\H,-2.4842913614,-0.8882823964,-0.6024888258\H,-
2.4847088745,0.8870686717,-0.6024360613\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-657.3677435\RMSD=5.885e-09\RMSF=1.633e-05\Dipole=-0.7463649,
-0.0002128,-0.4763938\PG=C01 [X(C5H11C11)]\@

n.C_CH3_3-CH2F

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H11F1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C_CH3_3
-CH2F.freq\0,1\C,-0.2053040599,-0.0116094456,-0.3372808663\C,-0.23237
31084,0.0362202371,1.1933677013\F,1.0650463109,0.0594131572,1.70849506
31\C,0.5199674906,1.2370179938,-0.8714095854\C,-1.6607550579,-0.035290
4556,-0.8371999406\H,-0.7391248237,-0.8467846706,1.6049986511\H,-0.748
8393631,0.9376419023,1.5492707766\H,-2.2007784225,-0.9144226302,-0.463
7602098\H,-1.6887991067,-0.0698550304,-1.9323303971\H,-2.2105923409,0.
859581407,-0.5195867795\H,1.5379763552,1.2932327458,-0.4735906089\H,-0.
0069269835,2.1551587966,-0.5824008768\H,0.5795250756,1.2151429087,-1.
9657806305\C,0.5335782009,-1.283618573,-0.7923401611\H,0.5929962481,-1.
3298065566,-1.8859290981\H,1.5520540658,-1.3037019385,-0.3923312967\H
,0.0164117056,-2.1872238883,-0.4458379859\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-297.0008223\RMSD=4.183e-09\RMSF=2.414e-05\Dipole=-0.531818
4,-0.0129006,-0.3193447\PG=C01 [X(C5H11F1)]\@

n.C_CH3_3-CH2OH

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H12O1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C_CH3_3
-CH2OH.freq\0,1\C,-0.2062935281,-0.0199543219,-0.3501238961\C,-0.2354
78727,0.0212067391,1.1866371052\O,1.0972490784,0.1009735211,1.68540833
51\C,0.4568281702,1.2609580927,-0.8899241097\C,-1.6591627197,-0.106061
8138,-0.8519626325\H,-0.7400874931,-0.8843175522,1.5640280447\H,-0.828
1433351,0.8918665855,1.5148142392\H,1.052127269,0.1279855031,2.6524098
794\H,-2.1595831086,-1.0092178594,-0.4803238375\H,-1.6873215827,-0.138
2447885,-1.9474552932\H,-2.2474156186,0.7625973834,-0.5300888231\H,1.4
786908662,1.3600144297,-0.5124437824\H,-0.1042159144,2.1536545687,-0.5
850854079\H,0.4928060791,1.2469642889,-1.9859927984\C,0.5819284794,-1.
2567613352,-0.8200486568\H,0.6202431923,-1.2994074407,-1.9153048118\H,
1.6072691577,-1.2335293002,-0.4396782993\H,0.1107078125,-2.1824781529,
-0.4656126514\Version=IA64L-G03RevC.02\State=1-A\HF=-272.9764229\RMSD
=2.915e-09\RMSF=6.180e-06\Dipole=-0.3951873,-0.0064022,0.4183739\PG=C0
1 [X(C5H12O1)]\@

n.C_CH3_3-CH2Ph

1\1\GINC-AC13\FOpt\RB3LYP\Gen\C11H16\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C_CH3_3-
CH2Ph.freq\0,1\C,-1.3402214919,0.0015123105,-1.4110119076\C,-1.301952
4254,0.1158467203,0.1468115117\C,0.0599758016,0.0561046076,0.808599738
8\C,0.610593629,-1.1660371629,1.2225263915\C,0.8031625523,1.2229211716
,1.0418578815\C,1.8647904242,-1.2245462674,1.8317428742\C,2.057905155,
1.1713032524,1.6505603602\C,2.595437943,-0.0546886792,2.0459288134\H,3
.5704895638,-0.097120525,2.5240254981\H,2.2677103386,-2.184276017,2.14
54321506\H,2.612273103,2.090563827,1.8222063325\H,0.0443793026,-2.0824

112084,1.0722902842\H,0.3883201376,2.1849065966,0.7496378715\H,-1.7904
266935,1.0600140526,0.4232277376\H,-1.9309236725,-0.6868873506,0.55482
07344\C,-2.8165064681,0.0879070811,-1.8453675544\C,-0.7567312477,-1.34
4981602,-1.8766345292\H,-3.2674433045,1.0393372983,-1.5367970643\H,-3.
4096102845,-0.7227065884,-1.4039017048\H,-2.9086132317,0.013101797,-2.
9357545884\H,0.2970439856,-1.4464416644,-1.596616288\H,-0.8240014824,-
1.4364884009,-2.9676400169\H,-1.3050078262,-2.1890293636,-1.4388875355
\C,-0.5551513967,1.1531981157,-2.0648829597\H,-0.6210111672,1.09143487
54,-3.1580580592\H,-0.9558161186,2.1295455953,-1.763428659\H,0.5048224
986,1.1252197903,-1.7913404152\\Version=IA64L-G03RevC.02\State=1-A\HF=
-428.8204531\RMSD=3.069e-09\RMSF=3.995e-06\Dipole=-0.0511824,0.0005266
,-0.0478613\PG=C01 [X(C11H16)]\@

n.C_CH3_3-CH_CH2_2

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C7H14\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H_CH2_2.freq\0,1\C,-1.6098352715,1.0250281331,-0.7563052593\C,-1.6103
488803,1.0245683814,0.7557922532\C,-0.3092373098,0.9019072826,0.000148
0839\H,-2.0092225719,0.1477225995,-1.2575258476\H,-1.8160882128,1.9570
728069,-1.2761998321\H,-2.0100661735,0.14694687,1.2561981481\H,-1.8169
65401,1.9562869684,1.2761259344\H,0.292247802,1.8119723021,0.000627051
7\C,0.5757727326,-0.3527446528,0.0000955973\C,1.465680139,-0.315120095
7,1.2597108996\C,1.4668427674,-0.3141925645,-1.25867155\H,2.0752031963
,0.5984264251,-1.2843779056\H,0.8593973856,-0.3363480667,-2.1710168842
\H,2.1504063867,-1.1718890886,-1.2852926142\H,0.8573986643,-0.33801903
59,2.1714803388\H,2.1492710626,-1.1727962424,1.2862949946\H,2.07396025
01,0.5975157279,1.2866861741\C,-0.2320234194,-1.6639692189,-0.00077272
15\H,0.4500047729,-2.5223321098,-0.0006654624\H,-0.8688245901,-1.75400
06814,0.8864649784\H,-0.8678271193,-1.7534220666,-0.8887828936\\Versio
n=IA64L-G03RevC.02\State=1-A\HF=-275.1515254\RMSD=5.569e-09\RMSF=4.399
e-05\Dipole=0.0225829,0.0004696,0.0000029\PG=C01 [X(C7H14)]\@

n.C_CH3_3-CH2CH=CH2

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C7H14\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H2CH=CH2.freq\0,1\C,0.3564172333,0.2701351743,-0.8780056303\C,0.34478
97263,0.2672638343,0.6808494869\H,1.407693279,0.2324351364,-1.20391460
1\H,-0.0440909651,1.2313335208,-1.2278076143\C,-0.3976026624,-0.848254
234,-1.5459710857\C,1.1960554511,1.4568860203,1.1640645277\C,-1.095364
2744,0.4270617115,1.2007491594\C,-1.4679422915,-0.691578989,-2.3271892
168\H,-0.0182209352,-1.856882952,-1.3777289661\H,-1.9672329116,-1.5370
320339,-2.7935647187\H,-1.883950947,0.2924819145,-2.5357072051\H,2.234
4864721,1.3689888956,0.8207049724\H,1.2099024072,1.5101331469,2.259580
9204\H,0.7985894085,2.4080478037,0.7886372889\H,-1.1143720661,0.439312
5935,2.2974530053\H,-1.736814314,-0.3922332494,0.8588779867\H,-1.53991
56193,1.3664795134,0.8486885476\C,0.9515071278,-1.0389970447,1.2285108
913\H,1.0127868116,-1.0066675776,2.3231412659\H,0.3471746687,-1.912699
3841,0.9600575354\H,1.9668028503,-1.1987961646,0.8435327879\\Version=I
A64L-G03RevC.02\State=1-A\HF=-275.1617267\RMSD=2.356e-09\RMSF=1.147e-0
6\Dipole=0.0806413,0.0030466,0.0694577\PG=C01 [X(C7H14)]\@

n.C_CH3_3-CH2CH3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C6H14\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H2CH3.freq\0,1\C,0.3788026987,0.2139598036,0.0336837408\C,0.379283216
,0.1607727143,1.5739032577\C,1.8339833016,0.1241697653,-0.4674819102\C
, -0.4065022932,-0.9858860173,-0.559930228\C,-1.8905996752,-1.096700598
2,-0.1880730734\H,0.103080442,-1.9114168837,-0.2550692449\H,-0.3200908
569,-0.9416865757,-1.6552834874\H,2.4384498148,0.952205892,-0.07707956

53\H,1.8794818189,0.1649927837,-1.5630076984\H,2.3062513107,-0.8134554
88,-0.1485256106\H,-0.6296447513,0.2701381659,1.9871548982\H,0.9933959
9,0.9689016009,1.9900480883\H,0.7899521785,-0.7898399325,1.937242946\C
, -0.2267666284,1.5513660772,-0.4351052975\H,-2.3364724278,-1.977686725
6,-0.664099124\H,-2.0367002823,-1.2020014933,0.8926897429\H,-2.4635057
956,-0.2232957714,-0.518871879\H,0.3709607187,2.3965668905,-0.07214521
7\H,-0.2557595175,1.6106458203,-1.5305369191\H,-1.2486023585,1.6898412
477,-0.0644958668\\Version=IA64L-G03RevC.02\State=1-A\HF=-237.0836716\
RMSD=9.595e-09\RMSF=1.094e-06\Dipole=-0.0099771,-0.0115883,-0.0049934\
PG=C01 [X(C6H14)]\\@

n.C_CH3_3-CH_CH3_2

1\1\GINC-AC2\FOpt\RB3LYP\Gen\C7H16\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-CH
_CH3_2.freq\\0,1\C,0.4787128445,-2.0094698048,-0.003235718\H,0.4031167
034,-2.1328198915,1.0838459535\H,1.5405261158,-1.9644710076,-0.2634296
482\H,0.0698100295,-2.9184699045,-0.4600665834\C,-0.3038266398,-0.7766
693225,-0.4918802629\C,-1.8016506751,-0.9894843685,-0.2052254323\H,-0.
1895154796,-0.7379291341,-1.5867834668\C,0.2607455536,0.5898295692,0.0
34779177\C,-0.5299291478,1.7577778547,-0.5940260816\C,1.7364115591,0.7
440894473,-0.3933319912\H,-2.4264417112,-0.1900706727,-0.6147949962\H,
-2.0028630172,-1.056670785,0.8707280433\H,-2.139723736,-1.9301563202,-
0.6558028109\H,2.1074754438,1.743031328,-0.1340571148\H,1.8507670944,0
.6188403791,-1.4777234247\H,2.3898112428,0.0171733268,0.0999952573\H,-
1.5690872217,1.7879071284,-0.250582767\H,-0.53867874,1.6875915972,-1.6
893189568\H,-0.0714706839,2.7176296678,-0.3270111854\C,0.1761739184,0.
7047165339,1.5700878306\H,0.5785945032,1.670054457,1.9011633794\H,-0.8
57282305,0.642379442,1.9290260753\H,0.7551372838,-0.0787590672,2.07180
7115\\Version=IA64L-G03RevC.02\State=1-A\HF=-276.3932308\RMSD=1.782e-0
9\RMSF=4.057e-05\Dipole=-0.0009395,-0.0050913,-0.0151056\PG=C01 [X(C7H
16)]\\@

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
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.C_CH3_3-CCH

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C6H10\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
CH.freq\\0,1\C,0.1513760358,0.2360403668,0.1027003666\C,0.173625244,0.
1889882197,1.6484899073\C,1.5986016732,0.1895707015,-0.4409325727\C,-0

.596915639,-0.9265155239,-0.4076913571\C,-1.2093599623,-1.8820303069,-
0.8222504423\H,-1.7501799335,-2.723902465,-1.1902856005\H,-0.842330391
7,0.2162140957,2.0559630074\H,0.659049804,-0.7252020185,2.0056424982\H
,0.7266940888,1.0501299483,2.0422363335\H,1.6070664421,0.2172799391,-1
.5355159864\H,2.1668475306,1.0507219613,-0.0694657636\H,2.1085917122,-
0.7246106963,-0.1197868253\C,-0.5409832812,1.5359054231,-0.3691741782\
H,0.0065605618,2.409389382,0.0045282891\H,-0.5707176612,1.5893431941,-
1.4624176539\H,-1.5696465755,1.5888833775,0.0022513602\\Version=IA64L-
G03RevC.02\State=1-A\HF=-234.5950975\RMSD=2.594e-09\RMSF=3.842e-05\Dip
ole=0.1183311,0.1837163,0.0806518\PG=C01 [X(C6H10)]\@

n.C_CH3_3-CH=C_CH3_2

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H16\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H=C_CH3_2.freq\0,1\H,-2.5782618095,-0.4591495616,-2.3911488605\C,-2.5
246590306,-0.4939850659,-1.2935331972\C,-1.0897194287,-0.6255520814,-0
.8228617294\C,-0.4211622338,-1.8691643692,-1.362086468\C,-0.5784017386
,0.3210782744,-0.0177548182\C,0.7635950534,0.5695189479,0.6607585871\C
,1.277693303,1.9461268134,0.1716023005\C,0.4990943224,0.6548319048,2.1
843665291\H,-1.2743737953,1.1270037754,0.2300657438\H,-3.0079309827,0.
4066547532,-0.9026694525\H,-3.1229811776,-1.3625585876,-0.9829892222\H
, -0.440212714,-1.8607797956,-2.4612611747\H,-0.9839188178,-2.762508337
7,-1.0557209365\H,0.6108812884,-2.0007849382,-1.0473019271\H,-0.261301
8026,1.4105693205,2.4148064997\H,1.4158895412,0.9264236345,2.722813716
3\H,0.145341616,-0.3060194699,2.5753815536\H,1.4909918806,1.9257216173
, -0.9032727787\H,2.1992270236,2.2255772785,0.6977999376\H,0.5369896717
,2.734523939,0.3511350031\C,1.8694368699,-0.4721150647,0.4202687278\H,
2.774979118,-0.1730205793,0.9624452242\H,1.5843476564,-1.4647275371,0.
7845183157\H,2.1350706017,-0.5513616671,-0.6391612316\\Version=IA64L-G
03RevC.02\State=1-A'\HF=-314.476846\RMSD=5.790e-09\RMSF=4.076e-06\Dipo
le=0.0318355,-0.0643484,-0.028968\PG=CS [SG(C6H4),X(C2H12)]\@

n.C_CH3_3-CH=CH2

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H12\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H=CH2.freq\0,1\H,2.3049782449,0.0004319666,-1.0647855453\C,2.20993622
69,0.0002680889,0.0175173696\H,3.1397645106,0.0003009804,0.5803973342\
C,1.0289114574,0.0000375044,0.636894642\C,-0.3531059865,-0.0000440085,
0.0089334986\H,1.0184064031,-0.0001185828,1.7295109896\C,-1.1069851781
, -1.2588371791,0.4974165823\C,-1.1073044768,1.2584123155,0.4977904557\
H,-0.605467983,-2.1730506074,0.1603179851\H,-2.1337981591,-1.269751428
9,0.1112705762\H,-1.1609691079,-1.2895921262,1.592513786\H,-0.60602012
45,2.1728535287,0.1609631467\H,-1.1612956604,1.2888286754,1.5928968053
\H,-2.1341203777,1.2691804723,0.111648223\C,-0.3011199186,0.0001909272
, -1.5272305976\H,-1.315930127,0.0001375543,-1.9417904281\H,0.216129190
1,0.8872940092,-1.9103047758\H,0.2163304453,-0.8866803329,-1.910569801
\\Version=IA64L-G03RevC.02\State=1-A\HF=-235.8482115\RMSD=6.664e-09\RM
SF=5.474e-06\Dipole=-0.1253317,-0.0000178,0.0108813\PG=C01 [X(C6H12)]\@

n.C_CH3_3-CH=CHCH3

1\1\GINC-AC14\FOpt\RB3LYP\Gen\C7H14\CYL509\29-Sep-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-C
H=CHCH3.freq\0,1\H,1.757417155,0.000017554,-1.1367739631\C,1.68581885
73,0.0000052398,-0.0494311189\C,2.9957615453,-0.0000005345,0.688584202
4\C,0.4845019148,-0.0000040916,0.5342988042\C,-0.8809614237,-0.0000006
182,-0.1300455028\H,0.4462694644,-0.000015982,1.6273564479\C,-1.649450
7577,-1.2582033306,0.3370973052\C,-1.649459763,1.2581849854,0.33712841
61\H,-1.1400126003,-2.1725628086,0.0122458314\H,-2.6664864081,-1.26848

06232,-0.0746089592\H,-1.7307521416,-1.2900259865,1.4304834234\H,-1.14
00282562,2.1725561984,0.0122995073\H,-1.7307612977,1.2899800462,1.4305
153297\H,-2.6664955084,1.2684651571,-0.0745775189\C,-0.7933166795,0.00
0018705,-1.6649918763\H,2.8467960591,-0.0000058955,1.7738856995\H,3.60
01521916,-0.8803113785,0.4297735669\H,3.6001552569,0.880310663,0.42978
23295\H,-1.7984334392,0.0000215837,-2.102753254\H,-0.2675935431,0.8870
619825,-2.0367238157\H,-0.2675890936,-0.8870126418,-2.0367460032\\Vers
ion=IA64L-G03RevC.02\State=1-A\HF=-275.1672515\RMSD=7.099e-09\RMSF=5.6
10e-06\Dipole=0.0168305,-0.0000003,-0.0144346\PG=C01 [X(C7H14)]\@

n.C_CH3_3-CHO

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H10O1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CHO.freq\0,1\O,1.0533586316,0.1155166194,-1.8213773497\C,1.057982317
1,0.0384105119,-0.6132595372\H,2.0236031096,0.0021784622,-0.0533675698
\C,-0.1764062987,-0.0177906294,0.2795567773\C,-1.4535545061,0.03633556
7,-0.5666305076\C,-0.0978359786,1.1850689213,1.2463722843\H,-1.4963823
391,-0.8031727527,-1.2676131403\H,-1.4955705731,0.9576300099,-1.156051
5782\H,-2.3403519337,-0.0039987064,0.0761870404\H,0.838130316,1.182141
8373,1.8184586274\H,-0.9264646166,1.1455485396,1.9627893505\H,-0.16287
55558,2.1358502817,0.7052505302\C,-0.0988471947,-1.3330040255,1.086912
6771\H,-0.9276268317,-1.3836050868,1.802471354\H,-0.164355446,-2.20796
09584,0.430235859\H,0.8369947843,-1.4028666533,1.6549481601\\Version=I
A64L-G03RevC.02\State=1-A\HF=-271.7737274\RMSD=5.615e-09\RMSF=5.356e-0
6\Dipole=-0.2418979,-0.0640665,1.0076456\PG=C01 [X(C5H10O1)]\@

n.C_CH3_3-CN

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C5H9N1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
CN.freq\0,1\N,0.0821584079,-0.0085368171,-2.3591225317\C,0.0419626106
, -0.0045954935,-1.1984571432\C,-0.0097240926,0.0009802081,0.2788554041
\C,0.8144234233,1.2014004916,0.797412523\C,0.5896121111,-1.3253515929,
0.7991880401\H,0.7841649279,1.2183134276,1.8926657436\H,1.8600775076,1
.128268237,0.4822786719\H,0.4095576152,2.1482690275,0.4264672459\H,0.0
238768252,-2.1863947627,0.4295536492\H,1.6317013818,-1.4384230646,0.48
40436377\H,0.5570286511,-1.3351147817,1.8944569968\C,-1.4849007007,0.1
325136406,0.7210985841\H,-1.5380783446,0.1379783471,1.8155847484\H,-1.
9272662105,1.0621765787,0.3495166828\H,-2.0844113192,-0.7049988127,0.3
507058968\\Version=IA64L-G03RevC.02\State=1-A\HF=-250.6973101\RMSD=4.5
12e-09\RMSF=1.056e-05\Dipole=-0.0541311,0.0056221,1.5535041\PG=C01 [X(
C5H9N1)]\@

n.C_CH3_3-COCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H12O1\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
COCH3.freq\0,1\C,-0.975088071,-0.1929699144,-1.8557907763\C,-0.89339
82963,0.0625366158,-0.3558092882\C,0.4892873554,0.0070088594,0.3313691
595\O,-1.9053025529,0.2975612918,0.2787846885\H,-2.0131328893,-0.40036
67705,-2.1236761713\H,-0.3333401856,-1.0189448043,-2.1791117001\H,-0.6
474205505,0.7016236693,-2.4004895956\C,0.8905447617,-1.4832293359,0.45
83666538\C,0.3862636844,0.6302961982,1.7325279025\H,1.351236603,0.5607
237444,2.2480019656\H,-0.3707636441,0.1217380533,2.3348337492\H,0.1032
851709,1.6867355072,1.6748531032\H,1.8566607604,-1.5639593586,0.970521
6507\H,0.9922522389,-1.9694668092,-0.5184002819\H,0.151221666,-2.04201
82377,1.0429869604\C,1.5476615335,0.7580162321,-0.5034965467\H,2.51531
10534,0.7296465924,0.0110143271\H,1.6889467934,0.3119756284,-1.4938452
687\H,1.2765376002,1.8118705196,-0.6399688738\\Version=IA64L-G03RevC.0
2\State=1-A\HF=-311.0953247\RMSD=7.022e-09\RMSF=3.109e-05\Dipole=0.893
236,-0.2082592,-0.5148708\PG=C01 [X(C6H12O1)]\@

n.C_CH3_3-CON_CH2CH3_2

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C9H19N1O1\CYL509\29-Sep-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3
_3-CON_CH2CH3_2.freq\\0,1\H,-0.9677227089,1.3139652734,-3.4489632429\C
,-1.1825639808,1.2800926201,-2.3742796754\C,0.095856281,0.9524959648,-
1.592171754\N,-0.0861823858,0.9311042903,-0.1400527018\C,-0.1462900448
,2.2557180917,0.5021925139\C,1.2188400335,2.7427790362,0.9956822755\C,
-0.0849773942,-0.1539762308,0.7137835523\O,-0.1637612246,0.0457566842,
1.9265456654\C,0.0319874406,-1.6237990005,0.2002647808\C,1.4713854528,
-1.8999877397,-0.297325222\C,-0.224958639,-2.5411801197,1.4153358782\H
,0.8654508705,1.7023530276,-1.821805834\H,0.4992873061,-0.0004215407,-
1.9261710464\H,-0.8427546002,2.1936672583,1.3399771879\H,-0.55898503,2
.9583595924,-0.2291471187\H,-1.9557945976,0.5257188722,-2.2000922953\H
,-1.592527089,2.2537404816,-2.0862476028\H,1.602660436,2.064697033,1.7
622076229\H,1.1298824884,3.7441219868,1.4333073788\H,1.94664794,2.7971
777125,0.1770875001\H,1.7457396547,-1.3273588064,-1.1883748528\H,1.577
5203594,-2.9628566688,-0.5456789186\H,2.1996609364,-1.6658115447,0.487
1126002\H,-1.2318608652,-2.3940636528,1.8168272938\H,0.4807515591,-2.3
379345839,2.2230579334\H,-0.1222853192,-3.5887917472,1.1081330537\C,-1
.0132113949,-1.9878191914,-0.8786764285\H,-0.9945700257,-3.0709940491,
-1.0479730369\H,-2.0246605476,-1.7242156645,-0.548404551\H,-0.83948079
52,-1.5110770692,-1.8456840072\\Version=IA64L-G03RevC.02\State=1-A\HF=
-484.3922277\RMSE=9.715e-09\RMSE=1.611e-05\Dipole=0.1136796,0.1627886,
-1.29466\PG=C01 [X(C9H19N1O1)]\@
```

n.C_CH3_3-CON_CH3_2

```
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C7H15N1O1\CYL509\29-Sep-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3
_3-CON_CH3_2.freq\\0,1\C,-0.441514754,-0.0401244909,-1.0759227767\C,-0
.415499974,-0.1563230405,0.4798486915\N,0.7315088653,0.1123558984,1.20
50088324\O,-1.4408009725,-0.4948165117,1.0680456193\C,-0.1749449257,1.
410037293,-1.5459529643\C,-1.8702710131,-0.4114757705,-1.5278847079\C,
2.0408370426,0.5232246683,0.7286564182\C,0.6701570691,-0.020821327,2.6
567619709\H,2.8027465953,-0.209431587,1.031037072\H,2.0751903905,0.619
6695362,-0.3501472742\H,2.3183775621,1.4922088741,1.1676965994\H,1.397
2373752,-0.7685946171,3.0016896562\H,0.9106324018,0.9371428835,3.13767
00977\H,-0.3343549329,-0.3297225779,2.9374801227\H,-1.9349714864,-0.34
30642494,-2.6203884504\H,-2.6124978394,0.2602466767,-1.0897542829\H,-2
.1311879798,-1.4281694174,-1.2240107417\H,-0.3319507851,1.4763676279,-
2.6291708151\H,0.8368937356,1.7693722891,-1.3426523559\H,-0.875904835,
2.1030693621,-1.0669297639\C,0.5258262022,-1.0483149873,-1.741295979\H
,0.3816913244,-1.0282313833,-2.8281415326\H,1.5833113004,-0.8488779042
,-1.5510067312\H,0.3130950138,-2.0671587779,-1.3980622972\\Version=IA6
4L-G03RevC.02\State=1-A\HF=-405.7611668\RMSE=7.844e-09\RMSE=2.093e-06\
Dipole=1.2227226,0.3727054,-0.3106376\PG=C01 [X(C7H15N1O1)]\@
```

n.C_CH3_3-CONH2

```
1\1\GINC-AC24\FOpt\RB3LYP\Gen\C5H11N1O1\CYL509\29-Sep-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3
_3-CONH2.freq\\0,1\C,-0.0188721585,0.0001950593,-0.5716007829\C,-0.066
8653776,0.0000040405,0.9754452639\N,1.1226623601,-0.0001846119,1.64787
43837\O,-1.1354900352,-0.0012709162,1.5739591135\C,-0.7729279485,-1.26
19334378,-1.0421967187\C,-0.7776673806,1.259438702,-1.0422275318\H,2.0
201714736,0.0052894139,1.1923518358\H,1.0880010654,0.0021309376,2.6575
888839\H,-0.8666102752,1.2632319133,-2.1350645492\H,-0.2534525191,2.17
49356432,-0.7421334184\H,-1.7795333734,1.2827078181,-0.6059583146\H,-0
.8617371048,-1.266162041,-2.1350459127\H,-1.7747662978,-1.2888707007,-
0.6060595288\H,-0.2453291577,-2.1754158033,-0.7419223396\C,1.403626996
```

2,0.0028125045,-1.1580910109\H,1.3540818191,0.0026269133,-2.2528169099
\H,1.9686664347,0.8961072644,-0.8629908982\H,1.9720269096,-0.888222957
6,-0.8627177601\\Version=IA64L-G03RevC.02\State=1-A\HF=-327.1532944\RM
SD=9.693e-09\RMSF=3.328e-05\Dipole=1.3133772,0.0053877,-0.3907127\PG=C
01 [X(C5H11N1O1)]\\@

n.C_CH3_3-CONHCH3

1\1\GINC-AC15\FOpt\RB3LYP\Gen\C6H13N1O1\CYL509\29-Sep-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3
_3-CONHCH3.freq\\0,1\H,-2.4824804822,0.6529294533,-2.4566619666\C,-2.4
576222975,0.669069623,-1.3602761097\N,-1.0935265124,0.7326709467,-0.86
62660052\C,-0.5553565129,-0.2408324612,-0.0724227783\C,0.9119072989,-0
.0572645197,0.3901341221\O,-1.1949683227,-1.2307924904,0.2722040967\C,
1.6966408138,-1.2866134537,-0.1162949779\C,0.8964337101,-0.0566699136,
1.9339415454\H,-0.5279696021,1.526404297,-1.1219010915\H,-2.8979200926
, -0.2527458423,-0.9783738639\H,-3.0478724862,1.5234647208,-1.007373456
\H,2.7230606562,-1.2680582621,0.2690227608\H,1.7468541254,-1.302114084
4,-1.2119338093\H,1.2113180206,-2.2081669718,0.2148255489\H,1.92070335
76,-0.0348444417,2.3247701905\H,0.3944092529,-0.9525812415,2.307780542
2\H,0.3661920384,0.8200614336,2.3255688933\C,1.5870340663,1.2290886544
, -0.1180481016\H,2.6164571054,1.278101869,0.2543661668\H,1.6419796248,
1.261927229,-1.2136871211\H,1.0754781788,2.1325975621,0.2376242689\\Ve
rsion=IA64L-G03RevC.02\State=1-A\HF=-366.4642064\RMSD=5.015e-09\RMSF=1
.972e-05\Dipole=0.4179624,1.1585296,-0.5320916\PG=C01 [X(C6H13N1O1)]\\@

n.C_CH3_3-COOC_CH3_3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C9H18O2\CYL509\29-Sep-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-COOC_CH3_3.freq\\0,1\H,-1.2147045917,-0.0192499984,-3.4913119324\C,-1
.2140114543,-0.0416608659,-2.3955955211\C,0.216359939,-0.2552543507,-1
.8888586592\C,1.1432210945,0.9092224327,-2.2539734307\O,0.2094230174,-
0.4556056249,-0.4272937814\C,-0.2261544295,0.497098928,0.4248540149\O,
-0.6455321679,1.5868245609,0.0900300001\C,-0.1202391007,0.0175759729,1
.8829430825\C,0.7821364959,-1.5810615114,-2.4044140037\C,-0.6264845391
,1.134155647,2.8090664679\C,-0.9827312536,-1.2516611282,2.0604556047\H
,0.8417199358,-1.5659042698,-3.4978503425\H,0.142835422,-2.4175634469,
-2.1037988653\H,1.7867436098,-1.7544458479,-2.0050247564\H,-1.62836493
21,0.8972201022,-2.0254727614\H,-1.859105843,-0.8665264011,-2.07332025
48\H,1.2411092261,0.971440381,-3.3437634076\H,2.1416883777,0.747336401
8,-1.8329439538\H,0.7518078407,1.8573440358,-1.8824299055\H,-0.5586886
427,0.8096248221,3.8538291872\H,-1.6684219655,1.3877251857,2.591806412
7\H,-0.0345670999,2.0466698863,2.6904241528\H,-0.9275560682,-1.5955828
713,3.1000099737\H,-0.6380729082,-2.0605991164,1.4104189727\H,-2.03564
37553,-1.0504107878,1.8300749208\C,1.3562756018,-0.3074503925,2.200651
4308\H,1.448496637,-0.634203305,3.2431180853\H,1.7360645042,-1.1036396
68,1.554437473\H,1.9932993324,0.5752250183,2.0691333351\\Version=IA64L
-G03RevC.02\State=1-A\HF=-504.280587\RMSD=5.126e-09\RMSF=7.602e-06\Dip
ole=0.2730294,-0.6476233,-0.1961073\PG=C01 [X(C9H18O2)]\\@

n.C_CH3_3-COOCH2CH3

1\1\GINC-AC14\FOpt\RB3LYP\Gen\C7H14O2\CYL509\29-Sep-2008\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-COOCH2CH3.freq\\0,1\C,0.5335906705,-0.0438692204,-1.279651761\C,0.528
516699,-0.1226949364,0.2523675272\O,1.4925535288,-0.3598663601,0.94943
50396\O,-0.7058540262,0.1070985498,0.7609510792\C,-0.817623386,0.05468
47242,2.2009909048\C,-2.2650739729,0.3375637134,2.557207292\C,0.071885
7821,1.3656648801,-1.7121489235\C,1.9598218369,-0.312990904,-1.7834371
416\H,-0.4947666535,-0.9334805414,2.5445310923\H,-0.1350912608,0.79239

37062,2.6353263201\H,-2.5694601061,1.327521072,2.2022617885\H,-2.39348
26661,0.3070931221,3.6447585533\H,-2.9311437556,-0.4079881887,2.110933
853\H,2.6659944967,0.4221941771,-1.3858254778\H,1.9835783943,-0.260685
6373,-2.877952408\H,2.3084194203,-1.3035129873,-1.4759520331\H,-0.9413
52375,1.5780193495,-1.3596236081\H,0.0799342773,1.4387144251,-2.805942
6969\H,0.7417217017,2.1397645078,-1.3196509514\C,-0.4394264702,-1.1053
418014,-1.8403208309\H,-0.4365211773,-1.0685141723,-2.93593911\H,-0.14
01728218,-2.1157917628,-1.5381180885\H,-1.4614004519,-0.931683321,-1.4
919385854\\Version=IA64L-G03RevC.02\State=1-A\HF=-425.6491345\RMSE=3.2
07e-09\RMSF=2.772e-05\Dipole=-0.7281532,0.1571858,-0.1148286\PG=C01 [X
(C7H14O2)]\\@

n.C_CH3_3-COOCH3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C6H12O2\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-COOCH3.freq\0,1\C,0.2162747506,0.0289626714,-0.9551774182\C,0.222073
9954,0.0790431652,0.5772706667\O,1.1740147273,0.3620936352,1.272977702
5\O,-0.991419006,-0.237269279,1.0927703096\C,-1.0761376471,-0.21495210
15,2.5259289996\H,-2.104739357,-0.4890750647,2.7632613602\C,-0.1592877
68,-1.3990851956,-1.4100677205\C,1.6176947632,0.397364486,-1.465935753
1\H,-0.3764799762,-0.9316241949,2.9645272502\H,-0.8458453591,0.7825020
246,2.9100537209\H,1.9058575424,1.4022316359,-1.1427985314\H,1.6337932
833,0.3668641536,-2.5613827385\H,2.3728299444,-0.2988179859,-1.0886534
24\H,0.5614630072,-2.1361997876,-1.0371626532\H,-0.1559238557,-1.45132
74722,-2.5050566714\H,-1.1540770829,-1.6817237195,-1.0543329657\C,-0.8
275422719,1.0366387956,-1.4869351959\H,-0.8318944889,1.0210015348,-2.5
830585392\H,-1.8334097861,0.7915073305,-1.1345668897\H,-0.590794575,2.
0582357685,-1.1673154857\\Version=IA64L-G03RevC.02\State=1-A\HF=-386.3
30144\RMSE=3.163e-09\RMSF=1.235e-05\Dipole=-0.6445171,-0.1811845,-0.14
45862\PG=C01 [X(C6H12O2)]\\@

n.C_CH3_3-COOH

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C5H10O2\CYL509\29-Sep-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3
-COOH.freq\0,1\C,0.0504593833,-0.0148207332,-0.5704680836\C,0.0807167
317,-0.0131029137,0.9587541479\O,1.0478721527,-0.2313484038,1.65556205
09\O,-1.1358853398,0.2694890532,1.4985700629\C,1.4573970318,-0.3412091
604,-1.0935429126\C,-0.3938925009,1.3812888836,-1.062586563\H,-1.00685
20008,0.2453275192,2.4653513118\H,1.7927011226,-1.3219928384,-0.743074
2714\H,2.1882610139,0.3982187906,-0.7525366083\H,1.4542960708,-0.34651
11196,-2.1893812457\H,-0.4102612363,1.3968604705,-2.1584500706\H,0.300
5148276,2.1598716607,-0.7261958667\H,-1.3941757421,1.6332136848,-0.699
1615101\C,-0.9600882584,-1.0820394208,-1.048556673\H,-0.9838473868,-1.
1012197999,-2.1442298007\H,-0.6748643291,-2.0819178589,-0.7014970111\H
, -1.9692211673,-0.8676756373,-0.685481332\\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-347.0235897\RMSE=5.060e-09\RMSF=3.750e-06\Dipole=-0.52504,
0.1189718,-0.2927887\PG=C01 [X(C5H10O2)]\\@

n.C_CH3_3-COPh

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C11H14O1\CYL509\29-Sep-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_
3-COPh.freq\0,1\C,-3.1899739119,0.1303435137,-0.1884884109\C,-3.27766
12755,-0.1970571005,1.167127228\C,-2.1105826121,-0.4069481491,1.901110
8501\C,-0.8622915021,-0.2912797367,1.2880998913\C,-0.756715551,0.03718
97239,-0.0739560138\C,-1.945290618,0.2451829252,-0.7981390175\C,0.5316
058744,0.1924946838,-0.8552251631\O,0.4500397425,0.4808159058,-2.04137
26748\C,1.9383569936,0.00489891,-0.2269716332\C,2.1158234516,-1.441638
467,0.2949494538\C,2.9899462209,0.2452195219,-1.3275815268\H,-1.860608
2267,0.4984339206,-1.8490718312\H,0.020281302,-0.4614634192,1.89003959

21\H,-2.1674839699,-0.6620606369,2.955851061\H,-4.0934225809,0.2959095
528,-0.7693220944\H,-4.2484781836,-0.2877786249,1.6472108895\H,3.99477
48377,0.1183331763,-0.9079916888\H,2.9106190356,1.2543631579,-1.741280
0143\H,2.8676721125,-0.4577966756,-2.1562028106\H,3.1399918303,-1.5714
47156,0.6644727642\H,1.9601847102,-2.1661505955,-0.5127206047\H,1.4345
994895,-1.7010161933,1.1083010515\C,2.1784890502,1.0417371675,0.897207
9349\H,3.2032304546,0.938806254,1.2735663546\H,2.0672646077,2.06213224
64,0.5126050081\H,1.5008199203,0.932349791,1.7467221656\\Version=IA64L
-G03RevC.02\State=1-A\HF=-502.8290682\RMSD=6.693e-09\RMSF=6.000e-06\Di
pole=-0.1665987,-0.2405669,1.0147642\PG=C01 [X(C11H14O1)]\\@

n.H-H2CCH2-H

1\1\GINC-AC13\FOpt\RB3LYP\Gen\C2H6\CYL509\23-Aug-2008\0\#B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.H-H2CCH2-H
.freq\\0,1\C,0.,0.,0.7652753363\H,-1.0209484437,-0.0000000001,1.164356
0784\H,0.510474222,-0.8841672882,1.1643560784\H,0.5104742218,0.8841672
883,1.1643560784\C,0.,0.,-0.7652753363\H,1.0209484437,0.0000000001,-1.
1643560784\H,-0.510474222,0.8841672882,-1.1643560784\H,-0.5104742218,-
0.8841672883,-1.1643560784\\Version=IA64L-G03RevC.02\State=1-A1G\HF=-7
9.8304207\RMSD=1.668e-09\RMSF=5.241e-06\Dipole=0.,0.,0.\PG=D03D [C3(C1
.C1),3SGD(H2)]\\@

n.BH2-H2CCH2-BH2

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C2H8B2\CYL509\13-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.BH2-H2CC
H2-BH2.freq\\0,1\C,0.0254938076,0.0104160918,-0.7710181846\H,1.006252
8083,-0.054048065,-1.1755612072\H,-0.4912145369,-0.9075840584,-1.16058
54457\B,-0.5942656824,1.2729371087,-1.4902472661\H,-0.7536139244,2.312
1919329,-0.9123263414\H,-0.8323988208,1.2371571742,-2.664679797\C,0.02
54938076,-0.0104160918,0.7710181846\H,-1.0062528083,0.054048065,1.1755
612072\H,0.4912145369,0.9075840584,1.1605854457\B,0.5942656824,-1.2729
371087,1.4902472661\H,0.7536139244,-2.3121919329,0.9123263414\H,0.8323
988208,-1.2371571742,2.664679797\\Version=IA64L-G03RevC.02\State=1-AG\
HF=-130.6850911\RMSD=2.915e-09\RMSF=1.296e-05\Dipole=0.,0.,0.\PG=CI [X
(C2H8B2)]\\@

n.CH3-H2CCH2-CH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10\CYL509\21-Aug-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH3-H2CCH
2-CH3.freq\\0,1\H,-0.7647100025,-0.0140350358,-1.3289478891\C,-0.73179
71886,-0.0022094845,-0.2298885106\H,-1.2098742619,-0.9369614326,0.0969
712803\C,-1.5345157106,1.1929662232,0.2930494495\H,-1.1002797416,2.141
4414851,-0.0469596494\H,-1.5484655437,1.2117163914,1.3899653317\H,-2.5
74281652,1.1607659712,-0.0521027218\H,0.7647100025,0.0140350358,1.3289
478891\C,0.7317971886,0.0022094845,0.2298885106\H,1.2098742619,0.93696
14326,-0.0969712803\C,1.5345157106,-1.1929662232,-0.2930494495\H,1.100
2797416,-2.1414414851,0.0469596494\H,1.5484655437,-1.2117163914,-1.389
9653317\H,2.574281652,-1.1607659712,0.0521027218\\Version=IA64L-G03Rev
C.02\State=1-AG\HF=-158.4580434\RMSD=9.956e-09\RMSF=5.092e-05\Dipole=0
.,0.,0.\PG=CI [X(C4H10)]\\@

n.NH2-H2CCH2-NH2

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H8N2\CYL509\13-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NH2-H2CC
H2-NH2.freq\\0,1\C,0.3247279795,0.6558341677,0.2419480086\H,0.32361876
42,0.674634958,1.3411039248\H,1.3807194574,0.6693435876,-0.0633344907\
N,-0.2960628652,1.8959185883,-0.2300308778\H,-0.2976841174,1.912481429
2,-1.2496260419\H,-1.2763505213,1.9172385304,0.0500369444\C,-0.3247279
795,-0.6558341677,-0.2419480086\H,-0.3236187642,-0.674634958,-1.341103

9248\H,-1.3807194574,-0.6693435876,0.0633344907\N,0.2960628652,-1.8959
185883,0.2300308778\H,0.2976841174,-1.9124814292,1.2496260419\H,1.2763
505213,-1.9172385304,-0.0500369444\\Version=IA64L-G03RevC.02\State=1-A
G\HF=-190.5111\RMSE=4.150e-09\RMSE=1.303e-04\Dipole=0.,0.,0.\PG=CI [X(
C2H8N2)]\\@

n.OH-H2CCH2-OH

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C2H6O2\CYL509\13-Jul-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OH-H2CCH
2-OH.freq\\0,1\C,0.3497453331,0.6414181226,0.2098914248\O,0.3524205787
,0.6701488134,1.6318610253\H,1.3695848006,0.6451274186,-0.2048043246\H
, -0.1895593555,1.4999733674,-0.2191597259\H,0.7950847017,1.4845075088,
1.9114927687\C,-0.3497453331,-0.6414181226,-0.2098914248\O,-0.35242057
87,-0.6701488134,-1.6318610253\H,-1.3695848006,-0.6451274186,0.2048043
246\H,0.1895593555,-1.4999733674,0.2191597259\H,-0.7950847017,-1.48450
75088,-1.9114927687\\Version=IA64L-G03RevC.02\State=1-AG\HF=-230.23571
48\RMSE=2.286e-09\RMSE=7.942e-05\Dipole=0.,0.,0.\PG=CI [X(C2H6O2)]\\@

n.F-H2CCH2-F

1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H4F2\CYL509\13-Jul-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.F-H2CCH2
-F.freq\\0,1\H,-0.7300307643,-0.0058952498,-1.3532023159\C,-0.71524670
72,-0.0101298039,-0.2572825296\H,-1.2410530925,-0.9018617852,0.1027411
923\F,-1.3632506754,1.1241435742,0.2132852668\H,0.7300307643,0.0058952
498,1.3532023159\C,0.7152467072,0.0101298039,0.2572825296\H,1.24105309
25,0.9018617852,-0.1027411923\F,1.3632506754,-1.1241435742,-0.21328526
68\\Version=IA64L-G03RevC.02\State=1-AG\HF=-278.2779902\RMSE=1.592e-09
\RMSE=1.305e-04\Dipole=0.,0.,0.\PG=CI [X(C2H4F2)]\\@

n.SiH3-H2CCH2-SiH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C2H10Si2\CYL509\13-Jul-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SiH3-H
2CCH2-SiH3.freq\\0,1\H,0.3373287451,0.7065791972,-1.3352857394\C,0.324
1109929,0.6616124132,-0.2377172921\H,1.3760936368,0.7047396574,0.07585
33703\Si,-0.5568634839,2.2108031142,0.4128036054\H,-1.976476036,2.2269
737757,-0.0395456341\H,-0.5473147452,2.2240844732,1.9027386906\H,0.105
557197,3.454239357,-0.0727540164\H,-0.3373287451,-0.7065791972,1.33528
57394\C,-0.3241109929,-0.6616124132,0.2377172921\H,-1.3760936368,-0.70
47396574,-0.0758533703\Si,0.5568634839,-2.2108031142,-0.4128036054\H,1
.976476036,-2.2269737757,0.0395456341\H,0.5473147452,-2.2240844732,-1.
9027386906\H,-0.105557197,-3.454239357,0.0727540164\\Version=IA64L-G03
RevC.02\State=1-AG\HF=-661.2114385\RMSE=7.152e-09\RMSE=2.723e-05\Dipol
e=0.,0.,0.\PG=CI [X(C2H10Si2)]\\@

n.PH2-H2CCH2-PH2

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C2H8P2\CYL509\13-Jul-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.PH2-H2CC
H2-PH2.freq\\0,1\C,0.3363780235,0.6414691391,0.2477236299\H,0.34741516
21,0.6690111706,1.3444747821\H,1.3885172518,0.6663682919,-0.0623255202
\P,-0.4239560343,2.2696839382,-0.3180419732\H,-0.5486795582,1.93764628
35,-1.699885424\H,-1.7825221044,1.9408118093,-0.0326549091\C,-0.336378
0235,-0.6414691391,-0.2477236299\H,-0.3474151621,-0.6690111706,-1.3444
747821\H,-1.3885172518,-0.6663682919,0.0623255202\P,0.4239560343,-2.26
96839382,0.3180419732\H,0.5486795582,-1.9376462835,1.699885424\H,1.782
5221044,-1.9408118093,0.0326549091\\Version=IA64L-G03RevC.02\State=1-A
G\HF=-763.7118498\RMSE=4.159e-09\RMSE=9.437e-05\Dipole=0.,0.,0.\PG=CI
[X(C2H8P2)]\\@

n.SH-H2CCH2-SH

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C2H6S2\CYL509\23-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.SH-H2CCH
2-SH.freq\|0,1\C,0.3503025884,0.6432411809,0.2146806138\S,0.3700090797
,0.7112606911,2.062420531\H,1.3774815227,0.6595964136,-0.1597548664\H,
-0.1833111311,1.5145623332,-0.1746912427\H,1.0172856119,1.8919483192,2
.1618621323\C,-0.3503025884,-0.6432411809,-0.2146806138\S,-0.370009079
7,-0.7112606911,-2.062420531\H,-1.3774815227,-0.6595964136,0.159754866
4\H,0.1833111311,-1.5145623332,0.1746912427\H,-1.0172856119,-1.8919483
192,-2.1618621323\|Version=IA64L-G03RevC.02\State=1-AG\HF=-876.1933278
\RMSD=4.628e-09\RMSF=2.142e-05\Dipole=0.,0.,0.\PG=CI [X(C2H6S2)]\|@
```

n.Cl-H2CCH2-Cl

```
1\1\GINC-AC29\FOpt\RB3LYP\Gen\C2H4Cl2\CYL509\13-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.Cl-H2CC
H2-Cl.freq\|0,1\H,-0.7088384399,-0.004396739,-1.3680361146\C,-0.706829
5545,0.0042271704,-0.2777114672\H,-1.2894031163,-0.8378775993,0.096926
82\H,0.7088384399,0.004396739,1.3680361146\C,0.7068295545,-0.004227170
4,0.2777114672\H,1.2894031163,0.8378775993,-0.09692682\Cl,1.5466616621
,-1.5227359232,-0.2534085411\Cl,-1.5466616621,1.5227359232,0.253408541
1\|Version=IA64L-G03RevC.02\State=1-AG\HF=-999.0190097\RMSD=1.283e-09\
RMSF=1.367e-04\Dipole=0.,0.,0.\PG=C02H [SGH(C2Cl2),X(H4)]\|@
```

n.Br-H2CCH2-Br

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C2H4Br2\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.Br-H2CC
H2-Br.freq\|0,1\H,-0.7137703195,-0.0012741088,-1.3697383008\C,-0.70106
0851,-0.0153303936,-0.2810091731\H,-1.2805367229,-0.8588538609,0.09095
86843\Br,-1.6640885238,1.6204482203,0.3055947841\H,0.7137703195,0.0012
741088,1.3697383008\C,0.701060851,0.0153303936,0.2810091731\H,1.280536
7229,0.8588538609,-0.0909586843\Br,1.6640885238,-1.6204482203,-0.30559
47841\|Version=IA64L-G03RevC.02\State=1-AG\HF=-5226.3929673\RMSD=4.246
e-09\RMSF=1.007e-04\Dipole=0.,0.,0.\PG=CI [X(C2H4Br2)]\|@
```

n.N_CH3_2-H2CCH2-N_CH3_2

```
1\1\GINC-AC30\FOpt\RB3LYP\Gen\C6H16N2\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.N_CH3_2
-H2CCH2-N_CH3_2.freq\|0,1\C,1.0281743647,-0.641557669,2.4229633704\H,1
.1249529677,-0.4999254988,3.506445608\H,2.0376792014,-0.6799565223,1.9
977214355\H,0.5527443942,-1.6282207664,2.2615209615\N,0.301963312,0.48
19916334,1.8549369342\C,0.3529519984,0.5668270717,0.3945311067\C,-1.02
60611029,0.6350501196,2.4253011293\H,1.4120202953,0.6041556318,0.10789
50217\H,-0.0825192429,1.5334920091,0.1097270688\H,-0.9401450243,0.7829
23146,3.5088588817\H,-1.7005898151,-0.2277939126,2.2636712634\H,-1.508
0013004,1.5238978362,2.0021116694\C,-1.0281743647,0.641557669,-2.42296
33704\H,-1.1249529677,0.4999254988,-3.506445608\H,-2.0376792014,0.6799
565223,-1.9977214355\H,-0.5527443942,1.6282207664,-2.2615209615\N,-0.3
01963312,-0.4819916334,-1.8549369342\C,-0.3529519984,-0.5668270717,-0.
3945311067\C,1.0260611029,-0.6350501196,-2.4253011293\H,-1.4120202953,
-0.6041556318,-0.1078950217\H,0.0825192429,-1.5334920091,-0.1097270688
\H,0.9401450243,-0.782923146,-3.5088588817\H,1.7005898151,0.2277939126
,-2.2636712634\H,1.5080013004,-1.5238978362,-2.0021116694\|Version=IA6
4L-G03RevC.02\State=1-AG\HF=-347.7414752\RMSD=4.027e-09\RMSF=4.000e-05
\Dipole=0.,0.,0.\PG=CI [X(C6H16N2)]\|@
```

n.NHCH3-H2CCH2-NHCH3

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H12N2\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.NHCH3-H
2CCH2-NHCH3.freq\|0,1\H,-1.8414432697,0.7167124517,-3.4039922587\C,-1.
8165643019,0.9082977986,-2.3260210967\N,-0.6730367434,0.2224829184,-1.
```

```
7354282492\C,-0.6143307174,0.3563404181,-0.2826717518\H,-0.5488517784,
1.4301472671,-0.0518094806\H,-1.5172198361,-0.0196964471,0.2340971245\
H,-2.7954121403,0.6169810668,-1.8998285413\H,-1.704382566,1.9898704502
,-2.1830579714\H,-0.7257402772,-0.7679333395,-1.9702662289\H,1.8414432
697,-0.7167124517,3.4039922587\C,1.8165643019,-0.9082977986,2.32602109
67\N,0.6730367434,-0.2224829184,1.7354282492\C,0.6143307174,-0.3563404
181,0.2826717518\H,0.5488517784,-1.4301472671,0.0518094806\H,1.5172198
361,0.0196964471,-0.2340971245\H,2.7954121403,-0.6169810668,1.89982854
13\H,1.704382566,-1.9898704502,2.1830579714\H,0.7257402772,0.767933339
5,1.9702662289\\Version=IA64L-G03RevC.02\State=1-AG\HF=-269.1274636\RM
SD=1.489e-09\RMSF=2.131e-05\Dipole=0.,0.,0.\PG=CI [X(C4H12N2)]\\@
```

n.NHCHO-H2CCH2-NHCHO

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1\1\GINC-AC27\FOpt\RB3LYP\Gen\C4H8N2O2\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCHO-
H2CCH2-NHCHO.freq\\0,1\O,-2.5653491462,0.866012773,-1.2699910933\C,-2.
716793581,-0.0223722272,-0.4464234101\N,-1.7121038611,-0.7926335778,0.
052596667\C,-0.3249589682,-0.6041106901,-0.3497769902\H,-0.2999126239,
-0.4575759341,-1.4337793725\H,0.2363115061,-1.5088459597,-0.1055535189
\H,-1.9311246457,-1.4662019966,0.7734643834\H,-3.7064531143,-0.2944647
47,-0.0293078981\O,2.5653491462,-0.866012773,1.2699910933\C,2.71679358
1,0.0223722272,0.4464234101\N,1.7121038611,0.7926335778,-0.052596667\C
,0.3249589682,0.6041106901,0.3497769902\H,0.2999126239,0.4575759341,1.
4337793725\H,-0.2363115061,1.5088459597,0.1055535189\H,1.9311246457,1.
4662019966,-0.7734643834\H,3.7064531143,0.294464747,0.0293078981\\Vers
ion=IA64L-G03RevC.02\State=1-AG\HF=-417.2047425\RMSD=2.975e-09\RMSF=1.
947e-05\Dipole=0.,0.,0.\PG=CI [X(C4H8N2O2)]\\@
```

n.NHCOCH3-H2CCH2-NHCOCH3

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1\1\GINC-AC27\FOpt\RB3LYP\Gen\C6H12N2O2\CYL509\14-Jul-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCOCH
H3-H2CCH2-NHCOCH3.freq\\0,1\C,0.1865965028,0.3177153554,-0.6759973489\
H,1.1519929451,0.8246560468,-0.5881575743\H,0.2671773521,-0.4664955646
,-1.4326103937\N,-0.7974957297,1.2938102164,-1.1191601225\H,-1.5230967
568,0.9969967894,-1.7548687495\C,-0.8275075151,2.5626810554,-0.6107142
482\O,-0.015727558,2.9513831245,0.2225524318\C,-1.9233935045,3.4682712
169,-1.1540142769\H,-1.4581054826,4.349911312,-1.6054569841\H,-2.54015
18537,3.8173418926,-0.3200864521\H,-2.5682783733,2.9883792531,-1.89704
64906\C,-0.1865965028,-0.3177153554,0.6759973489\H,-1.1519929451,-0.82
46560468,0.5881575743\H,-0.2671773521,0.4664955646,1.4326103937\N,0.79
74957297,-1.2938102164,1.1191601225\H,1.5230967568,-0.9969967894,1.754
8687495\C,0.8275075151,-2.5626810554,0.6107142482\O,0.015727558,-2.951
3831245,-0.2225524318\C,1.9233935045,-3.4682712169,1.1540142769\H,1.45
81054826,-4.349911312,1.6054569841\H,2.5401518537,-3.8173418926,0.3200
864521\H,2.5682783733,-2.9883792531,1.8970464906\\Version=IA64L-G03Rev
C.02\State=1-AG\HF=-495.8515834\RMSD=3.391e-09\RMSF=1.275e-05\Dipole=0
.,0.,0.\PG=CI [X(C6H12N2O2)]\\@
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n.NO2-H2CCH2-NO2

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1\1\GINC-AC30\FOpt\RB3LYP\Gen\C2H4N2O4\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NO2-H2
CCH2-NO2.freq\\0,1\O,-1.9589457056,0.0247539014,-1.3654269927\N,-1.866
0583364,-0.3877801294,-0.2114204167\C,-0.5181291354,-0.3052042636,0.46
43071686\O,-2.771163434,-0.8680753048,0.4561044189\H,-0.6714929873,0.2
816888091,1.3710741826\H,-0.2691268045,-1.3240013684,0.7646556162\O,1.
9589457056,-0.0247539014,1.3654269927\N,1.8660583364,0.3877801294,0.21
14204167\C,0.5181291354,0.3052042636,-0.4643071686\O,2.771163434,0.868
0753048,-0.4561044189\H,0.6714929873,-0.2816888091,-1.3710741826\H,0.2
691268045,1.3240013684,-0.7646556162\\Version=IA64L-G03RevC.02\State=1
```

-AG\HF=-488.8171926\RMSD=4.823e-09\RMSF=1.158e-04\Dipole=0.,0.,0.\PG=C
I [X(C2H4N2O4)]\@

n.OCF3-H2CCH2-OCF3

1\1\GINC-AC30\FOpt\RB3LYP\Gen\C4H4F6O2\CYL509\20-Aug-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\#n.OCF3-H
2CCH2-OCF3.freq\0,1\C,0.6912986651,-0.2142614568,0.226656511\O,0.6227
6534,-0.2840689958,1.6618004542\C,1.796315087,-0.4824766878,2.29826149
06\F,2.6662964303,0.5318999501,2.0985747687\F,2.4158969184,-1.61136180
58,1.8909638653\F,1.5489831305,-0.5775127112,3.6030501676\H,1.44899531
11,0.5120011937,-0.0827027115\H,0.9405036443,-1.1961282058,-0.18648843
2\C,-0.6901193682,0.2276250922,-0.2257108127\O,-0.620569647,0.30109982
89,-1.6606622951\C,-1.7964279058,0.480657118,-2.2984236877\F,-2.647299
8849,-0.5512629338,-2.1061384842\F,-2.4382145642,1.5951643456,-1.88600
12132\F,-1.548511836,0.5875278989,-3.6021781043\H,-1.4474721672,-0.499
8616034,0.0814982078\H,-0.9403429481,1.2083848614,0.1894476572\#Versio
n=IA64L-G03RevC.02\State=1-A\HF=-904.3333029\RMSD=7.225e-09\RMSF=2.108
e-06\Dipole=-0.0002346,0.0021185,0.0000345\PG=C01 [X(C4H4F6O2)]\@

n.OCH2CH3-H2CCH2-OCH2CH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C6H14O2\CYL509\27-Aug-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.OCH2CH3
-H2CCH2-OCH2CH3.freq\0,1\C,0.3453767449,0.6293922326,0.2521421997\H,0
.348116099,0.6347285708,1.3546395692\H,1.3964121469,0.6345135068,-0.08
07818349\O,-0.3594724565,1.7405404282,-0.2627696226\C,0.1889489436,2.9
850706439,0.1373025836\C,-0.646651249,4.0983362986,-0.4729994815\H,1.2
386897225,3.0607604503,-0.1948179107\H,0.1924519053,3.0611086031,1.238
299013\H,-0.2498909948,5.0777225873,-0.1837114036\H,-1.6849233844,4.02
92286572,-0.1326502593\H,-0.6389508247,4.0287439319,-1.5655745169\C,-0
.3453767449,-0.6293922326,-0.2521421997\H,-0.348116099,-0.6347285708,-
1.3546395692\H,-1.3964121469,-0.6345135068,0.0807818349\O,0.3594724565
, -1.7405404282,0.2627696226\C,-0.1889489436,-2.9850706439,-0.137302583
6\C,0.646651249,-4.0983362986,0.4729994815\H,-1.2386897225,-3.06076045
03,0.1948179107\H,-0.1924519053,-3.0611086031,-1.238299013\H,0.2498909
948,-5.0777225873,0.1837114036\H,1.6849233844,-4.0292286572,0.13265025
93\H,0.6389508247,-4.0287439319,1.5655745169\#Version=IA64L-G03RevC.02
\State=1-AG\HF=-387.4943855\RMSD=2.270e-09\RMSF=5.369e-05\Dipole=0.,0.
,0.\PG=CI [X(C6H14O2)]\@

n.OCH3-H2CCH2-OCH3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C4H10O2\CYL509\13-Jul-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.OCH3-H2
CCH2-OCH3.freq\0,1\C,-1.2071571922,-0.0000688273,-2.7279949745\O,-1.2
21431851,0.0000565187,-1.3174766412\C,0.0754780745,-0.0000865475,-0.75
69923309\H,-0.7023498108,-0.8932059953,-3.1307836963\H,-2.2483551488,0
.0000871676,-3.0610783951\H,-0.7020329325,0.8928192363,-3.1309382635\H
,0.6464388085,-0.8885645902,-1.0739110947\H,0.6467091087,0.8881544017,
-1.0740881482\C,1.2071571922,0.0000688273,2.7279949745\O,1.221431851,-
0.0000565187,1.3174766412\C,-0.0754780745,0.0000865475,0.7569923309\H,
0.7023498108,0.8932059953,3.1307836963\H,2.2483551488,-0.0000871676,3.
0610783951\H,0.7020329325,-0.8928192363,3.1309382635\H,-0.6464388085,0
.8885645902,1.0739110947\H,-0.6467091087,-0.8881544017,1.0740881482\#V
ersion=IA64L-G03RevC.02\State=1-AG\HF=-308.8559544\RMSD=3.837e-09\RMSF
=1.662e-04\Dipole=0.,0.,0.\PG=CI [X(C4H10O2)]\@

n.OCHO-H2CCH2-OCHO

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H6O4\CYL509\15-Jul-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.OCHO-H2C
CH2-OCHO.freq\0,1\C,0.7343145704,0.0004478442,0.1919992225\O,0.764427

```
4563,0.0003095331,1.6338139368\C,1.9901212709,0.0008146527,2.188809501
4\O,3.0353171581,0.0013336449,1.5889383706\H,1.2502384891,-0.885048414
2,-0.1904943601\H,1.2490982871,0.8866952383,-0.1902959277\H,1.88526314
9,0.0005937316,3.2839397615\C,-0.7343145704,-0.0004478442,-0.191999222
5\O,-0.7644274563,-0.0003095331,-1.6338139368\C,-1.9901212709,-0.00081
46527,-2.1888095014\O,-3.0353171581,-0.0013336449,-1.5889383706\H,-1.2
502384891,0.8850484142,0.1904943601\H,-1.2490982871,-0.8866952383,0.19
02959277\H,-1.885263149,-0.0005937316,-3.2839397615\\Version=IA64L-G03
RevC.02\State=1-AG\HF=-456.9286333\RMSD=6.323e-09\RMSF=5.491e-05\Dipol
e=0.,0.,0.\PG=CI [X(C4H6O4)]\\@
```

n.OCOCH3-H2CCH2-OCOCH3

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H10O4\CYL509\15-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCOCH3-
H2CCH2-OCOCH3.freq\\0,1\C,0.734395054,0.0000657071,0.1926849597\O,0.76
56850372,-0.0002904678,1.6307557333\C,2.0021430298,-0.0000434549,2.190
6883449\C,1.9072881581,-0.0020177574,3.6977501062\O,3.0243630784,0.000
7653793,1.5432721824\H,1.2494436991,0.8851269779,-0.192844075\H,1.2497
081272,-0.8846447152,-0.1933111784\H,2.9109154412,0.0066878984,4.12378
61182\H,1.3653232063,-0.8898879287,4.0397519952\H,1.348075382,0.874102
717,4.0419356379\C,-0.734395054,-0.0000657071,-0.1926849597\O,-0.76568
50372,0.0002904678,-1.6307557333\C,-2.0021430298,0.0000434549,-2.19068
83449\C,-1.9072881581,0.0020177574,-3.6977501062\O,-3.0243630784,-0.00
07653793,-1.5432721824\H,-1.2494436991,-0.8851269779,0.192844075\H,-1.
2497081272,0.8846447152,0.1933111784\H,-2.9109154412,-0.0066878984,-4.
1237861182\H,-1.3653232063,0.8898879287,-4.0397519952\H,-1.348075382,-
0.874102717,-4.0419356379\\Version=IA64L-G03RevC.02\State=1-AG\HF=-535
.5803683\RMSD=3.913e-09\RMSF=5.150e-05\Dipole=0.,0.,0.\PG=CI [X(C6H10O
4)]\\@
```

n.Si_CH3_3-H2CCH2-Si_CH3_3

```
1\1\GINC-AC27\FOpt\RB3LYP\Gen\C8H22Si2\CYL509\16-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Si_CH3
_3-H2CCH2-Si_CH3_3.freq\\0,1\H,1.280817154,-0.6857306541,-4.0336985355
\C,1.2643141836,-0.7323026784,-2.937851518\H,2.3058698035,-0.743581661
8,-2.5936046713\H,0.8131921739,-1.6916091019,-2.6575371918\Si,0.308300
5956,0.7336355492,-2.2058727905\C,-1.4779451004,0.7010773349,-2.843840
4728\C,0.3224583704,0.636202815,-0.3036451527\C,1.1361783336,2.3527428
594,-2.7474441408\H,-1.5081901744,0.7713583084,-3.9381326333\H,-2.0614
524083,1.5397620758,-2.4443481179\H,-1.9931939534,-0.224529848,-2.5607
352283\H,2.1750313483,2.4076264966,-2.3993944605\H,0.6079435703,3.2266
418786,-2.3466511057\H,1.1498665887,2.4492379091,-3.8400550542\H,1.366
5812794,0.7226495993,0.0324722284\H,-0.1823401322,1.5331060303,0.08546
80341\H,-1.280817154,0.6857306541,4.0336985355\C,-1.2643141836,0.73230
26784,2.937851518\H,-2.3058698035,0.7435816618,2.5936046713\H,-0.81319
21739,1.6916091019,2.6575371918\Si,-0.3083005956,-0.7336355492,2.20587
27905\C,1.4779451004,-0.7010773349,2.8438404728\C,-0.3224583704,-0.636
202815,0.3036451527\C,-1.1361783336,-2.3527428594,2.7474441408\H,1.508
1901744,-0.7713583084,3.9381326333\H,2.0614524083,-1.5397620758,2.4443
481179\H,1.9931939534,0.224529848,2.5607352283\H,-2.1750313483,-2.4076
264966,2.3993944605\H,-0.6079435703,-3.2266418786,2.3466511057\H,-1.14
98665887,-2.4492379091,3.8400550542\H,-1.3665812794,-0.7226495993,-0.0
324722284\H,0.1823401322,-1.5331060303,-0.0854680341\\Version=IA64L-G0
3RevC.02\State=1-AG\HF=-897.1717968\RMSD=7.711e-09\RMSF=2.405e-05\Dipo
le=0.,0.,0.\PG=CI [X(C8H22Si2)]\\@
```

n.P_CH3_2-H2CCH2-P_CH3_2

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H16P2\CYL509\15-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.P_CH3_2
```

-H2CCH2-P_CH3_2.freq\\0,1\C,2.9972907272,-0.3175001167,0.3853789179\H,
2.9336503701,-0.366038241,1.4781110071\H,4.0529364232,-0.1860316193,0.
1240076342\H,2.6557351311,-1.2720975362,-0.0306796759\H,2.037620255,1.
1614644967,-0.2319743225\C,2.0718202099,0.8137095103,-2.0669030905\C,0.
.268146438,0.6853732555,0.2158550559\H,1.4015293692,1.5087183679,-2.58
47155764\H,1.787139742,-0.2117616704,-2.328332324\H,3.0852760844,0.995
6819777,-2.440772077\H,0.2110684598,0.794448377,1.3063377641\H,-0.3557
006185,1.4890143493,-0.1955040498\C,-2.9972907272,0.3175001167,-0.3853
789179\H,-2.9336503701,0.366038241,-1.4781110071\H,-4.0529364232,0.186
0316193,-0.1240076342\H,-2.6557351311,1.2720975362,0.0306796759\H,-2.0
37620255,-1.1614644967,0.2319743225\C,-2.0718202099,-0.8137095103,2.06
69030905\C,-0.268146438,-0.6853732555,-0.2158550559\H,-1.4015293692,-1.
.5087183679,2.5847155764\H,-1.787139742,0.2117616704,2.328332324\H,-3.
0852760844,-0.9956819777,2.440772077\H,-0.2110684598,-0.794448377,-1.3
063377641\H,0.3557006185,-1.4890143493,0.1955040498\\Version=IA64L-G03
RevC.02\State=1-AG\HF=-920.9872581\RMSE=5.424e-09\RMSF=2.056e-05\Dipole
=0.,0.,0.\PG=CI [X(C6H16P2)]\\@

n.SC_CH3_2CN-H2CCH2-SC_CH3_2CN

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C10H16N2S2\CYL509\15-Jul-2008\0\\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SC_C
H3_2CN-H2CCH2-SC_CH3_2CN.freq\\0,1\C,-0.7082503376,-0.0469915398,0.285
9801045\H,-0.6704269212,-0.1168202841,1.3764609743\S,-1.513774717,-1.5
461379405,-0.4188233508\C,-3.301716091,-1.3061333704,0.0699171153\C,-3.
.4903128071,-1.3510645965,1.5983362725\C,-4.076388784,-2.4507416093,-0.
.6155641415\C,-3.7607330634,-0.0100538436,-0.4514752294\H,-3.132113313
2,-2.3114929278,1.9797199767\H,-2.9419617597,-0.5483504461,2.098295213
5\H,-4.551821994,-1.2422161696,1.8489552075\H,-3.9623175502,-2.4128752
11,-1.7019955001\H,-5.1411468709,-2.374994751,-0.3724114733\H,-3.70409
4892,-3.4140834435,-0.2532653391\N,-4.1084520572,1.0282546479,-0.84065
90197\H,-1.2972395015,0.831427218,0.0030480548\C,0.7082503376,0.046991
5398,-0.2859801045\H,0.6704269212,0.1168202841,-1.3764609743\S,1.51377
4717,1.5461379405,0.4188233508\C,3.301716091,1.3061333704,-0.069917115
3\C,3.4903128071,1.3510645965,-1.5983362725\C,4.076388784,2.4507416093
,0.6155641415\C,3.7607330634,0.0100538436,0.4514752294\H,3.1321133132,
2.3114929278,-1.9797199767\H,2.9419617597,0.5483504461,-2.0982952135\H
,4.551821994,1.2422161696,-1.8489552075\H,3.9623175502,2.412875211,1.7
019955001\H,5.1411468709,2.374994751,0.3724114733\H,3.704094892,3.4140
834435,0.2532653391\N,4.1084520572,-1.0282546479,0.8406590197\H,1.2972
395015,-0.831427218,-0.0030480548\\Version=IA64L-G03RevC.02\State=1-AG
\HF=-1296.5516164\RMSE=4.382e-09\RMSF=5.075e-06\Dipole=0.,0.,0.\PG=CI
[X(C10H16N2S2)]\\@

n.SCH2COOCH3-H2CCH2-SCH2COOCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H14O4S2\CYL509\15-Jul-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2C
OOCH3-H2CCH2-SCH2COOCH3.freq\\0,1\S,0.2693235635,-0.665615251,-2.13869
93774\C,0.2351066324,-0.6641574303,-0.295433455\H,1.2710501349,-0.8724
70769,-0.0103063234\H,-0.3856321518,-1.4953167589,0.0478321801\C,-1.51
82365953,-0.8823784539,-2.5345979124\C,-1.9927367243,-2.27060859,-2.16
65946316\O,-2.3287504993,-2.6072607909,-1.0490454879\O,-1.9642341158,-
3.1011187732,-3.2266576647\C,-2.3263832292,-4.4653208338,-2.9505030556
\H,-2.117954418,-0.1425454955,-1.9994803452\H,-1.6032295745,-0.7110119
022,-3.6094409824\H,-3.3431052963,-4.5193005256,-2.5528094832\H,-1.635
9020195,-4.9031140254,-2.2248858865\H,-2.2585153951,-4.9839905269,-3.9
069065258\S,-0.2693235635,0.665615251,2.1386993774\C,-0.2351066324,0.6
641574303,0.295433455\H,-1.2710501349,0.872470769,0.0103063234\H,0.385
6321518,1.4953167589,-0.0478321801\C,1.5182365953,0.8823784539,2.53459
79124\C,1.9927367243,2.27060859,2.1665946316\O,2.3287504993,2.60726079

09,1.0490454879\O,1.9642341158,3.1011187732,3.2266576647\C,2.326383229
2,4.4653208338,2.9505030556\H,2.117954418,0.1425454955,1.9994803452\H,
1.6032295745,0.7110119022,3.6094409824\H,3.3431052963,4.5193005256,2.5
528094832\H,1.6359020195,4.9031140254,2.2248858865\H,2.2585153951,4.98
39905269,3.9069065258\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1410.56
76572\RMSD=3.993e-09\RMSF=8.029e-06\Dipole=0.,0.,0.\PG=CI [X(C8H14O4S2
)J]\@

n.SCH2Ph-H2CCH2-SCH2Ph

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C16H18S2\CYL509\15-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2Ph
-H2CCH2-SCH2Ph.freq\\0,1\C,0.7245521358,-0.0504285665,0.2365993434\S,0
.7617225434,-0.0142509772,2.0755155926\C,2.5873145534,-0.0373689107,2.
3688223416\H,1.3157100211,0.7867568091,-0.1469085217\C,3.3361580421,1.
1694386454,1.8572373298\H,2.9978706527,-0.9586131864,1.9424752538\H,2.
6687978159,-0.1178308834,3.4581550272\C,4.2113033741,1.0550924321,0.77
01775544\C,3.1767072574,2.425455457,2.4612574448\C,4.9144420604,2.1658
409489,0.2967333431\C,3.8785473266,3.5340954696,1.9936013815\C,4.75061
66099,3.4080785194,0.9080182071\H,5.2972514679,4.2735807925,0.54337403
83\H,3.7466580333,4.4989940857,2.4762272124\H,5.5892365751,2.057020612
9,-0.5482507269\H,2.4909083359,2.5306254419,3.2984691111\H,4.349009065
2,0.0866609243,0.2939466244\H,1.1747974005,-0.9850470603,-0.1149961204
\C,-0.7245521358,0.0504285665,-0.2365993434\S,-0.7617225434,0.01425097
72,-2.0755155926\C,-2.5873145534,0.0373689107,-2.3688223416\H,-1.31571
00211,-0.7867568091,0.1469085217\C,-3.3361580421,-1.1694386454,-1.8572
373298\H,-2.9978706527,0.9586131864,-1.9424752538\H,-2.6687978159,0.11
78308834,-3.4581550272\C,-4.2113033741,-1.0550924321,-0.7701775544\C,-
3.1767072574,-2.425455457,-2.4612574448\C,-4.9144420604,-2.1658409489,
-0.2967333431\C,-3.8785473266,-3.5340954696,-1.9936013815\C,-4.7506166
099,-3.4080785194,-0.9080182071\H,-5.2972514679,-4.2735807925,-0.54337
40383\H,-3.7466580333,-4.4989940857,-2.4762272124\H,-5.5892365751,-2.0
570206129,0.5482507269\H,-2.4909083359,-2.5306254419,-3.2984691111\H,-
4.3490090652,-0.0866609243,-0.2939466244\H,-1.1747974005,0.9850470603,
0.1149961204\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1416.9258149\RMS
D=4.838e-09\RMSF=8.144e-06\Dipole=0.,0.,0.\PG=CI [X(C16H18S2)]\@

n.SCH3-H2CCH2-SCH3

1\1\GINC-AC11\FOpt\RB3LYP\Gen\C4H10S2\CYL509\27-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.SCH3-H2
CCH2-SCH3.freq\\0,1\S,0.7738087614,0.,-2.0743577462\C,0.7263983376,0.,
-0.2357779597\C,2.5831828481,0.,-2.3241413618\H,2.7555607515,0.,-3.403
5700954\H,1.2476103483,0.8883897329,0.1373198161\H,3.043566294,0.89474
11057,-1.8939424864\H,1.2476103483,-0.8883897329,0.1373198161\H,3.0435
66294,-0.8947411057,-1.8939424864\S,-0.7738087614,0.,2.0743577462\C,-0
.7263983376,0.,0.2357779597\C,-2.5831828481,0.,2.3241413618\H,-2.75556
07515,0.,3.4035700954\H,-1.2476103483,-0.8883897329,-0.1373198161\H,-3
.043566294,-0.8947411057,1.8939424864\H,-1.2476103483,0.8883897329,-0.
1373198161\H,-3.043566294,0.8947411057,1.8939424864\\Version=IA64L-G03
RevC.02\State=1-AG\HF=-954.8247163\RMSD=3.009e-09\RMSF=1.308e-05\Dipol
e=0.,0.,0.\PG=C02H [SGH(C4H2S2),X(H8)]\@

n.SO2CH3-H2CCH2-SO2CH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10O4S2\CYL509\22-Aug-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SO2CH
3-H2CCH2-SO2CH3.freq\\0,1\C,-1.738373119,-0.0000015791,-3.0481408419\S
, -1.8049481422,0.0000016127,-1.2420515056\C,-0.044352694,-0.000001409,
-0.7607236953\O,-2.387335898,1.2773373909,-0.80142946\O,-2.387341632,-
1.2773300656,-0.8014251622\H,0.4204552247,-0.8957262865,-1.1817817781\H,
0.4204590317,0.8957202348,-1.1817843806\H,-1.2301526683,-0.902545799

```
9,-3.3936617509\H,-1.2301482614,0.9025390007,-3.3936647879\H,-2.777030
9721,0.000000403,-3.387327865\C,1.7383731137,0.0000004254,3.0481408415
\S,1.8049481424,-0.0000013939,1.2420515053\C,0.0443526954,0.0000005401
,0.7607236912\O,2.3873369739,-1.2773364352,0.8014286005\O,2.3873405608
,1.2773310212,0.8014260268\H,-0.4204558403,0.8957249925,1.1817819213\H
,-0.4204584142,-0.8957215286,1.1817842286\H,1.2301511832,0.9025435705,
3.3936623757\H,1.2301497343,-0.9025412301,3.3936641599\H,2.7770309659,
-0.0000000124,3.3873278673\\Version=IA64L-G03RevC.02\State=1-A\HF=-125
5.6001787\RMSD=6.126e-09\RMSF=7.283e-05\Dipole=0.,-0.0000033,0.\PG=C01
[X(C4H10O4S2)]\\@
```

n.SOCH3-H2CCH2-SOCH3

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H10O2S2\CYL509\16-Jul-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SOCH3
-H2CCH2-SOCH3.freq\\0,1\C,-0.3412147917,0.6386384417,0.2424201297\S,-0
.4183399309,0.7512629892,2.0643115156\O,1.2342497487,0.7630433735,2.44
36370209\C,1.813202176,2.0716987674,2.494547304\H,0.1497171984,1.52508
12077,-0.1719230903\H,2.8596590133,1.9197202737,2.7755925726\H,1.31897
77792,2.6997282473,3.2447498295\H,1.7705043638,2.574687851,1.519922978
6\H,-1.3875891055,0.661731082,-0.0843274274\C,0.3412147917,-0.63863844
17,-0.2424201297\S,0.4183399309,-0.7512629892,-2.0643115156\O,-1.23424
97487,-0.7630433735,-2.4436370209\C,-1.813202176,-2.0716987674,-2.4945
47304\H,-0.1497171984,-1.5250812077,0.1719230903\H,-2.8596590133,-1.91
97202737,-2.7755925726\H,-1.3189777792,-2.6997282473,-3.2447498295\H,-
1.7705043638,-2.574687851,-1.5199229786\H,1.3875891055,-0.661731082,0.
0843274274\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1105.1983955\RMSD=
5.326e-09\RMSF=7.745e-06\Dipole=0.,0.,0.\PG=CI [X(C4H10O2S2)]\\@
```

n.Ph-H2CCH2-Ph

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C14H14\CYL509\15-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Ph-H2CCH
2-Ph.freq\\0,1\C,-0.0010765342,0.0008359981,-0.7758066757\H,1.03807536
42,-0.0028037399,-1.1278981838\H,-0.4518799153,-0.9358506446,-1.126824
6892\C,-0.7427152114,1.1845197434,-1.3577288668\C,-2.1390710264,3.4134
047829,-2.3692949651\C,-2.1187302062,1.1151604784,-1.6153585404\C,-0.0
792948828,2.3912925449,-1.6187447156\C,-0.768049807,3.4966582047,-2.11
96649074\C,-2.812839244,2.2171660666,-2.116259987\H,-2.6499405093,0.18
41943189,-1.4269221483\H,0.9906662593,2.4622306166,-1.4328997093\H,-0.
2327894731,4.4215102181,-2.3193948953\H,-3.8791097479,2.1398853357,-2.
3133536665\H,-2.6770259135,4.2720654916,-2.7621690417\C,0.0010765342,-
0.0008359981,0.7758066757\H,-1.0380753642,0.0028037399,1.1278981838\H,
0.4518799153,0.9358506446,1.1268246892\C,0.7427152114,-1.1845197434,1.
3577288668\C,2.1390710264,-3.4134047829,2.3692949651\C,2.1187302062,-1
.1151604784,1.6153585404\C,0.0792948828,-2.3912925449,1.6187447156\C,0
.768049807,-3.4966582047,2.1196649074\C,2.812839244,-2.2171660666,2.11
6259987\H,2.6499405093,-0.1841943189,1.4269221483\H,-0.9906662593,-2.4
622306166,1.4328997093\H,0.2327894731,-4.4215102181,2.3193948953\H,3.8
791097479,-2.1398853357,2.3133536665\H,2.6770259135,-4.2720654916,2.76
21690417\\Version=IA64L-G03RevC.02\State=1-AG\HF=-541.930358\RMSD=4.60
7e-09\RMSF=4.273e-05\Dipole=0.,0.,0.\PG=CI [X(C14H14)]\\@
```

n.C6H4CN-H2CCH2-C6H4CN

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C16H12N2\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4CN
-H2CCH2-C6H4CN.freq\\0,1\C,-0.0022598893,0.0020521925,-0.7764915869\H,
1.0348074799,-0.0002814246,-1.1329524937\H,-0.4582999949,-0.9300916057
,-1.1310524321\C,-0.7428765767,1.1901981368,-1.3477773371\C,-2.1369684
486,3.4269518962,-2.3396627599\C,-2.12096638,1.1241709383,-1.599488270
3\C,-0.0757403109,2.3968797326,-1.6040213609\C,-0.7562889075,3.5066716
```

85,-2.093989513\C,-2.817564555,2.22396617,-2.0894052223\H,-2.655144336
1,0.1952057647,-1.41500634\H,0.9942148595,2.4661371019,-1.4230446937\H
, -0.2285274973,4.4339045763,-2.2928807039\H,-3.8831855706,2.1596646687
, -2.2847777909\C,-2.8462401972,4.5648589879,-2.8472915677\N,-3.4219914
645,5.4884775836,-3.2584124513\C,0.0022598893,-0.0020521925,0.77649158
69\H,-1.0348074799,0.0002814246,1.1329524937\H,0.4582999949,0.93009160
57,1.1310524321\C,0.7428765767,-1.1901981368,1.3477773371\C,2.13696844
86,-3.4269518962,2.3396627599\C,2.12096638,-1.1241709383,1.5994882703\
C,0.0757403109,-2.3968797326,1.6040213609\C,0.7562889075,-3.506671685,
2.093989513\C,2.817564555,-2.22396617,2.0894052223\H,2.6551443361,-0.1
952057647,1.41500634\H,-0.9942148595,-2.4661371019,1.4230446937\H,0.22
85274973,-4.4339045763,2.2928807039\H,3.8831855706,-2.1596646687,2.284
7777909\C,2.8462401972,-4.5648589879,2.8472915677\N,3.4219914645,-5.48
84775836,3.2584124513\\Version=IA64L-G03RevC.02\State=1-AG\HF=-726.417
8093\RMSD=6.486e-09\RMSF=9.622e-06\Dipole=0.,0.,0.\PG=CI [X(C16H12N2)]
\\@

n.C6H4NO2-H2CCH2-C6H4NO2

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C14H12N2O4\CYL509\14-Jul-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4
NO2-H2CCH2-C6H4NO2.freq\\0,1\O,-5.5714255937,-0.8292806839,-3.71538633
12\N,-5.5170928299,-0.6571190447,-2.4977660697\C,-4.1905812601,-0.6794
140299,-1.8635040394\C,-4.0950172272,-0.4894769998,-0.4864422606\C,-2.
8351515481,-0.5147881194,0.1039452415\C,-1.6779660792,-0.7265607361,-0.
.6610994688\C,-1.8144056305,-0.9162179619,-2.0448167418\C,-3.064603119
9,-0.8946607274,-2.6555618164\C,-0.3112581537,-0.7113643361,-0.0146496
249\O,-6.4938804451,-0.4665203914,-1.7733655703\H,-0.3779052112,-1.089
6920638,1.0123108992\H,0.3665153511,-1.3831702635,-0.55458114\H,-0.929
541885,-1.0898648759,-2.6520249771\H,-2.7491706706,-0.3742170548,1.178
5055089\H,-4.9949757904,-0.3313451476,0.0949596209\H,-3.1818368098,-1.
044284964,-3.7217869157\O,5.5714255937,0.8292806839,3.7153863312\N,5.5
170928299,0.6571190447,2.4977660697\C,4.1905812601,0.6794140299,1.8635
040394\C,4.0950172272,0.4894769998,0.4864422606\C,2.8351515481,0.51478
81194,-0.1039452415\C,1.6779660792,0.7265607361,0.6610994688\C,1.81440
56305,0.9162179619,2.0448167418\C,3.0646031199,0.8946607274,2.65556181
64\C,0.3112581537,0.7113643361,0.0146496249\O,6.4938804451,0.466520391
4,1.7733655703\H,0.3779052112,1.0896920638,-1.0123108992\H,-0.36651535
11,1.3831702635,0.55458114\H,0.929541885,1.0898648759,2.6520249771\H,2.
7491706706,0.3742170548,-1.1785055089\H,4.9949757904,0.3313451476,-0.
0949596209\H,3.1818368098,1.044284964,3.7217869157\\Version=IA64L-G03R
evC.02\State=1-AG\HF=-950.9344672\RMSD=3.855e-09\RMSF=1.285e-05\Dipole
=0.,0.,0.\PG=CI [X(C14H12N2O4)]\\@

n.C6H4OCH3-H2CCH2-C6H4OCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C16H18O2\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4OC
H3-H2CCH2-C6H4OCH3.freq\\0,1\C,-3.7740573593,-0.9957305622,1.423731749
2\C,-3.7122392658,-0.6556350153,2.7828079997\C,-2.4764996697,-0.338553
0519,3.3560954002\C,-1.3233900486,-0.3633333699,2.5653928799\C,-1.3638
169449,-0.6974699338,1.2094050933\C,-2.6159866475,-1.0139229345,0.6570
377613\C,-0.1147365327,-0.679699477,0.3558940766\O,-4.9039519956,-0.66
86972846,3.4535823889\C,-4.8986923581,-0.3352609341,4.8310423075\H,-0.
1677985844,-1.467584787,-0.4063298569\H,0.7645431066,-0.9054986885,0.9
722607002\H,-2.682517639,-1.2857940024,-0.3945797145\H,-0.3684477288,-
0.1192072635,3.0267052685\H,-2.3966038448,-0.0785748058,4.4056526379\H
, -4.7396579861,-1.2463964777,0.9951775548\H,-4.2850593546,-1.034487109
3,5.4151083058\H,-5.9369014652,-0.4060066593,5.1612480229\H,-4.5345794
926,0.6873441936,4.9992436381\C,3.7740573593,0.9957305622,-1.423731749
2\C,3.7122392658,0.6556350153,-2.7828079997\C,2.4764996697,0.338553051

9,-3.3560954002\C,1.3233900486,0.3633333699,-2.5653928799\C,1.36381694
49,0.6974699338,-1.2094050933\C,2.6159866475,1.0139229345,-0.657037761
3\C,0.1147365327,0.679699477,-0.3558940766\O,4.9039519956,0.6686972846
, -3.4535823889\C,4.8986923581,0.3352609341,-4.8310423075\H,0.167798584
4,1.467584787,0.4063298569\H,-0.7645431066,0.9054986885,-0.9722607002\
H,2.682517639,1.2857940024,0.3945797145\H,0.3684477288,0.1192072635,-3
.0267052685\H,2.3966038448,0.0785748058,-4.4056526379\H,4.7396579861,1
.2463964777,-0.9951775548\H,4.2850593546,1.0344871093,-5.4151083058\H,
5.9369014652,0.4060066593,-5.1612480229\H,4.5345794926,-0.6873441936,-
4.9992436381\\Version=IA64L-G03RevC.02\State=1-AG\HF=-770.9748193\RMSD
=7.759e-09\RMSF=7.043e-07\Dipole=0.,0.,0.\PG=CI [X(C16H18O2)]\@

n.C6H4OH-H2CCH2-C6H4OH

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C14H14O2\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4OH
-H2CCH2-C6H4OH.freq\\0,1\C,-3.8718705818,0.9202791957,1.2196227332\C,-
3.8222158038,0.7244490358,2.6035796784\C,-2.587529223,0.5391495847,3.2
318673176\C,-1.4151409222,0.54849324,2.4753748085\C,-1.4404535905,0.74
07369795,1.0893108193\C,-2.6916473806,0.9264019618,0.4819898111\C,-0.1
69416052,0.707614429,0.2689763442\O,-5.0094467265,0.7297741725,3.28652
18002\H,0.6758088266,1.0651804332,0.8705637471\H,-0.253397299,1.394177
3002,-0.5830948501\H,-2.743261732,1.0853583313,-0.5932761862\H,-0.4612
123884,0.4080307634,2.9795238348\H,-2.5409950666,0.3934302587,4.310084
1247\H,-4.8361829715,1.0702229993,0.7440550815\H,-4.8290666019,0.58658
80705,4.2284750351\C,3.8718705818,-0.9202791957,-1.2196227332\C,3.8222
158038,-0.7244490358,-2.6035796784\C,2.587529223,-0.5391495847,-3.2318
673176\C,1.4151409222,-0.54849324,-2.4753748085\C,1.4404535905,-0.7407
369795,-1.0893108193\C,2.6916473806,-0.9264019618,-0.4819898111\C,0.16
9416052,-0.707614429,-0.2689763442\O,5.0094467265,-0.7297741725,-3.286
5218002\H,-0.6758088266,-1.0651804332,-0.8705637471\H,0.253397299,-1.3
941773002,0.5830948501\H,2.743261732,-1.0853583313,0.5932761862\H,0.46
12123884,-0.4080307634,-2.9795238348\H,2.5409950666,-0.3934302587,-4.3
100841247\H,4.8361829715,-1.0702229993,-0.7440550815\H,4.8290666019,-0
.5865880705,-4.2284750351\\Version=IA64L-G03RevC.02\State=1-AG\HF=-692
.3618044\RMSD=5.181e-09\RMSF=7.227e-06\Dipole=0.,0.,0.\PG=CI [X(C14H14
O2)]\@

n.CF2CF3-H2CCH2-CF2CF3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H4F10\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF2CF3-
H2CCH2-CF2CF3.freq\\0,1\F,1.5950637574,1.1022635888,-1.6174923467\C,1.
5731415318,1.0905070152,-0.2510957565\C,3.0407394442,1.0451496346,0.22
21863603\C,0.720668082,-0.0561482447,0.2554253815\F,1.0580180817,2.287
249086,0.1613182144\F,3.6235742101,-0.0931341768,-0.1947911604\F,3.092
0095935,1.0799706453,1.5658484997\F,3.7309359327,2.0829605335,-0.26092
73652\H,0.7425235413,-0.0432388649,1.3486387942\H,1.1739293375,-0.9939
62147,-0.0775065986\F,-1.5950637574,-1.1022635888,1.6174923467\C,-1.57
31415318,-1.0905070152,0.2510957565\C,-3.0407394442,-1.0451496346,-0.2
221863603\C,-0.720668082,0.0561482447,-0.2554253815\F,-1.0580180817,-2
.287249086,-0.1613182144\F,-3.6235742101,0.0931341768,0.1947911604\F,-
3.0920095935,-1.0799706453,-1.5658484997\F,-3.7309359327,-2.0829605335
,0.2609273652\H,-0.7425235413,0.0432388649,-1.3486387942\H,-1.17392933
75,0.993962147,0.0775065986\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1
229.4671963\RMSD=6.787e-09\RMSF=2.222e-05\Dipole=0.,0.,0.\PG=CI [X(C6H
4F10)]\@

n.CF2H-H2CCH2-CF2H

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H6F4\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF2H-H2C

CH2-CF2H.freq\0,1\C,0.3963551797,-0.690881752,-1.7666301537\C,0.3588900575,-0.6271630461,-0.2561107859\H,1.38844252,-0.6504841669,0.1162505526\H,0.9061835128,-1.5804572414,-2.1530800408\F,1.0377601289,0.4124757618,-2.2704588181\F,-0.8794518804,-0.6857583559,-2.2715324275\H,-0.1434739572,-1.526626845,0.115060311\C,-0.3963551797,0.690881752,1.7666301537\C,-0.3588900575,0.6271630461,0.2561107859\H,-1.38844252,0.6504841669,-0.1162505526\H,-0.9061835128,1.5804572414,2.1530800408\F,-1.0377601289,-0.4124757618,2.2704588181\F,0.8794518804,0.6857583559,2.2715324275\H,0.1434739572,1.526626845,-0.115060311\\Version=IA64L-G03RevC.02\State=1-AG\HF=-555.4017375\RMSD=8.359e-09\RMSF=9.662e-05\Dipole=0.,0.,0.\PG=CI [X(C4H6F4)]\\@

n.CF3-H2CCH2-CF3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H4F6\CYL509\14-Jul-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF3-H2CCH2-CF3.freq\0,1\F,0.6878993817,1.0831972126,-2.7298371436\C,0.7265026993,1.1419633617,-1.3832190309\F,2.0272725561,1.1578418123,-1.0125775517\C,-0.0144654558,-0.0224104445,-0.765327588\F,0.191263677,2.3271207265,-1.0109483301\H,-1.0444311387,0.0055542384,-1.1327474442\H,0.4467981723,-0.943593126,-1.1330896706\F,-0.6878993817,-1.0831972126,2.7298371436\C,-0.7265026993,-1.1419633617,1.3832190309\F,-2.0272725561,-1.1578418123,1.0125775517\C,0.0144654558,0.0224104445,0.765327588\F,-0.191263677,-2.3271207265,1.0109483301\H,1.0444311387,-0.0055542384,1.1327474442\H,-0.4467981723,0.943593126,1.1330896706\\Version=IA64L-G03RevC.02\State=1-AG\HF=-753.906447\RMSD=3.711e-09\RMSF=7.551e-05\Dipole=0.,0.,0.\PG=CI [X(C4H4F6)]\\@

n.CC12H-H2CCH2-CC12H

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H6Cl4\CYL509\21-Aug-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC12H-H2CCH2-CC12H.freq\0,1\C,0.7734661042,0.000175427,-1.8157860332\C,0.7067747226,0.0002930913,-0.2929714115\H,1.8058313033,0.0006117375,-2.1593039811\H,1.2559620488,0.8835586194,0.0516437665\H,1.2567651911,-0.8824055263,0.0518154628\C,-0.7734661042,-0.000175427,1.8157860332\C,-0.7067747226,-0.0002930913,0.2929714115\H,-1.8058313033,-0.0006117375,2.1593039811\H,-1.2559620488,-0.8835586194,-0.0516437665\H,-1.2567651911,0.8824055263,-0.0518154628\C1,-0.0248248533,-1.4868367708,2.5281835808\C1,-0.0261778272,1.487305602,2.5278933238\C1,0.0261778272,-1.487305602,-2.5278933238\C1,0.0248248533,1.4868367708,-2.5281835808\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1996.826987\RMSD=8.975e-09\RMSF=3.012e-05\Dipole=0.,0.,0.\PG=CI [X(C4H6Cl4)]\\@

n.CC13-H2CCH2-CC13

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H4Cl6\CYL509\21-Aug-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC13-H2CCH2-CC13.freq\0,1\C,0.8009473989,-0.0017219633,-1.8054672414\C,0.7157415788,-0.0086234966,-0.2750020332\H,1.2704949132,0.86542322,0.0772839819\H,1.2456110258,-0.9016241686,0.0679302662\C,-0.8009471911,0.0017219576,1.8054672563\C,-0.7157415008,0.0086235453,0.2750020283\H,-1.2704948246,-0.8654231826,-0.0772839709\H,-1.2456109543,0.9016242183,-0.0679302287\C1,-0.0345426355,-1.4822012672,2.4925470429\C1,-2.5426855949,0.0237255361,2.2819581359\C1,0.006832649,1.4561222717,2.508100951\C1,2.5426854993,-0.0237260953,-2.2819581865\C1,0.034543099,1.4822015906,-2.492547046\C1,-0.0068331272,-1.4561220561,-2.5081009037\\Version=IA64L-G03RevC.02\State=1-A\HF=-2915.9896237\RMSD=1.543e-09\RMSF=9.842e-05\Dipole=0.0000007,0.,0.\PG=C01 [X(C4H4Cl6)]\\@

n.CH2Cl-H2CCH2-CH2Cl

1\1\GINC-AC17\FOpt\RB3LYP\Gen\C4H8Cl2\CYL509\13-Jul-2008\0\\#B3LYP/GEN

```
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Cl-H
2CCH2-CH2Cl.freq\\0,1\\H,0.3875385408,0.6714624351,-1.3331171126\\C,0.36
26305314,0.6360224613,-0.2371762587\\H,1.4044469356,0.628231566,0.10558
55088\\C,-0.3265177363,1.8896531193,0.2875603729\\H,-0.3311962473,1.9221
380454,1.3793216452\\H,-1.3549731055,1.9667779845,-0.0720813166\\H,-0.38
75385408,-0.6714624351,1.3331171126\\C,-0.3626305314,-0.6360224613,0.23
71762587\\H,-1.4044469356,-0.628231566,-0.1055855088\\C,0.3265177363,-1.
8896531193,-0.2875603729\\H,0.3311962473,-1.9221380454,-1.3793216452\\H,
1.3549731055,-1.9667779845,0.0720813166\\Cl,-0.521730603,-3.3994834915,
0.2648116334\\Cl,0.521730603,3.3994834915,-0.2648116334\\Version=IA64L-
G03RevC.02\\State=1-AG\\HF=-1077.6483179\\RMSD=1.669e-09\\RMSF=2.011e-05\\D
ipole=0.,0.,0.\\PG=CI [X(C4H8Cl2)]\\@
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n.CH2F-H2CCH2-CH2F

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1\\1\\GINC-AC28\\FOpt\\RB3LYP\\Gen\\C4H8F2\\CYL509\\27-Aug-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2F-H2C
CH2-CH2F.freq\\0,1\\C,0.7194985351,0.0000002132,0.2653003995\\C,0.775502
1079,-0.0000009378,1.7846656409\\F,2.102544709,-0.0000004768,2.20431819
43\\H,0.2851100656,-0.8903750956,2.1995406009\\H,0.2851090065,0.89037199
17,2.1995419849\\H,1.2624277982,-0.8812111729,-0.1009887377\\H,1.2624267
029,0.8812128491,-0.1009873667\\C,-0.719498535,-0.0000002853,-0.2653003
995\\C,-0.7755021078,0.000000989,-1.7846656409\\F,-2.1025447091,0.000000
4932,-2.2043181942\\H,-0.2851101179,0.8903752065,-2.1995405331\\H,-0.285
1089543,-0.8903718808,-2.1995420531\\H,-1.2624278343,0.8812110462,0.100
9888164\\H,-1.2624266667,-0.8812129759,0.1009872875\\Version=IA64L-G03R
evC.02\\State=1-A\\HF=-356.9093873\\RMSD=4.152e-09\\RMSF=3.850e-05\\Dipole=
0.,0.,0.\\PG=C01 [X(C4H8F2)]\\@
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n.CH2OH-H2CCH2-CH2OH

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1\\1\\GINC-AC23\\FOpt\\RB3LYP\\Gen\\C4H10O2\\CYL509\\22-Aug-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2OH-H
2CCH2-CH2OH.freq\\0,1\\C,0.7160822558,0.,0.2729062228\\C,0.7661398034,0.
,1.7952807605\\O,2.1350533554,0.,2.1892026996\\H,1.263501554,0.880307765
9,-0.0894037761\\H,1.263501554,-0.8803077659,-0.0894037761\\H,0.24022364
03,-0.8877723515,2.1850920083\\H,0.2402236403,0.8877723515,2.1850920083
\\H,2.1660050698,0.,3.1576631968\\C,-0.7160822558,0.,-0.2729062228\\C,-0.
7661398034,0.,-1.7952807605\\O,-2.1350533554,0.,-2.1892026996\\H,-1.2635
01554,-0.8803077659,0.0894037761\\H,-1.263501554,0.8803077659,0.0894037
761\\H,-0.2402236403,0.8877723515,-2.1850920083\\H,-0.2402236403,-0.8877
723515,-2.1850920083\\H,-2.1660050698,0.,-3.1576631968\\Version=IA64L-G
03RevC.02\\State=1-AG\\HF=-308.8643082\\RMSD=4.754e-09\\RMSF=4.878e-05\\Dip
ole=0.,0.,0.\\PG=C02H [SGH(C4H2O2),X(H8)]\\@
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n.CH2Ph-H2CCH2-CH2Ph

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1\\1\\GINC-AC24\\FOpt\\RB3LYP\\Gen\\C16H18\\CYL509\\27-Aug-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Ph-H2
CCH2-CH2Ph.freq\\0,1\\C,0.7100923224,0.0000012047,0.2887174967\\C,0.7351
371273,-0.0000018655,1.8304802388\\C,2.1379350053,-0.0000037443,2.40035
74443\\C,2.811389237,-1.2027136499,2.6539557847\\C,2.8113917528,1.202704
4817,2.653957229\\C,4.1182819171,-1.2059277723,3.1432453693\\C,4.1182844
248,1.2059152831,3.1432467539\\C,4.7772061226,-0.0000070952,3.389153516
7\\H,5.7937354194,-0.0000083462,3.7735549144\\H,4.620134068,-2.150608687
7,3.3370428038\\H,4.6201385878,2.1505948997,3.3370453164\\H,2.3026946932
,-2.1470976705,2.4703194053\\H,2.302699158,2.1470897685,2.4703219647\\H,
0.1879900895,0.8794781557,2.1955688436\\H,0.1879891676,-0.8794827232,2.
1955654603\\H,1.2600438699,-0.8777769996,-0.0790079085\\H,1.2600439534,0
.8777807743,-0.0790046333\\C,-0.7100923426,0.0000021093,-0.2887174583\\C
,-0.7351371411,0.000003792,-1.8304802004\\C,-2.1379350163,0.0000037143,
-2.4003574129\\C,-2.8113890684,1.2027133068,-2.6539593689\\C,-2.81139192
```

78,-1.2027048251,-2.6539536228\C,-4.1182814851,1.205926286,-3.14324894
22\C,-4.1182848319,-1.2059167693,-3.1432432428\C,-4.7772061009,0.00000
47723,-3.3891535723\H,-5.7937353724,0.0000055314,-3.7735550329\H,-4.62
01337198,2.1506065556,-3.3370493345\H,-4.620138884,-2.1505970317,-3.33
70389184\H,-2.3026939806,2.1470975428,-2.4703256146\H,-2.3026998762,-2
.147089896,-2.4703157385\H,-0.1879890558,-0.8794758982,-2.1955680733\H
, -0.1879902237,0.8794849797,-2.1955661475\H,-1.2600437242,0.8777807238
,0.0790072882\H,-1.2600441405,-0.877777051,0.0790053271\\Version=IA64L
-G03RevC.02\State=1-A\HF=-620.5578484\RMSD=7.827e-09\RMSF=3.762e-05\Di
pole=0.,0.0000001,0.\PG=C01 [X(C16H18)]\\@

n.CH_CH2_2-H2CCH2-CH_CH2_2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H14\CYL509\27-Aug-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH_CH2_2-
H2CCH2-CH_CH2_2.freq\0,1\C,-2.607419924,1.2705944507,-0.5379650841\C,
-2.9318238251,1.057719476,0.9223520328\C,-1.493802085,1.1630365629,0.4
774695628\H,-2.7562925052,0.4340782726,-1.2172710401\H,-2.8212423258,2
.2403224182,-0.979592434\H,-3.2992815443,0.0795300438,1.2239758988\H,-
3.3655633338,1.8828911541,1.4810889141\H,-0.9930764242,2.0994436935,0.
724561375\C,-0.5839976895,-0.0503072701,0.497365379\H,-1.1770768397,-0
.9486058773,0.2705176792\H,-0.1839240453,-0.1976529952,1.5106654007\C,
2.607419924,-1.2705944507,0.5379650841\C,2.9318238251,-1.057719476,-0.
9223520328\C,1.493802085,-1.1630365629,-0.4774695628\H,2.7562925052,-0
.4340782726,1.2172710401\H,2.8212423258,-2.2403224182,0.979592434\H,3.
2992815443,-0.0795300438,-1.2239758988\H,3.3655633338,-1.8828911541,-1
.4810889141\H,0.9930764242,-2.0994436935,-0.724561375\C,0.5839976895,0
.0503072701,-0.497365379\H,1.1770768397,0.9486058773,-0.2705176792\H,0
.1839240453,0.1976529952,-1.5106654007\\Version=IA64L-G03RevC.02\State
=1-AG\HF=-313.2213503\RMSD=5.227e-09\RMSF=9.083e-06\Dipole=0.,0.,0.\PG
=CI [X(C8H14)]\\@

n.CH2CH=CH2-H2CCH2-CH2CH=CH2

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H14\CYL509\21-Aug-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2CH=CH2
-H2CCH2-CH2CH=CH2.freq\0,1\H,0.3117030353,0.6976631776,-1.333995736\C
,0.31269278,0.6591504137,-0.2358918154\H,1.3686272,0.6921810737,0.0700
847983\C,-0.4137014588,1.9031516765,0.3107549286\C,0.2303869699,3.1938
230304,-0.1169134117\H,-0.423107238,1.8467694756,1.4104797492\H,-1.463
535048,1.8896289573,-0.0112703246\H,1.2678507781,3.331046239,0.1949612
282\C,-0.3568557309,4.1463349708,-0.8422471911\H,0.1657123928,5.056068
8283,-1.1261136009\H,-1.3881675505,4.0542730337,-1.1781460379\H,-0.311
7030353,-0.6976631776,1.333995736\C,-0.31269278,-0.6591504137,0.235891
8154\H,-1.3686272,-0.6921810737,-0.0700847983\C,0.4137014588,-1.903151
6765,-0.3107549286\C,-0.2303869699,-3.1938230304,0.1169134117\H,0.4231
07238,-1.8467694756,-1.4104797492\H,1.463535048,-1.8896289573,0.011270
3246\H,-1.2678507781,-3.331046239,-0.1949612282\C,0.3568557309,-4.1463
349708,0.8422471911\H,-0.1657123928,-5.0560688283,1.1261136009\H,1.388
1675505,-4.0542730337,1.1781460379\\Version=IA64L-G03RevC.02\State=1-A
G\HF=-313.2393114\RMSD=2.772e-09\RMSF=6.154e-06\Dipole=0.,0.,0.\PG=CI
[X(C8H14)]\\@

n.CH2CH3-H2CCH2-CH2CH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H14\CYL509\21-Aug-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2CH3-H2
CCH2-CH2CH3.freq\0,1\C,-0.3820422405,0.6071917643,0.271186387\H,0.074
9569194,1.5288102068,-0.1198071397\C,-0.4221063531,0.6745566613,1.8030
994409\H,-1.4114999685,0.5924915093,-0.1175415187\H,0.6062814381,0.690
125571,2.191613309\H,-0.8795353824,-0.2456562355,2.1938964752\C,-1.187
0583603,1.8904519179,2.3359107267\H,-1.197061151,1.9091767967,3.431749

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3645\H,-0.7322433108,2.8273307881,1.9909166371\H,-2.2292872834,1.88444
44655,1.9933625806\C,0.3820422405,-0.6071917643,-0.271186387\H,-0.0749
569194,-1.5288102068,0.1198071397\C,0.4221063531,-0.6745566613,-1.8030
994409\H,1.4114999685,-0.5924915093,0.1175415187\H,-0.6062814381,-0.69
0125571,-2.191613309\H,0.8795353824,0.2456562355,-2.1938964752\C,1.187
0583603,-1.8904519179,-2.3359107267\H,1.197061151,-1.9091767967,-3.431
7493645\H,0.7322433108,-2.8273307881,-1.9909166371\H,2.2292872834,-1.8
844444655,-1.9933625806\\Version=IA64L-G03RevC.02\State=1-AG\HF=-237.0
854815\RMSD=7.206e-09\RMSF=3.962e-05\Dipole=0.,0.,0.\PG=CI [X(C6H14)]\
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n.CH_CH3_2-H2CCH2-CH_CH3_2

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H18\CYL509\14-Jul-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH_CH3_2-
H2CCH2-CH_CH3_2.freq\0,1\C,0.0547419997,-2.6772984618,-0.7593336398\H
,-0.0141325727,-2.8007380014,0.3280692462\H,1.1185315239,-2.6371457401
,-1.0241894581\H,-0.3694067445,-3.5789865926,-1.2171744012\C,-0.688984
1425,-1.4201571845,-1.2379114862\C,-2.181301226,-1.4908923654,-0.87655
88453\H,-0.6246746271,-1.407452805,-2.336508482\C,-0.018529177,-0.1093
818228,-0.7609141867\H,-0.5432268946,0.7306743068,-1.2363071555\H,1.00
65059514,-0.0912254298,-1.1558733851\H,-2.7193906445,-0.6009061147,-1.
2255477489\H,-2.3337015359,-1.5698446523,0.2064494932\H,-2.6525840318,
-2.3676645062,-1.3367013826\C,-0.0547419997,2.6772984618,0.7593336398\
H,0.0141325727,2.8007380014,-0.3280692462\H,-1.1185315239,2.6371457401
,1.0241894581\H,0.3694067445,3.5789865926,1.2171744012\C,0.6889841425,
1.4201571845,1.2379114862\C,2.181301226,1.4908923654,0.8765588453\H,0.
6246746271,1.407452805,2.336508482\C,0.018529177,0.1093818228,0.760914
1867\H,0.5432268946,-0.7306743068,1.2363071555\H,-1.0065059514,0.09122
54298,1.1558733851\H,2.7193906445,0.6009061147,1.2255477489\H,2.333701
5359,1.5698446523,-0.2064494932\H,2.6525840318,2.3676645062,1.33670138
26\\Version=IA64L-G03RevC.02\State=1-AG\HF=-315.7081428\RMSD=2.177e-09
\RMSF=4.431e-05\Dipole=0.,0.,0.\PG=CI [X(C8H18)]\@
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n.C_CH3_3-H2CCH2-C_CH3_3

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1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H22\CYL509\14-Jul-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
H2CCH2-C_CH3_3.freq\0,1\C,-0.3467485792,0.6013615517,0.3296167969\C,-
0.3632747469,0.6296128711,1.8840006241\C,1.068378951,0.6675414655,2.45
39450071\C,-1.1117321969,-0.5916406108,2.4534458705\H,0.1314688497,1.5
292488955,-0.0130789206\H,-1.3893305162,0.652249769,-0.0131494889\C,-1
.1028413076,1.9100064929,2.3221051701\H,-2.129126519,-0.6573740019,2.0
473392631\H,-1.1936681028,-0.520730689,3.5451064624\H,-0.5976365975,-1
.5316041584,2.224331685\H,-0.5984834214,2.8084263952,1.9448522497\H,-1
.1467016432,1.9859282512,3.4156411531\H,-2.1330626767,1.9221320273,1.9
44813371\H,1.6338505459,1.516072499,2.0482873611\H,1.6258093723,-0.247
4006319,2.2248677214\H,1.0474672018,0.773650192,3.5456259599\C,0.34674
85792,-0.6013615517,-0.3296167969\C,0.3632747469,-0.6296128711,-1.8840
006241\C,-1.068378951,-0.6675414655,-2.4539450071\C,1.1117321969,0.591
6406108,-2.4534458705\H,-0.1314688497,-1.5292488955,0.0130789206\H,1.3
893305162,-0.652249769,0.0131494889\C,1.1028413076,-1.9100064929,-2.32
21051701\H,2.129126519,0.6573740019,-2.0473392631\H,1.1936681028,0.520
730689,-3.5451064624\H,0.5976365975,1.5316041584,-2.224331685\H,0.5984
834214,-2.8084263952,-1.9448522497\H,1.1467016432,-1.9859282512,-3.415
6411531\H,2.1330626767,-1.9221320273,-1.944813371\H,-1.6338505459,-1.5
16072499,-2.0482873611\H,-1.6258093723,0.2474006319,-2.2248677214\H,-1
.0474672018,-0.773650192,-3.5456259599\\Version=IA64L-G03RevC.02\State
=1-AG\HF=-394.3358649\RMSD=6.001e-09\RMSF=3.802e-06\Dipole=0.,0.,0.\PG
=CI [X(C10H22)]\@
```

n.CCH-H2CCH2-CCH

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H6\CYL509\21-Aug-2008\0\#\B3LYP/GEN 6D
INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CCH-H2CCH2
-CCH.freq\0,1\C,0.0022439951,-0.009408137,-0.7762359774\H,1.040582059
6,-0.0225695393,-1.130436064\H,-0.4542955971,-0.9446639586,-1.12357756
48\C,-0.7068005752,1.1358743121,-1.3450350813\C,-1.2963042927,2.088461
9551,-1.7955573247\H,-1.8153929907,2.927566776,-2.1997598127\C,-0.0022
439951,0.009408137,0.7762359774\H,-1.0405820596,0.0225695393,1.1304360
64\H,0.4542955971,0.9446639586,1.1235775648\C,0.7068005752,-1.13587431
21,1.3450350813\C,1.2963042927,-2.0884619551,1.7955573247\H,1.81539299
07,-2.927566776,2.1997598127\Version=IA64L-G03RevC.02\State=1-AG\HF=-
232.1030962\RMSD=3.940e-09\RMSF=4.099e-05\Dipole=0.,0.,0.\PG=CI [X(C6H
6)]\@
```

n.CH=C_CH3_2-H2CCH2-CH=C_CH3_2

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H18\CYL509\14-Jul-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CH=C_CH3
_2-H2CCH2-CH=C_CH3_2.freq\0,1\H,-3.5361208228,-1.830912162,-2.8273294
686\C,-3.5333106999,-1.8382043574,-1.7279647544\C,-2.1227598581,-1.828
9523146,-1.1863139612\C,-1.7049421129,-0.8417244273,-0.3785325236\C,-1
.2793923891,-2.9998886091,-1.6296856966\C,-0.3518288826,-0.6441836632,
0.249858923\H,0.3041765508,-1.503258325,0.070328439\H,-0.4639498527,-0
.5688940329,1.3414386343\H,-2.4252636846,-0.0546198327,-0.1444015643\H
,-4.0693440239,-2.7485444628,-1.4235695755\H,-4.1099170899,-0.97443233
16,-1.3820539694\H,-1.2181041809,-3.0389302268,-2.7263294015\H,-1.7349
711016,-3.9484945243,-1.3123496321\H,-0.2596143337,-2.9724844141,-1.23
91500365\H,3.5361208228,1.830912162,2.8273294686\C,3.5333106999,1.8382
043574,1.7279647544\C,2.1227598581,1.8289523146,1.1863139612\C,1.70494
21129,0.8417244273,0.3785325236\C,1.2793923891,2.9998886091,1.62968569
66\C,0.3518288826,0.6441836632,-0.249858923\H,-0.3041765508,1.50325832
5,-0.070328439\H,0.4639498527,0.5688940329,-1.3414386343\H,2.425263684
6,0.0546198327,0.1444015643\H,4.0693440239,2.7485444628,1.4235695755\H
,4.1099170899,0.9744323316,1.3820539694\H,1.2181041809,3.0389302268,2.
7263294015\H,1.7349711016,3.9484945243,1.3123496321\H,0.2596143337,2.9
724844141,1.2391500365\Version=IA64L-G03RevC.02\State=1-AG\HF=-391.88
3564\RMSD=5.935e-09\RMSF=4.010e-06\Dipole=0.,0.,0.\PG=CI [X(C10H18)]\@
```

n.CH=CH2-H2CCH2-CH=CH2

```
1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H10\CYL509\14-Jul-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CH=CH2-H2
CCH2-CH=CH2.freq\0,1\C,-0.0169530301,0.0241233147,-0.7641131762\H,1.0
124489521,0.0251057648,-1.1535458657\H,-0.464231311,-0.9044381294,-1.1
50140318\C,-0.7543317414,1.193346662,-1.3641571208\C,-1.3727226616,2.1
796830268,-0.7127359481\H,-0.7670143413,1.2081497386,-2.4553755177\H,-
1.4050982067,2.236614947,0.3719508821\H,-1.8767975009,2.9784185436,-1.
2498783751\C,0.0169530301,-0.0241233147,0.7641131762\H,-1.0124489521,-
0.0251057648,1.1535458657\H,0.464231311,0.9044381294,1.150140318\C,0.7
543317414,-1.193346662,1.3641571208\C,1.3727226616,-2.1796830268,0.712
7359481\H,0.7670143413,-1.2081497386,2.4553755177\H,1.4050982067,-2.23
6614947,-0.3719508821\H,1.8767975009,-2.9784185436,1.2498783751\Version=
IA64L-G03RevC.02\State=1-AG\HF=-234.6096457\RMSD=5.407e-09\RMSF=1.6
62e-04\Dipole=0.,0.,0.\PG=CI [X(C6H10)]\@
```

n.CH=CHCH3-H2CCH2-CH=CHCH3

```
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H14\CYL509\27-Aug-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CH=CHCH3-
H2CCH2-CH=CHCH3.freq\0,1\H,-3.4527969178,-0.9378019145,-3.3317401248\
C,-3.3470720066,-1.4787273826,-2.3813078537\C,-1.9485735213,-1.3698148
```

881,-1.8433632985\C,-1.6149333014,-0.8524614628,-0.6578929014\C,-0.214
0433678,-0.7339213151,-0.1226461413\H,0.4908816202,-1.2090714678,-0.81
7924925\H,-0.128839505,-1.2782455673,0.82935431\H,-2.4070027327,-0.465
2610988,-0.0120643523\H,-1.1555846829,-1.7542767079,-2.4884676186\H,-4
.0813970637,-1.0719598146,-1.6775407538\H,-3.616524563,-2.524146851,-2
.5852549118\H,3.4527969178,0.9378019145,3.3317401248\C,3.3470720066,1.
4787273826,2.3813078537\C,1.9485735213,1.3698148881,1.8433632985\C,1.6
149333014,0.8524614628,0.6578929014\C,0.2140433678,0.7339213151,0.1226
461413\H,-0.4908816202,1.2090714678,0.817924925\H,0.128839505,1.278245
5673,-0.82935431\H,2.4070027327,0.4652610988,0.0120643523\H,1.15558468
29,1.7542767079,2.4884676186\H,4.0813970637,1.0719598146,1.6775407538\
H,3.616524563,2.524146851,2.5852549118\\Version=IA64L-G03RevC.02\State
=1-AG\HF=-313.2505599\RMSD=3.285e-09\RMSF=8.410e-06\Dipole=0.,0.,0.\PG
=CI [X(C8H14)]\\@

n.CHO-H2CCH2-CHO

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H6O2\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CHO-H2CC
H2-CHO.freq\\0,1\C,-0.0043800185,0.0046346575,-0.7621080283\H,1.018950
1768,-0.0142826228,-1.1641456423\H,-0.4682232945,-0.9091218407,-1.1609
953867\C,-0.7214499644,1.194158112,-1.353351525\O,-1.2489876945,2.0729
014759,-0.7062689496\H,-0.7397370199,1.2213709212,-2.4660009442\C,0.00
43800185,-0.0046346575,0.7621080283\H,-1.0189501768,0.0142826228,1.164
1456423\H,0.4682232945,0.9091218407,1.1609953867\C,0.7214499644,-1.194
158112,1.353351525\O,1.2489876945,-2.0729014759,0.7062689496\H,0.73973
70199,-1.2213709212,2.4660009442\\Version=IA64L-G03RevC.02\State=1-AG\
HF=-306.4601101\RMSD=5.952e-09\RMSF=1.867e-05\Dipole=0.,0.,0.\PG=CI [X
(C4H6O2)]\\@

n.CN-H2CCH2-CN

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C4H4N2\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CN-H2CCH
2-CN.freq\\0,1\C,0.0053402119,-0.0112783762,-0.7751905975\H,1.03692135
76,-0.0225802932,-1.1437447698\H,-0.4777296036,-0.9239106886,-1.141066
5149\C,-0.6889250066,1.1537470277,-1.3289273776\N,-1.2426490558,2.0829
12398,-1.7487617018\C,-0.0053402119,0.0112783762,0.7751905975\H,-1.036
9213576,0.0225802932,1.1437447698\H,0.4777296036,0.9239106886,1.141066
5149\C,0.6889250066,-1.1537470277,1.3289273776\N,1.2426490558,-2.08291
2398,1.7487617018\\Version=IA64L-G03RevC.02\State=1-AG\HF=-264.3013877
\RMSD=3.518e-09\RMSF=2.768e-05\Dipole=0.,0.,0.\PG=CI [X(C4H4N2)]\\@

n.COCH3-H2CCH2-COCH3

1\1\GINC-AC9\FOpt\RB3LYP\Gen\C6H10O2\CYL509\27-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\\n.COCH3-H2
CCH2-COCH3.freq\\0,1\C,0.7305295759,0.0016603803,0.2652155091\C,0.7705
044677,0.0444369893,1.787202783\C,2.1490364819,0.0969232116,2.42307921
19\O,-0.2440644733,0.0451011547,2.460345824\H,1.4715316711,-0.72286799
72,-0.0980841198\H,1.0828419315,0.9708859848,-0.1148403471\H,2.7692453
23,0.8723379851,1.9577637067\H,2.0572104939,0.2851573932,3.4946414252\
H,2.6659285473,-0.8593108524,2.2690484827\C,-0.6554820119,-0.293203703
6,-0.2973475497\C,-0.7910322544,0.0353351288,-1.778415416\C,-2.0587499
719,-0.4477302654,-2.4617753453\O,0.0631616383,0.657817531,-2.38286418
97\H,-1.4072099181,0.2892059813,0.2537204674\H,-0.9404259064,-1.340376
1286,-0.1292731014\H,-2.0488803927,-1.543276243,-2.5320506211\H,-2.123
435225,-0.0254234253,-3.4665505227\H,-2.9484215688,-0.1742126288,-1.88
19836021\\Version=IA64L-G03RevC.02\State=1-A\HF=-385.1113666\RMSD=3.45
2e-09\RMSF=3.983e-06\Dipole=0.1376382,-0.5349587,-0.0588779\PG=C01 [X(
C6H10O2)]\\@

n.CON_CH2CH3_2-H2CCH2-CON_CH2CH3_2

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C12H24N2O2\CYL509\14-Jul-2008\0\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.CON_
CH2CH3_2-H2CCH2-CON_CH2CH3_2.freq\|0,1\C,-0.0250753957,0.0309909221,-0
.7626677081\H,0.9965661348,0.0174113127,-1.1630470931\H,-0.4984788979,
-0.8747805135,-1.1542614927\C,-0.7526214354,1.2871555332,-1.2430000972
\O,-1.0964392343,2.1670004238,-0.4527690114\N,-1.0045908548,1.39991846
12,-2.5880030172\C,-0.6108963102,0.4138128289,-3.5949841061\C,-1.70250
27729,2.603214182,-3.0551971424\H,-0.2898161053,0.9627783464,-4.488996
3933\C,-1.7285092226,-0.5694880012,-3.9631996583\H,0.2669444444,-0.132
9534966,-3.2439354868\H,-2.4139331313,2.8961585245,-2.2802933418\H,-2.
2719380604,2.3323746483,-3.9516335888\C,-0.7523503883,3.7663130007,-3.
3535728195\H,-2.0290338161,-1.1653641975,-3.0949087593\H,-1.3897031258
,-1.2555692595,-4.7481030303\H,-2.6148995948,-0.0429044456,-4.33377277
74\H,-0.2245099422,4.0606908615,-2.4419356803\H,-1.3129506109,4.633191
1281,-3.7228273259\H,-0.010452052,3.495209141,-4.114133213\C,0.0250753
957,-0.0309909221,0.7626677081\H,-0.9965661348,-0.0174113127,1.1630470
931\H,0.4984788979,0.8747805135,1.1542614927\C,0.7526214354,-1.2871555
332,1.2430000972\O,1.0964392343,-2.1670004238,0.4527690114\N,1.0045908
548,-1.3999184612,2.5880030172\C,0.6108963102,-0.4138128289,3.59498410
61\C,1.7025027729,-2.603214182,3.0551971424\H,0.2898161053,-0.96277834
64,4.4889963933\C,1.7285092226,0.5694880012,3.9631996583\H,-0.26694444
44,0.1329534966,3.2439354868\H,2.4139331313,-2.8961585245,2.2802933418
\H,2.2719380604,-2.3323746483,3.9516335888\C,0.7523503883,-3.766313000
7,3.3535728195\H,2.0290338161,1.1653641975,3.0949087593\H,1.3897031258
,1.2555692595,4.7481030303\H,2.6148995948,0.0429044456,4.3337727774\H,
0.2245099422,-4.0606908615,2.4419356803\H,1.3129506109,-4.6331911281,3
.7228273259\H,0.010452052,-3.495209141,4.114133213\|Version=IA64L-G03R
evC.02\State=1-AG\HF=-731.7235583\RMSD=2.390e-09\RMSF=2.776e-05\Dipole
=0.,0.,0.\PG=CI [X(C12H24N2O2)]\|@
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n.CON_CH3_2-H2CCH2-CON_CH3_2

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H16N2O2\CYL509\14-Jul-2008\0\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.CON_C
H3_2-H2CCH2-CON_CH3_2.freq\|0,1\H,-3.283122366,1.7159552007,-3.3926210
247\C,-3.2994386704,1.705806971,-2.2943158116\N,-1.9450147432,1.669621
6827,-1.7638789678\H,-3.8291202561,0.8206197441,-1.9455232263\H,-3.824
0214357,2.6077335117,-1.9508148334\C,-1.5655014157,0.6134753109,-0.967
9840247\O,-2.3426650861,-0.2996133655,-0.6934573622\C,-0.1334983367,0.
6157826368,-0.4315172587\H,0.0557566158,1.5221575913,0.1546549439\H,0.
5860613071,0.6476056447,-1.2574472591\C,-1.1005418755,2.7896708526,-2.
1399970721\H,-0.999995559,2.8461273326,-3.2330493\H,-0.1044526434,2.70
01040763,-1.7106435246\H,-1.5399106684,3.7361409337,-1.794737183\H,3.2
83122366,-1.7159552007,3.3926210247\C,3.2994386704,-1.705806971,2.2943
158116\N,1.9450147432,-1.6696216827,1.7638789678\H,3.8291202561,-0.820
6197441,1.9455232263\H,3.8240214357,-2.6077335117,1.9508148334\C,1.565
5014157,-0.6134753109,0.9679840247\O,2.3426650861,0.2996133655,0.69345
73622\C,0.1334983367,-0.6157826368,0.4315172587\H,-0.0557566158,-1.522
1575913,-0.1546549439\H,-0.5860613071,-0.6476056447,1.2574472591\C,1.1
005418755,-2.7896708526,2.1399970721\H,0.999995559,-2.8461273326,3.233
0493\H,0.1044526434,-2.7001040763,1.7106435246\H,1.5399106684,-3.73614
09337,1.794737183\|Version=IA64L-G03RevC.02\State=1-AG\HF=-574.4604365
\RMSD=3.225e-09\RMSF=5.704e-05\Dipole=0.,0.,0.\PG=CI [X(C8H16N2O2)]\|@
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n.CONH2-H2CCH2-CONH2

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1\1\GINC-AC18\FOpt\RB3LYP\Gen\C4H8N2O2\CYL509\20-Aug-2008\0\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\|n.CONH2-
H2CCH2-CONH2.freq\|0,1\C,0.7054409274,-0.2169093915,0.2677208149\C,0.7
465152061,-0.0218540419,1.7811400079\N,1.8757951172,-0.5014408437,2.39
```

11222297\O,-0.1518692695,0.5183325549,2.4118445812\H,1.1940089597,-1.1589796205,-0.0092463785\H,1.2911159992,0.5811633586,-0.206466105\H,2.0194875785,-0.2556683101,3.3611135263\H,2.6812290617,-0.7892842267,1.8548734281\C,-0.7177721927,-0.154282329,-0.2781241233\C,-0.7430326468,0.127383124,-1.7781908938\N,-1.9005231974,-0.2411246298,-2.4118738582\O,0.1904176035,0.6412038379,-2.3793625619\H,-1.2500687167,0.653117122,0.2410636123\H,-1.2682840424,-1.0758783173,-0.0533260166\H,-2.0256593352,0.0668690844,-3.3665441725\H,-2.7240273796,-0.5056960881,-1.8913374823\\Version=IA64L-G03RevC.02\State=1-A\HF=-417.225345\RMSD=6.946e-09\RMSE=1.051e-05\Dipole=-0.0274778,-0.8242945,-0.0234667\PG=C01 [X(C4H8N2O2)]\\@

n.CONHCH3-H2CCH2-CONHCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C6H12N2O2\CYL509\14-Jul-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CONHCH3-H2CCH2-CONHCH3.freq\\0,1\C,-1.2323259219,0.000648062,1.5958854693\O,-1.1686194458,-0.0005524234,2.8192792132\C,0.058928863,-0.0000060148,0.7638700936\H,0.6189355856,0.8780921935,1.1094703346\H,0.6182008488,-0.8785807608,1.1094729568\N,-2.411806793,0.0002856001,0.9092573765\H,-2.3958187848,0.0002859343,-0.0991421982\C,-3.7012324623,-0.0004019602,1.578648159\H,-3.5095820927,-0.0001482248,2.6522409517\H,-4.2824070198,-0.8922829861,1.316223727\H,-4.2834176559,0.8907433922,1.3159800343\C,1.2323259219,-0.000648062,-1.5958854693\O,1.1686194458,0.0005524234,-2.8192792132\C,-0.058928863,0.0000060148,-0.7638700936\H,-0.6189355856,-0.8780921935,-1.1094703346\H,-0.6182008488,0.8785807608,-1.1094729568\N,2.411806793,-0.0002856001,-0.9092573765\H,2.3958187848,-0.0002859343,0.0991421982\C,3.7012324623,0.0004019602,-1.578648159\H,3.5095820927,0.0001482248,-2.6522409517\H,4.2824070198,0.8922829861,-1.316223727\H,4.2834176559,-0.8907433922,-1.3159800343\\Version=IA64L-G03RevC.02\State=1-AG\HF=-495.8400146\RMSD=3.171e-09\RMSE=7.606e-05\Dipole=0.,0.,0.\PG=CI [X(C6H12N2O2)]\\@

n.COOC_CH3_3-H2CCH2-COOC_CH3_3

1\1\GINC-AC28\FOpt\RB3LYP\Gen\C12H22O4\CYL509\28-Aug-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOC_CH3_3-H2CCH2-COOC_CH3_3.freq\\0,1\C,0.3549901539,0.58247524,0.3481552552\H,0.4158718702,0.5255349188,1.4396752895\H,1.3929928878,0.5558622429,-0.0059456604\C,-0.2441325574,1.9211093245,-0.0488870719\O,-1.0160105416,2.0787266767,-0.9742134552\O,0.2256978522,2.8938601574,0.7547457225\C,-0.1411808468,4.3112510545,0.5623130642\C,0.3340370104,4.7932578339,-0.8123204822\C,0.6350684967,5.0095308632,1.6816463327\C,-1.6510021595,4.4908104625,0.7527389555\H,0.4480547564,6.0882190104,1.6534305163\H,1.7109268493,4.8405853571,1.5698462568\H,0.3270941942,4.6294857134,2.6611044089\H,0.1702661015,5.8734501787,-0.8978430775\H,-0.2074783392,4.2927157077,-1.6165578751\H,1.4061255836,4.6026938671,-0.9331799412\H,-1.8978431108,5.5583843396,0.7327011102\H,-1.9627958914,4.0892562446,1.7232459386\H,-2.211902743,3.9866097607,-0.0356605667\C,-0.4170751409,-0.5956140437,-0.2401889075\H,-0.6433070675,-0.3973028137,-1.2951925341\H,-1.387724623,-0.7311148433,0.2475081283\C,0.3659826186,-1.8953492816,-0.1624277385\O,1.5654573649,-1.9625332353,0.0209187124\O,-0.4583575093,-2.9430630046,-0.3509935479\C,0.0400939831,-4.3326266768,-0.3869885335\C,0.6611438781,-4.7002673789,0.9647515419\C,-1.2383357684,-5.1370939281,-0.6350073061\C,1.0257618347,-4.5055649557,-1.5473025513\H,-1.0068979634,-6.2063825088,-0.6839654142\H,-1.9599934578,-4.9748790468,0.1721587523\H,-1.7055968137,-4.8393535389,-1.5792163879\H,0.914760673,-5.7664085314,0.9729656408\H,1.5674795458,-4.1230134963,1.153790238\H,-0.0531639602,-4.51580211,1.774740029\H,1.2945938051,-5.5635293376,-1.6442126016\H,0.565910859,-4.1854224993,-2.4887597127\H,1.9362204997,-3.9270244503,-1.3831873433\\Version=IA64L-G03RevC.02\State=1-A\HF=-771

.4768694\RMSD=5.481e-09\RMSF=1.003e-06\Dipole=-0.2020379,-0.0427592,0.3505354\PG=C01 [X(C12H22O4)]\@

n.COOCH2CH3-H2CCH2-COOCH2CH3

1\1\GINC-AC3\FOpt\RB3LYP\Gen\C8H14O4\CYL509\20-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\ \n.COOCH2CH3-H2CCH2-COOCH2CH3.freq\ \0,1\C,0.3524170519,0.606901234,0.3008432675\H,0.3307867778,0.6176333132,1.3954748339\H,1.414316688,0.5643442857,0.0287187631\C,-0.2180470005,1.9107854928,-0.2208018189\O,-0.9328762416,2.0254674519,-1.1947218951\O,0.1952018154,2.9525533423,0.5312045694\C,-0.2450674357,4.2612405584,0.0982042463\H,-1.3396003669,4.276954836,0.0826447896\H,0.1016978772,4.4286259855,-0.9266849139\C,0.3271677735,5.2779695182,1.06784391\H,0.016382896,6.2867107249,0.774707868\H,1.4212587071,5.2419374983,1.0723479649\H,-0.0276538691,5.090383537,2.0863541728\C,-0.373760253,-0.6088218026,-0.2696467304\H,-0.5117223736,-0.4831373909,-1.3507032285\H,-1.3821152208,-0.7122040899,0.1442496483\C,0.3938727465,-1.8949753503,-0.0367708582\O,1.5665569722,-1.9684462923,0.2666451033\O,-0.3963759071,-2.9706550801,-0.2366989053\C,0.2415455245,-4.2615709927,-0.093146133\H,1.0760939722,-4.3228469247,-0.7991507991\H,0.657575391,-4.3381518317,0.9165744215\C,-0.8106424104,-5.3214594251,-0.3594557097\H,-0.3671038397,-6.318261711,-0.2607933343\H,-1.6374377793,-5.2400633246,0.3534490843\H,-1.2174479513,-5.2236956782,-1.3710412907\ \Version=IA64L-G03RevC.02\State=1-A\HF=-614.2137146\RMSD=6.405e-09\RM
SF=2.552e-06\Dipole=-0.2397039,-0.0216298,0.3510715\PG=C01 [X(C8H14O4)]\@

n.COOCH3-H2CCH2-COOCH3

1\1\GINC-AC6\FOpt\RB3LYP\Gen\C6H10O4\CYL509\20-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\ \n.COOCH3-H2CCH2-COOCH3.freq\ \0,1\C,-1.8773140799,0.0710817195,0.439700029\O,-1.8899264791,0.4572662827,1.5894468177\C,-0.6407625261,-0.1032053651,-0.4181687756\H,-0.6004472484,0.7272568937,-1.1337961278\H,-0.7492130659,-1.0079663355,-1.0250966878\O,-2.9932715532,-0.2395218799,-0.2551656773\C,-4.2306250231,-0.0600722487,0.4538155432\H,-4.2580609247,-0.6928838415,1.3448853326\H,-5.0136396393,-0.3503718279,-0.2472345695\H,-4.3530027402,0.9833623625,0.7564547619\C,1.8785604138,0.0422939316,-0.4380831359\O,1.8998855622,0.4595128291,-1.5768137397\C,0.63828802,-0.1282877433,0.415149077\H,0.7269684217,-1.0512008559,0.9974674562\H,0.6157260317,0.6832854425,1.1528773317\O,2.9872732546,-0.3116222762,0.2475608349\C,4.2284196791,-0.1400789626,-0.4567478659\H,4.3747434362,0.9086740568,-0.7288795602\H,5.0045639968,-0.4685671072,0.2350250789\H,4.2412765537,-0.7470564213,-1.365918132\ \Version=IA64L-G03RevC.02\State=1-A\HF=-535.5756989\RMSD=5.779e-09\RMSF=5.513e-06\Dipole=-0.0040436,-0.3774548,-0.005225\PG=C01 [X(C6H10O4)]\@

n.COOH-H2CCH2-COOH

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C4H6O4\CYL509\14-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.COOH-H2CCH2-COOH.freq\ \0,1\C,-0.7166197403,0.0001100862,0.2611726764\C,-0.7710246354,0.0000819263,1.7717770604\O,0.1827190632,0.0000792773,2.5191152292\O,-2.0510204081,0.0005613802,2.2194803372\H,-1.2722381188,0.8694677955,-0.108282877\H,-1.2725336924,-0.8690091375,-0.1083998748\H,-1.9954681759,0.0006922835,3.1935684563\C,0.7166197403,-0.0001100862,-0.2611726764\C,0.7710246354,-0.0000819263,-1.7717770604\O,-0.1827190632,-0.0000792773,-2.5191152292\O,2.0510204081,-0.0005613802,-2.2194803372\H,1.2722381188,-0.8694677955,0.108282877\H,1.2725336924,0.8690091375,0.1083998748\H,1.9954681759,-0.0006922835,-3.1935684563\ \Version=IA64L-G03RevC.02\State=1-AG\HF=-456.9621625\RMSD=4.105e-09\RMSF=1.435e-04\Dipole=0.,0.,0.\PG=CI [X(C4H6O4)]\@

n.COPh-H2CCH2-COPh

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1\1\GINC-AC26\FOpt\RB3LYP\Gen\C16H14O2\CYL509\14-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COPh-H
2CCH2-COPh.freq\\0,1\C,-5.6119013812,0.0005182247,0.6533685243\C,-5.58
54035149,0.000461616,2.0513942462\C,-4.3631468013,0.0005472911,2.72600
24299\C,-3.1680837711,0.0006879681,2.0068745379\C,-3.185229676,0.00075
75903,0.6035611816\C,-4.4202284658,0.000661502,-0.0645407302\C,-1.9349
015031,0.0009353022,-0.2249992253\O,-1.9993607854,0.0003047555,-1.4470
846342\C,-0.5874633363,0.0003093274,0.4860137435\H,-0.5279695044,-0.86
87758414,1.1532381495\H,-0.5271497263,0.8694186231,1.1531303514\H,-4.4
156900759,0.0007134031,-1.1496562295\H,-2.2255951927,0.0007493839,2.54
53424144\H,-4.3396530835,0.0005016168,3.8122512447\H,-6.5625585016,0.0
00451537,0.1269720447\H,-6.5157450284,0.0003488919,2.6132590924\C,5.61
19013812,-0.0005182247,-0.6533685243\C,5.5854035149,-0.000461616,-2.05
13942462\C,4.3631468013,-0.0005472911,-2.7260024299\C,3.1680837711,-0.
0006879681,-2.0068745379\C,3.185229676,-0.0007575903,-0.6035611816\C,4
.4202284658,-0.000661502,0.0645407302\C,1.9349015031,-0.0009353022,0.2
249992253\O,1.9993607854,-0.0003047555,1.4470846342\C,0.5874633363,-0.
0003093274,-0.4860137435\H,0.5279695044,0.8687758414,-1.1532381495\H,0
.5271497263,-0.8694186231,-1.1531303514\H,4.4156900759,-0.0007134031,1
.1496562295\H,2.2255951927,-0.0007493839,-2.5453424144\H,4.3396530835,
-0.0005016168,-3.8122512447\H,6.5625585016,-0.000451537,-0.1269720447\
H,6.5157450284,-0.0003488919,-2.6132590924\\Version=IA64L-G03RevC.02\St
ate=1-AG\HF=-768.5913022\RMSD=9.686e-09\RMSF=3.587e-05\Dipole=0.,0.,0
.\PG=CI [X(C16H14O2)]\\@
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n.H-MeHCCHMe-H

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1\1\GINC-LC62\FOpt\RB3LYP\Gen\C4H10\CYL509\28-Jun-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\H-MeHCCHMe-
H.freq\\0,1\C,-0.3380692254,0.6082621247,-0.3228497858\H,-0.6445839641
,1.310954508,0.4652535624\C,-1.552355289,0.2409848214,-1.181472184\H,-
1.2703514345,-0.4333148521,-1.9997170196\H,-2.0129677312,1.1299103679,
-1.6275408049\H,-2.3201604634,-0.2677468658,-0.5852034444\H,0.39789542
92,1.1459056078,-0.9379891253\C,0.3380692254,-0.6082621247,0.322849785
8\H,0.6445839641,-1.310954508,-0.4652535624\C,1.552355289,-0.240984821
4,1.181472184\H,1.2703514345,0.4333148521,1.9997170196\H,2.0129677312,
-1.1299103679,1.6275408049\H,2.3201604634,0.2677468658,0.5852034444\H,
-0.3978954292,-1.1459056078,0.9379891253\\Version=IA32L-G03RevC.02\Sta
te=1-AG\HF=-158.458045\RMSD=4.828e-09\RMSF=5.077e-05\Dipole=0.,0.,0.\P
G=CI [X(C4H10)]\\@
```

n.BH2-MeHCCHMe-BH2

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1\1\GINC-LC144\FOpt\RB3LYP\Gen\C4H12B2\CYL509\28-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\BH2-MeHC
CHMe-BH2.freq\\0,1\H,-2.0087563984,-0.4439436112,-1.5484790649\B,-1.98
59307177,-0.0919781746,-0.4008837167\C,-0.648105454,-0.0924853824,0.41
17160248\H,-3.0289905902,0.1665289804,0.1301526212\C,-0.6636138207,-1.
4835310257,1.1195573918\H,-1.5533810142,-1.6228355074,1.7442338609\H,0
.213298211,-1.5812754003,1.7726175761\H,-0.6272548124,-2.3071521137,0.
3955389603\H,-0.67062903,0.6619006982,1.2129315266\H,2.0087563984,0.44
39436112,1.5484790649\B,1.9859307177,0.0919781746,0.4008837167\C,0.648
105454,0.0924853824,-0.4117160248\H,3.0289905902,-0.1665289804,-0.1301
526212\C,0.6636138207,1.4835310257,-1.1195573918\H,1.5533810142,1.6228
355074,-1.7442338609\H,-0.213298211,1.5812754003,-1.7726175761\H,0.627
2548124,2.3071521137,-0.3955389603\H,0.67062903,-0.6619006982,-1.21293
15266\\Version=IA32L-G03RevC.02\State=1-AG\HF=-209.3070759\RMSD=8.208e
-09\RMSF=7.814e-06\Dipole=0.,0.,0.\PG=CI [X(C4H12B2)]\\@
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n.CH3-MeHCCHMe-CH3

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1\1\GINC-LC74\FOpt\RB3LYP\Gen\C6H14\CYL509\28-Jun-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH3-MeHCCHM
e-CH3.freq\0,1\H,1.6593698653,-0.9909522707,-1.4858134263\C,1.4931398
399,-1.2116599926,-0.42709922\H,2.4766630043,-1.3546938307,0.035723896
5\H,0.957330236,-2.1683865255,-0.3637314395\C,0.7131530169,-0.09698167
97,0.2915408106\C,0.6940265336,-0.3836546223,1.8030908364\H,1.70998264
62,-0.5602940268,2.1753990811\H,0.1017073459,-1.2818284587,2.024167306
2\H,0.2737363914,0.4447789937,2.3812551995\H,1.2586469205,0.8481759752
,0.1360903026\H,-1.6593698653,0.9909522707,1.4858134263\C,-1.493139839
9,1.2116599926,0.42709922\H,-2.4766630043,1.3546938307,-0.0357238965\H
,-0.957330236,2.1683865255,0.3637314395\C,-0.7131530169,0.0969816797,-
0.2915408106\C,-0.6940265336,0.3836546223,-1.8030908364\H,-1.709982646
2,0.5602940268,-2.1753990811\H,-0.1017073459,1.2818284587,-2.024167306
2\H,-0.2737363914,-0.4447789937,-2.3812551995\H,-1.2586469205,-0.84817
59752,-0.1360903026\Version=IA32L-G03RevC.02\State=1-AG\HF=-237.08250
56\RMSD=3.834e-09\RMSF=8.724e-06\Dipole=0.,0.,0.\PG=C02H [SGH(C2H2),X(
C4H12)]\@
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n.NH2-MeHCCHMe-NH2

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1\1\GINC-LC83\FOpt\RB3LYP\Gen\C4H12N2\CYL509\28-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\NH2-MeHCC
HMe-NH2.freq\0,1\H,-1.4352700647,1.6231145282,-0.7744581467\N,-0.4261
747627,1.7557834891,-0.6923176076\C,0.1301343011,0.7381504669,0.214531
5975\H,-0.0480482581,1.6400516049,-1.6303342909\C,-0.3951258534,1.0351
640767,1.6238166083\H,0.0781233472,0.4038083501,2.382590287\H,-1.48043
55469,0.8698189116,1.677714618\H,-0.2027955095,2.0811107136,1.87838636
94\H,1.2216439247,0.8885180461,0.215413883\H,1.4352700647,-1.623114528
2,0.7744581467\N,0.4261747627,-1.7557834891,0.6923176076\C,-0.13013430
11,-0.7381504669,-0.2145315975\H,0.0480482581,-1.6400516049,1.63033429
09\C,0.3951258534,-1.0351640767,-1.6238166083\H,-0.0781233472,-0.40380
83501,-2.382590287\H,1.4804355469,-0.8698189116,-1.677714618\H,0.20279
55095,-2.0811107136,-1.8783863694\H,-1.2216439247,-0.8885180461,-0.215
413883\Version=IA32L-G03RevC.02\State=1-AG\HF=-269.1419862\RMSD=9.583
e-09\RMSF=1.438e-05\Dipole=0.,0.,0.\PG=CI [X(C4H12N2)]\@
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n.OH-MeHCCHMe-OH

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1\1\GINC-LC146\FOpt\RB3LYP\Gen\C4H10O2\CYL509\29-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\OH-MeHCC
HMe-OH.freq\0,1\C,0.3451717655,-0.6444010765,0.2317687429\O,0.4211314
093,-0.5557715558,1.6571642477\C,-0.4019677532,-1.9010200984,-0.210266
2199\H,0.8217387052,-1.3777998403,1.9779863474\H,-0.4813100118,-1.9411
856379,-1.299730076\H,-1.4108640641,-1.9125790003,0.2182215136\H,0.123
9866959,-2.8030436765,0.1296145755\H,1.3582203774,-0.6505307019,-0.204
8267703\C,-0.3451717655,0.6444010765,-0.2317687429\O,-0.4211314093,0.5
557715558,-1.6571642477\C,0.4019677532,1.9010200984,0.2102662199\H,-0.
8217387052,1.3777998403,-1.9779863474\H,0.4813100118,1.9411856379,1.29
9730076\H,1.4108640641,1.9125790003,-0.2182215136\H,-0.1239866959,2.80
30436765,-0.1296145755\H,-1.3582203774,0.6505307019,0.2048267703\Vers
ion=IA32L-G03RevC.02\State=1-AG\HF=-308.8756679\RMSD=2.981e-09\RMSF=9.
770e-06\Dipole=0.,0.,0.\PG=CI [X(C4H10O2)]\@
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n.F-MeHCCHMe-F

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1\1\GINC-LC9\FOpt\RB3LYP\Gen\C4H8F2\CYL509\28-Jun-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\F-MeHCCHMe-
F.freq\0,1\C,0.6095152193,0.3820408133,-0.2606979377\C,1.9347650564,-
0.222820248,0.161091415\F,0.5167749352,1.6861875872,0.246464904\H,2.76
64613235,0.3701303795,-0.2311953167\H,2.0163593793,-1.2447292291,-0.21
9843387\H,2.0116042368,-0.2491401714,1.2537799645\H,0.5435938258,0.450
```

3397833,-1.3548216432\C,-0.6095152193,-0.3820408133,0.2606979377\C,-1.9347650564,0.222820248,-0.161091415\F,-0.5167749352,-1.6861875872,-0.246464904\H,-2.7664613235,-0.3701303795,0.2311953167\H,-2.0163593793,1.2447292291,0.219843387\H,-2.0116042368,0.2491401714,-1.2537799645\H,-0.5435938258,-0.4503397833,1.3548216432\\Version=IA32L-G03RevC.02\State=1-AG\HF=-356.9239578\RMSD=2.518e-09\RMSF=4.296e-05\Dipole=0.,0.,0.\PG=CI [X(C4H8F2)]\\@

n.SiH3-MeHCCHMe-SiH3

1\1\GINC-LC127\FOpt\RB3LYP\Gen\C4H14Si2\CYL509\29-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\SiH3-MeHCCHMe-SiH3.freq\\0,1\H,-1.4954238794,-0.1726713493,-3.0956396685\Si,-1.6684155633,0.0538239647,-1.6331485227\C,0.0431500399,-0.0002498137,-0.7773462434\H,-2.3752961248,1.3526698259,-1.4626369992\H,-2.544169683,-1.0261431285,-1.0934671573\C,0.8307538477,-1.2069999535,-1.3325900741\H,1.8680041931,-1.2186367096,-0.9765230199\H,0.8661990592,-1.1951074841,-2.4274351736\H,0.3732053314,-2.1563773658,-1.0262453307\H,0.5683161008,0.9169367067,-1.0876793798\H,1.4954238794,0.1726713493,3.0956396685\Si,1.6684155633,-0.0538239647,1.6331485227\C,-0.0431500399,0.0002498137,0.7773462434\H,2.3752961248,-1.3526698259,1.4626369992\H,2.544169683,1.0261431285,1.0934671573\C,-0.8307538477,1.2069999535,1.3325900741\H,-1.8680041931,1.2186367096,0.9765230199\H,-0.8661990592,1.1951074841,2.4274351736\H,-0.3732053314,2.1563773658,1.0262453307\H,-0.5683161008,-0.9169367067,1.0876793798\\Version=IA32L-G03RevC.02\State=1-AG\HF=-739.8294883\RMSD=3.756e-09\RMSF=4.743e-06\Dipole=0.,0.,0.\PG=CI [X(C4H14Si2)]\\@

n.PH2-MeHCCHMe-PH2

1\1\GINC-LC112\FOpt\RB3LYP\Gen\C4H12P2\CYL509\29-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\PH2-MeHCCHMe-PH2.freq\\0,1\H,-2.5379738901,0.5525403653,-0.484964173\P,-1.6309176735,1.650680294,-0.3883161063\H,-1.7953944957,1.7789519497,1.018550014\C,-0.0180337384,0.6383960169,-0.4389627774\C,0.256389462,0.3759462511,-1.9324388628\H,1.2653251961,-0.0115974912,-2.0974699498\H,0.1565630964,1.2965383273,-2.5165393121\H,-0.4523915038,-0.3559145286,-2.3407958557\H,0.749008264,1.3331104497,-0.0661681022\H,2.5379738901,-0.5525403653,0.484964173\P,1.6309176735,-1.650680294,0.3883161063\H,1.7953944957,-1.7789519497,-1.018550014\C,0.0180337384,-0.6383960169,0.4389627774\C,-0.256389462,-0.3759462511,1.9324388628\H,-1.2653251961,0.0115974912,2.0974699498\H,-0.1565630964,-1.2965383273,2.5165393121\H,0.4523915038,0.3559145286,2.3407958557\H,-0.749008264,-1.3331104497,0.0661681022\\Version=IA32L-G03RevC.02\State=1-AG\HF=-842.3304371\RMSD=3.060e-09\RMSF=8.513e-06\Dipole=0.,0.,0.\PG=CI [X(C4H12P2)]\\@

n.SH-MeHCCHMe-SH

1\1\GINC-LC9\FOpt\RB3LYP\Gen\C4H10S2\CYL509\29-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\SH-MeHCCHMe-SH.freq\\0,1\C,0.3585023768,-0.6349524677,0.251962941\S,0.4958094356,-0.4968530471,2.1116065637\C,-0.3547777396,-1.9339300964,-0.1325324151\H,0.8150902871,-1.7910305306,2.3198907956\H,-0.4028450498,-2.0460279005,-1.2213753282\H,-1.3762939884,-1.9507910382,0.26146008\H,0.1799210247,-2.8041470555,0.2626936036\H,1.3775178111,-0.6366178156,-0.1497865255\C,-0.3585023768,0.6349524677,-0.251962941\S,-0.4958094356,0.4968530471,-2.1116065637\C,0.3547777396,1.9339300964,0.1325324151\H,-0.8150902871,1.7910305306,-2.3198907956\H,0.4028450498,2.0460279005,1.2213753282\H,1.3762939884,1.9507910382,-0.26146008\H,-0.1799210247,2.8041470555,-0.2626936036\H,-1.3775178111,0.6366178156,0.1497865255\\Version=IA32L-G03RevC.02\State=1-AG\HF=-954.8213797\RMSD=9.922e-09\RMSF=4.036e-06\Dipole=0.,0.,0.\PG=CI [X(C4H10S2)]\\@

n.Cl-MeHCCHMe-Cl

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1\1\GINC-LC127\FOpt\RB3LYP\Gen\C4H8Cl2\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\Cl-MeHCC
HMe-Cl.freq\0,1\C,0.4957869563,0.5804805681,0.0864916684\C,-0.0069562
201,1.7483579128,0.9253596124\H,0.7349755365,2.5508738902,0.9367843394
\H,-0.1850495266,1.4214532124,1.9533254202\H,-0.9413274595,2.147008504
6,0.5171121066\H,1.4412985349,0.1943298096,0.4750514058\C,-0.495782003
2,-0.5804855378,-0.0864963593\C,0.0069646807,-1.7483705688,-0.92535173
7\H,-0.7349676742,-2.5508860531,-0.9367730698\H,0.1850634651,-1.421475
2628,-1.9533194875\H,0.9413334777,-2.1470183855,-0.5170959496\H,-1.441
290762,-0.1943362999,-0.4750644894\Cl,0.9050847956,1.2197304438,-1.592
9800355\Cl,-0.9050916235,-1.2197212475,1.5929777189\Version=IA32L-G03
RevC.02\State=1-A\HF=-1077.6517485\RMSD=4.129e-09\RMSF=3.926e-05\Dipol
e=0.0000047,-0.0000071,0.0000002\PG=C01 [X(C4H8Cl2)]\@
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n.Br-MeHCCHMe-Br

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1\1\GINC-LC78\FOpt\RB3LYP\Gen\C4H8Br2\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\Br-MeHCC
HMe-Br.freq\0,1\Br,0.5491838066,-1.4391972931,-1.7977271987\C,0.256887
4203,-0.7163309877,0.0696587207\C,1.565049576,-0.8925661208,0.82798702
97\H,2.3561753178,-0.2709466551,0.3969298145\H,1.8880935068,-1.9356944
406,0.7930551113\H,1.4286821249,-0.6056210624,1.8748232118\H,-0.529149
0885,-1.3608233329,0.4669061953\Br,-0.5491838066,1.4391972931,1.797727
1987\C,-0.2568874203,0.7163309877,-0.0696587207\C,-1.565049576,0.89256
61208,-0.8279870297\H,-2.3561753178,0.2709466551,-0.3969298145\H,-1.88
80935068,1.9356944406,-0.7930551113\H,-1.4286821249,0.6056210624,-1.87
48232118\H,0.5291490885,1.3608233329,-0.4669061953\Version=IA32L-G03R
evC.02\State=1-AG\HF=-5305.0234383\RMSD=4.395e-09\RMSF=2.497e-05\Dipol
e=0.,0.,0.\PG=CI [X(C4H8Br2)]\@
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n.N_CH3_2-MeHCCHMe-N_CH3_2

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1\1\GINC-LC86\FOpt\RB3LYP\Gen\C8H20N2\CYL509\29-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\N_CH3_2-M
eHCCHMe-N_CH3_2.freq\0,1\C,2.6399614909,-0.2672365979,1.1701043848\H,
3.7153406658,-0.379897005,0.9756273806\H,2.320080366,-1.1262320222,1.7
697915466\H,2.515956805,0.6416286953,1.7883812987\N,1.9264947799,-0.25
67901065,-0.0921983075\C,0.4940458756,-0.6022148475,-0.0868978767\C,2.
3565386317,0.801421788,-0.9850160233\C,0.1764741556,-1.4378292791,-1.3
394800655\H,3.4383234722,0.717998007,-1.1519030402\H,2.1632346572,1.82
5971513,-0.6111651272\H,1.8667372579,0.7020569152,-1.9588033371\H,0.92
26513759,-2.2312200256,-1.4440017159\H,0.1994309314,-0.8309932351,-2.2
527574304\H,-0.8133372518,-1.8988820044,-1.2776335956\H,0.3602373116,-
1.2579376027,0.783431418\C,-2.6399614909,0.2672365979,-1.1701043848\H,
-3.7153406658,0.379897005,-0.9756273806\H,-2.320080366,1.1262320222,-1.
7697915466\H,-2.515956805,-0.6416286953,-1.7883812987\N,-1.9264947799
,0.2567901065,0.0921983075\C,-0.4940458756,0.6022148475,0.0868978767\C
,-2.3565386317,-0.801421788,0.9850160233\C,-0.1764741556,1.4378292791,
1.3394800655\H,-3.4383234722,-0.717998007,1.1519030402\H,-2.1632346572
,-1.825971513,0.6111651272\H,-1.8667372579,-0.7020569152,1.9588033371\
H,-0.9226513759,2.2312200256,1.4440017159\H,-0.1994309314,0.8309932351
,2.2527574304\H,0.8133372518,1.8988820044,1.2776335956\H,-0.3602373116
,1.2579376027,-0.783431418\Version=IA32L-G03RevC.02\State=1-AG\HF=-42
6.3615602\RMSD=2.992e-09\RMSF=2.509e-05\Dipole=0.,0.,0.\PG=CI [X(C8H20
N2)]\@
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n.NHCH3-MeHCCHMe-NHCH3

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1\1\GINC-LC18\FOpt\RB3LYP\Gen\C6H16N2\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\NHCH3-MeH
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CCHMe-NHCH3.freq\0,1\C,2.4494861301,-1.4241241694,0.6958259608\H,3.5104484227,-1.4506036012,0.4227579751\H,2.122361271,-2.4622745612,0.8280037383\H,2.3634439832,-0.9204134255,1.6748505741\N,1.6948666965,-0.817940058,-0.3939514719\C,0.2354988283,-0.7101448749,-0.2153602891\C,-0.4516104839,-1.1944844503,-1.5022673112\H,2.0881879617,0.087473453,-0.6380910869\H,-0.1985223,-0.5388196685,-2.3442932375\H,-1.5427246385,-1.2247533897,-1.408572526\H,-0.0966860167,-2.1995115651,-1.7492766062\H,-0.0401663209,-1.4003238518,0.5976445641\C,-2.4494861301,1.4241241694,-0.6958259608\H,-3.5104484227,1.4506036012,-0.4227579751\H,-2.122361271,2.4622745612,-0.8280037383\H,-2.3634439832,0.9204134255,-1.6748505741\N,-1.6948666965,0.817940058,0.3939514719\C,-0.2354988283,0.7101448749,0.2153602891\C,0.4516104839,1.1944844503,1.5022673112\H,-2.0881879617,-0.087473453,0.6380910869\H,0.1985223,0.5388196685,2.3442932375\H,1.5427246385,1.2247533897,1.408572526\H,0.0966860167,2.1995115651,1.7492766062\H,0.0401663209,1.4003238518,-0.5976445641\Version=IA32L-G03RevC.02\State=1-AG\HF=-347.7481793\RMSD=3.280e-09\RMSF=1.005e-05\Dipole=0.,0.,0.\PG=CI [X(C6H16N2)]\@

n.NHCHO-MeHCCHMe-NHCHO

1\1\GINC-LC12\FOpt\RB3LYP\Gen\C6H12N2O2\CYL509\28-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\NHCHO-MeHCCHMe-NHCHO.freq\0,1\H,1.7270459793,-0.8512484031,-3.1705562599\C,0.9157004989,-0.4653258762,-2.5201784814\O,0.1053824586,0.36330513,-2.9092788145\N,0.9559770962,-1.0152405628,-1.2783820065\C,-0.0157610827,-0.7510952492,-0.2047068358\H,1.6889398153,-1.6872523472,-1.0976527269\C,-1.4163050426,-1.2352451239,-0.6049966136\H,-1.3842564654,-2.2985946772,-0.8641975148\H,-1.7829971383,-0.680314639,-1.4729512546\H,0.3282143819,-1.3257135079,0.6589854529\H,-1.7270459793,0.8512484031,3.1705562599\C,-0.9157004989,0.4653258762,2.5201784814\O,-0.1053824586,-0.36330513,2.9092788145\N,-0.9559770962,1.0152405628,1.2783820065\C,0.0157610827,0.7510952492,0.2047068358\H,-1.6889398153,1.6872523472,1.0976527269\C,1.4163050426,1.2352451239,0.6049966136\H,1.3842564654,2.2985946772,0.8641975148\H,1.7829971383,0.680314639,1.4729512546\H,-0.3282143819,1.3257135079,-0.6589854529\H,2.1197132823,1.1089070603,-0.2224187922\H,-2.1197132823,-1.1089070603,0.2224187922\Version=IA32L-G03RevC.02\State=1-AG\HF=-495.8322921\RMSD=3.236e-09\RMSF=6.295e-06\Dipole=0.,0.,0.\PG=CI [X(C6H12N2O2)]\@

n.NHCOCH3-MeHCCHMe-NHCOCH3

1\1\GINC-LC75\FOpt\RB3LYP\Gen\C8H16N2O2\CYL509\29-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\NHCOCH3-MeHCCHMe-NHCOCH3.freq\0,1\H,-1.2733411992,3.1018556898,-2.8472299672\C,-0.3733102442,3.4083674935,-2.3047232424\C,0.0355575713,2.4561700024,-1.186795227\H,-0.5412257737,4.4015686252,-1.8758714932\H,0.4566607105,3.4961884148,-3.0119891613\N,-0.8142816805,1.4113986986,-0.9656850022\O,1.0647237173,2.6357169491,-0.5404362639\C,-0.655772234,0.4080693791,0.0987970118\H,-1.6328874115,1.3368506357,-1.5509660227\C,-0.7543394365,1.0572630659,1.4864320398\H,0.0618888978,1.768377534,1.6388942604\H,-0.7166379189,0.2966483643,2.271135334\H,-1.703617072,1.5953283263,1.5807817368\H,-1.4863444631,-0.2909402585,-0.0258646272\H,1.2733411992,-3.1018556898,2.8472299672\C,0.3733102442,-3.4083674935,2.3047232424\C,-0.0355575713,-2.4561700024,1.186795227\H,0.5412257737,-4.4015686252,1.8758714932\H,-0.4566607105,-3.4961884148,3.0119891613\N,0.8142816805,-1.4113986986,0.9656850022\O,-1.0647237173,-2.6357169491,0.5404362639\C,0.655772234,-0.4080693791,-0.0987970118\H,1.6328874115,-1.3368506357,1.5509660227\C,0.7543394365,-1.0572630659,-1.4864320398\H,-0.0618888978,-1.768377534,-1.6388942604\H,0.7166379189,-0.2966483643,-2.271135334\H,1.703617072,-1.5953283263,-1.5807817368\H,1.4863444631,0.2909402585,0.0258646272\Version=IA32L-G03RevC.02\State=1-AG\HF=-574.4780929

\RMSD=3.545e-09\RMSF=2.566e-06\Dipole=0.,0.,0.\PG=CI [X(C8H16N2O2)]\@

n.NO2-MeHCCHMe-NO2

1\1\GINC-LC73\FOpt\RB3LYP\Gen\C4H8N2O4\CYL509\28-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\NO2-MeHC
CHMe-NO2.freq\0,1\O,-1.4607058822,-1.4255587236,-1.9922487078\N,-1.44
01977881,-0.8329713108,-0.9207867267\C,-0.1021275024,-0.734169144,-0.2
059386166\O,-2.4131627447,-0.3343868094,-0.3578271602\C,-0.1243059149,
-1.7170977092,0.9655607099\H,0.8540630138,-1.7291525898,1.4535989123\H
, -0.3332084114,-2.7285541517,0.6048759384\H,-0.8880401546,-1.435800920
1,1.6961521055\H,0.6369013956,-1.0234154448,-0.9520957151\O,1.46070588
22,1.4255587236,1.9922487078\N,1.4401977881,0.8329713108,0.9207867267\
C,0.1021275024,0.734169144,0.2059386166\O,2.4131627447,0.3343868094,0.
3578271602\C,0.1243059149,1.7170977092,-0.9655607099\H,-0.8540630138,1.
.7291525898,-1.4535989123\H,0.3332084114,2.7285541517,-0.6048759384\H,
0.8880401546,1.4358009201,-1.6961521055\H,-0.6369013956,1.0234154448,0.
.9520957151\Version=IA32L-G03RevC.02\State=1-AG\HF=-567.4532861\RMSD=
7.427e-09\RMSF=4.614e-05\Dipole=0.,0.,0.\PG=CI [X(C4H8N2O4)]\@

n.OCF3-MeHCCHMe-OCF3

1\1\GINC-LC131\FOpt\RB3LYP\Gen\C6H8F6O2\CYL509\28-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\OCF3-Me
HCCHMe-OCF3.freq\0,1\C,-0.0285349004,0.3583189265,-0.6864821616\O,-1.
1823541484,-0.1473017527,-1.4270218109\C,-2.4090357027,0.3753150364,-1.
.257999744\F,-2.5558184738,1.587518072,-1.8363797235\F,-2.7513279658,0.
5305681231,0.0482320759\F,-3.2926695528,-0.4540970882,-1.8199706714\C
,0.0310062607,1.8789960144,-0.5952106496\H,0.9841398808,2.1679072782,-
0.1463285668\H,-0.7734900335,2.2833969285,0.0255919489\H,-0.0368558689
,2.3239738785,-1.5909076113\H,0.7997525982,-0.0012135848,-1.2986545534
\C,0.0285349004,-0.3583189265,0.6864821616\O,1.1823541484,0.1473017527
,1.4270218109\C,2.4090357027,-0.3753150364,1.257999744\F,2.5558184738,
-1.587518072,1.8363797235\F,2.7513279658,-0.5305681231,-0.0482320759\F
,3.2926695528,0.4540970882,1.8199706714\C,-0.0310062607,-1.8789960144,
0.5952106496\H,-0.9841398808,-2.1679072782,0.1463285668\H,0.7734900335
, -2.2833969285,-0.0255919489\H,0.0368558689,-2.3239738785,1.5909076113
\H,-0.7997525982,0.0012135848,1.2986545534\Version=IA32L-G03RevC.02\St
ate=1-AG\HF=-982.9656505\RMSD=4.957e-09\RMSF=7.341e-05\Dipole=0.,0.,0.
\PG=CI [X(C6H8F6O2)]\@

n.OCH2CH3-MeHCCHMe-OCH2CH3

1\1\GINC-LC122\FOpt\RB3LYP\Gen\C8H18O2\CYL509\29-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\OCH2CH3-
MeHCCHMe-OCH2CH3.freq\0,1\H,-0.9183127635,-4.2735980133,1.9905831089\
C,-0.9764378188,-3.7406475536,1.0349234802\C,-0.8061642223,-2.24393900
11,1.2484049897\O,-0.9138942026,-1.6192870152,-0.0255647601\C,-0.74421
20571,-0.1978308713,-0.0884802518\C,-1.6717185969,0.5696588626,0.85589
8367\H,-1.5807404756,-1.8706368308,1.9341756213\H,0.1698063114,-2.0381
854922,1.7151131075\H,-0.1957149375,-4.1274493311,0.3717798658\H,-1.94
79426783,-3.9514158317,0.5762648707\H,-1.3815501257,0.449714801,1.9057
576173\H,-2.7036332542,0.2219145274,0.7377338832\H,-1.632623415,1.6384
569639,0.6302803026\H,-1.0372067937,0.0312379243,-1.12058065\H,0.91831
27635,4.2735980133,-1.9905831089\C,0.9764378188,3.7406475536,-1.034923
4802\C,0.8061642223,2.2439390011,-1.2484049897\O,0.9138942026,1.619287
0152,0.0255647601\C,0.7442120571,0.1978308713,0.0884802518\C,1.6717185
969,-0.5696588626,-0.855898367\H,1.5807404756,1.8706368308,-1.93417562
13\H,-0.1698063114,2.0381854922,-1.7151131075\H,0.1957149375,4.1274493
311,-0.3717798658\H,1.9479426783,3.9514158317,-0.5762648707\H,1.381550
1257,-0.449714801,-1.9057576173\H,2.7036332542,-0.2219145274,-0.737733
8832\H,1.632623415,-1.6384569639,-0.6302803026\H,1.0372067937,-0.03123

79243,1.12058065\\Version=IA32L-G03RevC.02\\State=1-AG\\HF=-466.120527\\R
MSD=6.545e-09\\RMSF=4.112e-06\\Dipole=0.,0.,0.\\PG=CI [X(C8H18O2)]\\@

n.OCH3-MeHCCHMe-OCH3

1\\1\\GINC-LC117\\FOpt\\RB3LYP\\Gen\\C6H14O2\\CYL509\\28-Jun-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\OCH3-MeH
CCHMe-OCH3.freq\\0,1\\C,-1.4324592436,-1.3397731799,-2.2593363254\\O,-1.
3202336457,-0.6588022041,-1.027731348\\C,0.0060809532,-0.5792592171,-0.
5072525144\\H,-1.1843776925,-2.4082971425,-2.1775950536\\H,-2.4750475897
, -1.2496825945,-2.5770447646\\H,-0.7855674461,-0.8917905785,-3.03078605
92\\C,0.4508564242,-1.8997285321,0.123211244\\H,1.4481231013,-1.79211592
69,0.5564431551\\H,0.4828312856,-2.7055239572,-0.6176939908\\H,-0.248015
0136,-2.1921795873,0.9156018411\\H,0.7020420002,-0.3061167125,-1.319237
5169\\C,1.4324592436,1.3397731799,2.2593363254\\O,1.3202336457,0.6588022
041,1.027731348\\C,-0.0060809532,0.5792592171,0.5072525144\\H,1.18437769
25,2.4082971425,2.1775950536\\H,2.4750475897,1.2496825945,2.5770447646\\
H,0.7855674461,0.8917905785,3.0307860592\\C,-0.4508564242,1.8997285321,
-0.123211244\\H,-1.4481231013,1.7921159269,-0.5564431551\\H,-0.482831285
6,2.7055239572,0.6176939908\\H,0.2480150136,2.1921795873,-0.9156018411\\
H,-0.7020420002,0.3061167125,1.3192375169\\Version=IA32L-G03RevC.02\\St
ate=1-AG\\HF=-387.4902377\\RMSD=4.210e-09\\RMSF=2.813e-05\\Dipole=0.,0.,0.
\\PG=CI [X(C6H14O2)]\\@

n.OCHO-MeHCCHMe-OCHO

1\\1\\GINC-LC115\\FOpt\\RB3LYP\\Gen\\C6H10O4\\CYL509\\29-Jun-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\OCHO-MeH
CCHMe-OCHO.freq\\0,1\\C,0.0420296196,-0.7637090196,-0.1107451254\\O,0.08
34326348,-1.4566866674,1.1785491274\\C,1.1221098376,-1.2928292311,2.011
0913062\\H,0.9727043422,-1.9513853317,2.8814906753\\O,2.0700729548,-0.55
68333114,1.8722340517\\C,1.1887794769,-1.2065370832,-1.0145140167\\H,2.1
527116383,-0.8482151745,-0.6469773592\\H,1.0338542509,-0.8208982974,-2.
0261870899\\H,1.2132247482,-2.2995174884,-1.0698857853\\H,-0.9080258614,
-1.1057128148,-0.5217576964\\C,-0.0420296196,0.7637090196,0.1107451254\\
O,-0.0834326348,1.4566866674,-1.1785491274\\C,-1.1221098376,1.292829231
1,-2.0110913062\\H,-0.9727043422,1.9513853317,-2.8814906753\\O,-2.070072
9548,0.5568333114,-1.8722340517\\C,-1.1887794769,1.2065370832,1.0145140
167\\H,-2.1527116383,0.8482151745,0.6469773592\\H,-1.0338542509,0.820898
2974,2.0261870899\\H,-1.2132247482,2.2995174884,1.0698857853\\H,0.908025
8614,1.1057128148,0.5217576964\\Version=IA32L-G03RevC.02\\State=1-AG\\HF
=-535.5593878\\RMSD=6.187e-09\\RMSF=1.418e-05\\Dipole=0.,0.,0.\\PG=CI [X(C
6H10O4)]\\@

n.OCOCH3-MeHCCHMe-OCOCH3

1\\1\\GINC-LC48\\FOpt\\RB3LYP\\Gen\\C8H14O4\\CYL509\\29-Jun-2008\\0\\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\OCOCH3-Me
HCCHMe-OCOCH3.freq\\0,1\\C,0.3470894567,-0.1344429624,-0.6712358492\\O,1
.6187925726,-0.7415624461,-0.3207887002\\C,2.6533931275,-0.5508538842,-
1.1781967636\\C,3.8953240549,-1.2470913035,-0.6722853258\\O,2.575353298,
0.0908823941,-2.2019115045\\C,-0.4292501026,-1.0696228822,-1.5906009532
\\H,4.7135271539,-1.0848369384,-1.3745614884\\H,3.7061109227,-2.31984959
9,-0.5614690836\\H,4.1694660785,-0.8610122869,0.3150274532\\H,0.12443952
09,-1.2227501506,-2.5208160321\\H,-0.5891781749,-2.0405722268,-1.108293
074\\H,0.5495204812,0.8122392761,-1.1807707233\\C,-0.3470894567,0.134442
9624,0.6712358492\\O,-1.6187925726,0.7415624461,0.3207887002\\C,-2.65339
31275,0.5508538842,1.1781967636\\C,-3.8953240549,1.2470913035,0.6722853
258\\O,-2.575353298,-0.0908823941,2.2019115045\\C,0.4292501026,1.0696228
822,1.5906009532\\H,-4.7135271539,1.0848369384,1.3745614884\\H,-3.706110
9227,2.319849599,0.5614690836\\H,-4.1694660785,0.8610122869,-0.31502745
32\\H,-0.1244395209,1.2227501506,2.5208160321\\H,0.5891781749,2.04057222

68,1.108293074\H,-0.5495204812,-0.8122392761,1.1807707233\H,-1.4025114
205,-0.6352519242,-1.8346184126\H,1.4025114205,0.6352519242,1.83461841
26\Version=IA32L-G03RevC.02\State=1-AG\HF=-614.2178113\RMSD=3.737e-09
\RMSF=5.300e-06\Dipole=0.,0.,0.\PG=CI [X(C8H14O4)]\@

n.Si_CH3_3-MeHCCHMe-Si_CH3_3

1\1\GINC-LC49\FOpt\RB3LYP\Gen\C10H26Si2\CYL509\29-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\Si_CH3_
3-MeHCCHMe-Si_CH3_3.freq\0,1\H,3.3034684477,-0.3353721012,-1.76482708
83\C,3.4065392904,-0.3840896169,-0.673332874\H,4.4451031732,-0.1217550
547,-0.4345075435\H,3.2523499906,-1.4258116878,-0.3754489107\Si,2.2166
956014,0.8355197997,0.1703218714\C,0.3808297898,0.5667394386,-0.381072
4889\C,2.380597426,0.7166225279,2.0588166196\C,2.7984594127,2.56795605
23,-0.3544410539\C,-0.3726621774,1.9142562158,-0.3251250837\H,3.864874
4315,2.6885049643,-0.1256458199\H,2.2591114542,3.368153429,0.164620170
1\H,2.6772569126,2.7309262082,-1.4326525695\H,3.4104434654,0.932130830
5,2.3694348424\H,2.1218742246,-0.2765044482,2.4429284293\H,1.730453757
2,1.4438420098,2.5608091774\H,0.1554028329,2.6988467074,-0.8761181236\
H,-0.4945819609,2.2640186117,0.7086781584\H,-1.3752599926,1.8440398617
, -0.7604347518\H,0.436656488,0.2700874152,-1.4418353565\H,-3.303468447
7,0.3353721012,1.7648270883\C,-3.4065392904,0.3840896169,0.673332874\H
, -4.4451031732,0.1217550547,0.4345075435\H,-3.2523499906,1.4258116878,
0.3754489107\Si,-2.2166956014,-0.8355197997,-0.1703218714\C,-0.3808297
898,-0.5667394386,0.3810724889\C,-2.380597426,-0.7166225279,-2.0588166
196\C,-2.7984594127,-2.5679560523,0.3544410539\C,0.3726621774,-1.91425
62158,0.3251250837\H,-3.8648744315,-2.6885049643,0.1256458199\H,-2.259
1114542,-3.368153429,-0.1646201701\H,-2.6772569126,-2.7309262082,1.432
6525695\H,-3.4104434654,-0.9321308305,-2.3694348424\H,-2.1218742246,0.
2765044482,-2.4429284293\H,-1.7304537572,-1.4438420098,-2.5608091774\H
, -0.1554028329,-2.6988467074,0.8761181236\H,0.4945819609,-2.2640186117
, -0.7086781584\H,1.3752599926,-1.8440398617,0.7604347518\H,-0.43665648
8,-0.2700874152,1.4418353565\Version=IA32L-G03RevC.02\State=1-AG\HF=-
975.7826376\RMSD=2.214e-09\RMSF=6.054e-06\Dipole=0.,0.,0.\PG=CI [X(C10
H26Si2)]\@

n.P_CH3_2-MeHCCHMe-P_CH3_2

1\1\GINC-LC24\FOpt\RB3LYP\Gen\C8H20P2\CYL509\29-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\P_CH3_2-M
eHCCHMe-P_CH3_2.freq\0,1\C,-0.6923095037,0.7604514482,3.1468758167\H,
-0.8761641572,0.4801472606,4.1903783874\H,-1.6199407493,1.1596258696,2
.7288727539\H,0.0588854682,1.5582483774,3.1548785624\P,0.021087733,-0.
7364285119,2.282438344\C,-1.516094837,-1.7508896097,1.9737220444\C,0.5
452390229,-0.1418497752,0.5343559622\H,-1.2550204959,-2.6347843561,1.3
81774477\H,-2.325699281,-1.215843079,1.4661895954\H,-1.8900835523,-2.1
069556041,2.9400350447\C,1.5897824173,-1.181078088,0.0766156774\H,2.30
42750559,-1.393658313,0.8774947444\H,2.1568581816,-0.8369192312,-0.790
7295108\H,1.1115707089,-2.1302684515,-0.197507952\H,1.0758043211,0.799
326293,0.7431927881\C,0.6923095037,-0.7604514482,-3.1468758167\H,0.876
1641572,-0.4801472606,-4.1903783874\H,1.6199407493,-1.1596258696,-2.72
88727539\H,-0.0588854682,-1.5582483774,-3.1548785624\P,-0.021087733,0.
7364285119,-2.282438344\C,1.516094837,1.7508896097,-1.9737220444\C,-0.
5452390229,0.1418497752,-0.5343559622\H,1.2550204959,2.6347843561,-1.3
81774477\H,2.325699281,1.215843079,-1.4661895954\H,1.8900835523,2.1069
556041,-2.9400350447\C,-1.5897824173,1.181078088,-0.0766156774\H,-2.30
42750559,1.393658313,-0.8774947444\H,-2.1568581816,0.8369192312,0.7907
295108\H,-1.1115707089,2.1302684515,0.197507952\H,-1.0758043211,-0.799
326293,-0.7431927881\Version=IA32L-G03RevC.02\State=1-AG\HF=-999.5955
908\RMSD=6.265e-09\RMSF=1.384e-05\Dipole=0.,0.,0.\PG=CI [X(C8H20P2)]\@
@

n.SC_CH3_2CN-MeHCCHMe-SC_CH3_2CN

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C12H20N2S2\CYL509\21-Aug-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\SC_CH3
_2CN-MeHCCHMe-SC_CH3_2CN.freq\0,1\N,-0.2056793962,-3.0008161456,-2.01
21902074\C,-0.3824428696,-3.1033022411,-0.867854561\C,-0.622408782,-3.
2489614361,0.5724538759\S,-0.0616958726,-1.7177397907,1.5077433077\C,-
0.5224907425,-0.1746317308,0.5492750759\C,-1.9771905069,-0.1871118991,
0.0697914528\C,0.2749888384,-4.3836241756,1.1191192989\C,-2.1069155851
, -3.5806692352,0.8310965799\H,0.1510203365,-4.4572632885,2.2044018625\
H,-0.0208315601,-5.3384531018,0.6715060774\H,-2.2680745231,-3.68107177
67,1.9081853472\H,-2.3688704936,-4.5278817264,0.3447121896\H,-2.771286
3036,-2.803467529,0.4518420712\H,-2.6464829138,-0.4606880642,0.8900706
411\H,-2.1249740659,-0.8871335167,-0.7593108686\H,-0.4289233924,0.5584
557463,1.3573673767\N,0.2097999157,2.9982533017,2.0136749713\C,0.38522
69423,3.1019613617,0.869243665\C,0.6235333265,3.2491588474,-0.57118601
47\S,0.0594200348,1.7199974518,-1.5078236354\C,0.5194485828,0.17488727
18,-0.5521695688\C,1.9745641318,0.1850583824,-0.0739260348\C,-0.272979
1394,4.385793217,-1.1151994636\C,2.1081697443,3.5791323302,-0.83129054
44\H,-1.3267548838,4.2027076089,-0.8933624073\H,-0.1502527702,4.460742
6425,-2.2005336603\H,0.0247151043,5.3395998605,-0.6666516446\H,2.26813
92161,3.6805696046,-1.9084594794\H,2.3720086405,4.5254206675,-0.344127
6435\H,2.7719449579,2.8005948673,-0.4537405883\H,2.643315066,0.4598722
392,-0.8942318436\H,2.1237164214,0.8830819722,0.7566135369\H,2.2574552
742,-0.8089864873,0.2809648803\H,0.4244762212,-0.5569498814,-1.3612356
447\H,-2.2605833379,0.8059166571,-0.2875869498\H,1.3287891316,-4.19939
33188,0.8983460759\Version=IA64L-G03RevC.02\State=1-A\HF=-1375.168621
8\RMSD=3.447e-09\RMSF=9.720e-07\Dipole=-0.0008093,0.0006324,-0.0005316
\PG=C01 [X(C12H20N2S2)]\@

n.SCH2COOCH3-MeHCCHMe-SCH2COOCH3

1\1\GINC-LC84\FOpt\RB3LYP\Gen\C10H18O4S2\CYL509\29-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\SCH2CO
OCH3-MeHCCHMe-SCH2COOCH3.freq\0,1\S,1.2161067588,0.8330080992,-1.7231
469341\C,0.3559566963,-0.372188907,-0.5774549401\C,1.4209178901,-1.372
011116,-0.1124951377\C,0.0137373928,0.9985440024,-3.1103237138\C,-0.09
18562752,-0.2868309092,-3.9009206032\O,-0.7941943578,-1.2286330617,-3.
5919262025\O,0.7154282274,-0.2735585045,-4.979032382\C,0.7348311435,-1
.4874955169,-5.7497124982\H,0.4008762155,1.8067789623,-3.7344555858\H,
-0.9730406581,1.2692641588,-2.7299811183\H,-0.2647600532,-1.7186599885
, -6.1268375079\H,1.0864305138,-2.3219638058,-5.1372866081\H,1.42338637
5,-1.2986609118,-6.5734829771\H,0.9712007877,-2.1320851548,0.533666455
6\H,1.8697087296,-1.8767982809,-0.9719465485\H,2.22437118,-0.871643304
3,0.4421203681\H,-0.3840364669,-0.8952114225,-1.191551078\S,-1.2161067
588,-0.8330080992,1.7231469341\C,-0.3559566963,0.372188907,0.577454940
1\C,-1.4209178901,1.372011116,0.1124951377\C,-0.0137373928,-0.99854400
24,3.1103237138\C,0.0918562752,0.2868309092,3.9009206032\O,0.794194357
8,1.2286330617,3.5919262025\O,-0.7154282274,0.2735585045,4.979032382\C
, -0.7348311435,1.4874955169,5.7497124982\H,-0.4008762155,-1.8067789623
, 3.7344555858\H,0.2647600532,1.7186599885,6.1268375079\H,-1.0864305138
, 2.3219638058,5.1372866081\H,-1.423386375,1.2986609118,6.5734829771\H,
-1.8697087296,1.8767982809,0.9719465485\H,-2.22437118,0.8716433043,-0.
4421203681\H,0.3840364669,0.8952114225,1.191551078\H,0.9730406581,-1.2
692641588,2.7299811183\H,-0.9712007877,2.1320851548,-0.5336664556\Ver
sion=IA32L-G03RevC.02\State=1-AG\HF=-1489.1909903\RMSD=3.445e-09\RMSF=
3.742e-06\Dipole=0.,0.,0.\PG=CI [X(C10H18O4S2)]\@

n.SCH2Ph-MeHCCHMe-SCH2Ph

1\1\GINC-LC144\FOpt\RB3LYP\Gen\C18H22S2\CYL509\29-Jun-2008\0\#\B3LYP/G

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EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\SCH2Ph-
MeHCCMe-SCH2Ph.freq\\0,1\\C,0.2128983811,-0.0506996688,0.743202165\\S,1
.3150319342,1.4032971678,1.1306052539\\C,2.1211168901,0.8139094914,2.68
91690763\\C,3.1488419124,1.8209477942,3.141722843\\H,2.5889923959,-0.155
2436679,2.4856224929\\H,1.3588539367,0.6731040573,3.4611032294\\C,4.4660
732987,1.7604147389,2.6675180134\\C,2.8003954413,2.8438457382,4.0332482
026\\C,5.4153579013,2.6944064096,3.081567366\\C,3.7475292974,3.780392614
7,4.448251408\\C,5.0583598348,3.707513807,3.9738625719\\H,5.7978276778,4
.4346742905,4.2985062314\\H,3.4617931286,4.5654677661,5.1433574047\\H,6.
4341717812,2.6303229314,2.7086074003\\H,1.7797952412,2.9043235436,4.404
0354803\\H,4.7464013459,0.9748822637,1.9696777046\\H,0.8354152427,-0.948
1428668,0.8596947465\\C,-0.2128983811,0.0506996688,-0.743202165\\S,-1.31
50319342,-1.4032971678,-1.1306052539\\C,-2.1211168901,-0.8139094914,-2.
6891690763\\C,0.9661227061,0.1030426942,-1.7219516461\\C,-3.1488419124,-
1.8209477942,-3.141722843\\H,-2.5889923959,0.1552436679,-2.4856224929\\H
,-1.3588539367,-0.6731040573,-3.4611032294\\C,-4.4660732987,-1.76041473
89,-2.6675180134\\C,-2.8003954413,-2.8438457382,-4.0332482026\\C,-5.4153
579013,-2.6944064096,-3.081567366\\C,-3.7475292974,-3.7803926147,-4.448
251408\\C,-5.0583598348,-3.707513807,-3.9738625719\\H,-5.7978276778,-4.4
346742905,-4.2985062314\\H,-3.4617931286,-4.5654677661,-5.1433574047\\H,
-6.4341717812,-2.6303229314,-2.7086074003\\H,-1.7797952412,-2.904323543
6,-4.4040354803\\H,-4.7464013459,-0.9748822637,-1.9696777046\\H,0.615107
1239,0.1002975665,-2.7585249698\\H,1.6169887328,-0.7671869196,-1.584917
0354\\H,-0.8354152427,0.9481428668,-0.8596947465\\H,1.5656086715,1.00600
74539,-1.5732139186\\C,-0.9661227061,-0.1030426942,1.7219516461\\H,-0.61
51071239,-0.1002975665,2.7585249698\\H,-1.6169887328,0.7671869196,1.584
9170354\\H,-1.5656086715,-1.0060074539,1.5732139186\\Version=IA32L-G03R
evC.02\\State=1-AG\\HF=-1495.5483326\\RMSD=2.795e-09\\RMSF=4.507e-06\\Dipol
e=0.,0.,0.\\PG=CI [X(C18H22S2)]\\@
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n.SCH3-MeHCCMe-SCH3

```
1\\1\\GINC-LC138\\FOpt\\RB3LYP\\Gen\\C6H14S2\\CYL509\\29-Jun-2008\\0\\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\SCH3-MeH
CCHMe-SCH3.freq\\0,1\\S,0.4220079185,-0.4688809438,-2.1886624638\\C,0.10
87351675,-0.6755678323,-0.3635754526\\C,-0.992064365,-1.7121333204,-0.1
113905301\\C,-1.173977718,0.1771744031,-2.8047290838\\H,-1.0521511791,0.
2927866331,-3.8851021673\\H,-1.4152380141,1.1556837144,-2.3789649426\\H,
-1.9964814645,-0.5191213294,-2.6215459948\\H,-1.0588468243,-1.957211651
4,0.9521157142\\H,-1.9740693857,-1.3333350827,-0.4172426409\\H,-0.787675
1001,-2.6266937312,-0.6752330653\\H,1.0701797179,-1.091843067,-0.036130
529\\S,-0.4220079185,0.4688809438,2.1886624638\\C,-0.1087351675,0.675567
8323,0.3635754526\\C,0.992064365,1.7121333204,0.1113905301\\C,1.17397771
8,-0.1771744031,2.8047290838\\H,1.0521511791,-0.2927866331,3.8851021673
\\H,1.4152380141,-1.1556837144,2.3789649426\\H,1.9964814645,0.5191213294
,2.6215459948\\H,1.0588468243,1.9572116514,-0.9521157142\\H,1.9740693857
,1.3333350827,0.4172426409\\H,0.7876751001,2.6266937312,0.6752330653\\H,
-1.0701797179,1.091843067,0.036130529\\Version=IA32L-G03RevC.02\\State=
1-AG\\HF=-1033.4488312\\RMSD=5.758e-09\\RMSF=1.070e-05\\Dipole=0.,0.,0.\\PG
=CI [X(C6H14S2)]\\@
```

n.SO2CH3-MeHCCMe-SO2CH3

```
1\\1\\GINC-LC44\\FOpt\\RB3LYP\\Gen\\C6H14O4S2\\CYL509\\29-Jun-2008\\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\SO2CH3-
MeHCCMe-SO2CH3.freq\\0,1\\C,-0.5704757492,-0.4362521815,0.2800186444\\S
,-0.5766946806,-0.3830884535,2.158210147\\C,0.4938669526,-1.7475655029,
2.6854369157\\O,0.0299074002,0.8895066792,2.5919229283\\O,-1.9318298959,
-0.7429284972,2.6071449565\\H,0.069401775,-2.6866608571,2.3250474153\\H,
0.4739168455,-1.723636734,3.7777820907\\H,1.5115719524,-1.6070356014,2.
3224038636\\C,-1.9842404351,-0.0496896409,-0.1708016462\\H,-2.1020836399
```

, -0.2875933186, -1.2298060019\H, -2.1797754077, 1.0155314168, -0.005295116
\H, -2.7283687074, -0.6149625565, 0.3924525887\H, -0.3836258263, -1.4853132
441, 0.02489104\C, 0.5704757492, 0.4362521815, -0.2800186444\S, 0.576694680
6, 0.3830884535, -2.158210147\C, -0.4938669526, 1.7475655029, -2.6854369157
\O, -0.0299074002, -0.8895066792, -2.5919229283\O, 1.9318298959, 0.74292849
72, -2.6071449565\H, -0.069401775, 2.6866608571, -2.3250474153\H, -0.473916
8455, 1.723636734, -3.7777820907\H, -1.5115719524, 1.6070356014, -2.3224038
636\C, 1.9842404351, 0.0496896409, 0.1708016462\H, 2.1020836399, 0.28759331
86, 1.2298060019\H, 2.1797754077, -1.0155314168, 0.005295116\H, 2.728368707
4, 0.6149625565, -0.3924525887\H, 0.3836258263, 1.4853132441, -0.02489104\\
Version=IA32L-G03RevC.02\State=1-AG\HF=-1334.2218244\RMSD=2.579e-09\RM
SF=1.240e-05\Dipole=0., 0., 0.\PG=CI [X(C6H14O4S2)]\@

n. SOCH3-MeHCCHMe-SOCH3

1\1\GINC-LC37\FOpt\RB3LYP\Gen\C6H14O2S2\CYL509\29-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\SOCH3-M
eHCCHMe-SOCH3.freq\0, 1\C, -0.5956493234, -0.2814358535, 0.4079801305\S, -
0.6028855763, 0.2573489258, 2.1840202357\O, 0.5925844284, -0.7396176867, 2.
8581261251\C, 1.8473880264, -0.0926284914, 3.0965189882\C, -0.7463371932, -
1.8057195192, 0.3470785389\H, 2.4736838969, -0.8434007015, 3.5880346602\H,
1.7342944226, 0.7742255723, 3.758053013\H, 2.3285065, 0.2287887775, 2.16469
16047\H, 0.1027690222, -2.290182559, 0.8390551843\H, -0.7898201757, -2.1530
696252, -0.688417455\H, -1.6567855465, -2.1186395736, 0.8659397633\H, -1.51
59815291, 0.2021972361, 0.048772086\C, 0.5956493234, 0.2814358535, -0.40798
01305\S, 0.6028855763, -0.2573489258, -2.1840202357\O, -0.5925844284, 0.739
6176867, -2.8581261251\C, -1.8473880264, 0.0926284914, -3.0965189882\C, 0.7
463371932, 1.8057195192, -0.3470785389\H, -2.4736838969, 0.8434007015, -3.5
880346602\H, -1.7342944226, -0.7742255723, -3.758053013\H, -2.3285065, -0.2
287887775, -2.1646916047\H, -0.1027690222, 2.290182559, -0.8390551843\H, 0.
7898201757, 2.1530696252, 0.688417455\H, 1.6567855465, 2.1186395736, -0.865
9397633\H, 1.5159815291, -0.2021972361, -0.048772086\Version=IA32L-G03Re
vC.02\State=1-AG\HF=-1183.8198268\RMSD=6.035e-09\RMSF=2.012e-05\Dipole
=0., 0., 0.\PG=CI [X(C6H14O2S2)]\@

n. Ph-MeHCCHMe-Ph

1\1\GINC-LC102\FOpt\RB3LYP\Gen\C16H18\CYL509\29-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\Ph-MeHCCH
Me-Ph.freq\0, 1\H, -5.3896069015, -2.0927494346, 0.1208145038\C, -4.344731
6314, -1.7993315175, 0.1769963228\C, -3.3480666427, -2.6458987156, -0.30818
49247\C, -2.0070651118, -2.263508108, -0.2341928659\C, -1.6311486857, -1.03
5024793, 0.3245616181\C, -2.6459348326, -0.1958823403, 0.8109104698\C, -3.9
872940956, -0.5707968379, 0.7369797489\H, -3.6118547321, -3.605515073, -0.7
456182616\C, -0.1620603259, -0.6403001014, 0.4176362164\C, 0.2704557931, -0.
.4943872302, 1.8897322047\H, -2.387347149, 0.7626171629, 1.2547460162\H, -1.
.2371541552, -2.9310471746, -0.6155878077\H, -4.7550377345, 0.0970420666, 1.
.1196815504\H, 1.3455002861, -0.3077371606, 1.9686596644\H, 0.0354925156, -
1.4049060775, 2.4512193668\H, -0.2503708437, 0.3388281722, 2.3767860182\H,
0.4207113852, -1.4641357015, -0.017846072\H, 5.3896069015, 2.0927494346, -0.
.1208145038\C, 4.3447316314, 1.7993315175, -0.1769963228\C, 3.3480666427, 2.
.6458987156, 0.3081849247\C, 2.0070651118, -2.263508108, 0.2341928659\C, 1.6
311486857, 1.035024793, -0.3245616181\C, 2.6459348326, 0.1958823403, -0.810
9104698\C, 3.9872940956, 0.5707968379, -0.7369797489\H, 3.6118547321, 3.605
515073, 0.7456182616\C, 0.1620603259, 0.6403001014, -0.4176362164\C, -0.270
4557931, 0.4943872302, -1.8897322047\H, 2.387347149, -0.7626171629, -1.2547
460162\H, 1.2371541552, 2.9310471746, 0.6155878077\H, 4.7550377345, -0.0970
420666, -1.1196815504\H, -1.3455002861, 0.3077371606, -1.9686596644\H, -0.0
354925156, 1.4049060775, -2.4512193668\H, 0.2503708437, -0.3388281722, -2.3
767860182\H, -0.4207113852, 1.4641357015, 0.017846072\Version=IA32L-G03R
evC.02\State=1-AG\HF=-620.5540818\RMSD=4.046e-09\RMSF=1.640e-05\Dipole

=0.,0.,0.\PG=CI [X(C16H18)]\@

n.C6H4CN-MeHCCHMe-C6H4CN

1\1\GINC-LC21\FOpt\RB3LYP\Gen\C18H16N2\CYL509\28-Jun-2008\0\#\B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C6H4CN-M
eHCCHMe-C6H4CN.freq\0,1\N,-7.2373983888,-0.4993858944,0.5876198753\C,
-6.0852490191,-0.3382821017,0.5715843413\C,-4.6655001827,-0.1402696072
,0.5514169126\C,-3.8003711519,-1.1785912846,0.936542776\C,-2.424664510
2,-0.9793860946,0.9159840413\C,-1.8708838772,0.2464478177,0.5113430797
\C,-2.7475560564,1.2718436943,0.1303821135\C,-4.1277061961,1.091483837
2,0.1476330579\H,-4.2138206305,-2.1316358378,1.250848752\C,-0.36499510
81,0.4712182758,0.5060705408\C,0.2067341094,0.347243583,1.9324376628\H
, -2.3425589322,2.2305070078,-0.1838296161\H,-1.7734033548,-1.793261367
3,1.2228183787\H,-4.7921860209,1.8966071916,-0.149321639\H,1.268305506
2,0.610203164,1.9550387558\H,0.1070222322,-0.675212653,2.315605638\H,-
0.3254345344,1.0127238133,2.6199296474\H,-0.1949056262,1.5025164846,0.
1678910044\N,7.2373983888,0.4993858944,-0.5876198753\C,6.0852490191,0.
3382821017,-0.5715843413\C,4.6655001827,0.1402696072,-0.5514169126\C,3
.8003711519,1.1785912846,-0.936542776\C,2.4246645102,0.9793860946,-0.9
159840413\C,1.8708838772,-0.2464478177,-0.5113430797\C,2.7475560564,-1
.2718436943,-0.1303821135\C,4.1277061961,-1.0914838372,-0.1476330579\H
,4.2138206305,2.1316358378,-1.250848752\C,0.3649951081,-0.4712182758,-
0.5060705408\C,-0.2067341094,-0.347243583,-1.9324376628\H,2.3425589322
, -2.2305070078,0.1838296161\H,1.7734033548,1.7932613673,-1.2228183787\H
,4.7921860209,-1.8966071916,0.149321639\H,-1.2683055062,-0.610203164,
-1.9550387558\H,-0.1070222322,0.675212653,-2.315605638\H,0.3254345344,
-1.0127238133,-2.6199296474\H,0.1949056262,-1.5025164846,-0.1678910044
\Version=IA32L-G03RevC.02\State=1-AG\HF=-805.0417205\RMSD=5.627e-09\R
MSF=9.225e-06\Dipole=0.,0.,0.\PG=CI [X(C18H16N2)]\@

n.C6H4NO2-MeHCCHMe-C6H4NO2

1\1\GINC-LC136\FOpt\RB3LYP\Gen\C16H16N2O4\CYL509\28-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C6H4N
O2-MeHCCHMe-C6H4NO2.freq\0,1\O,-4.8354367403,4.4980119629,-1.76067618
85\N,-4.1611540067,3.7550329334,-2.4738984427\C,-3.2925583082,2.773148
42,-1.8088765447\O,-4.162252011,3.7762616396,-3.7048195633\C,-3.265364
1608,2.7232347867,-0.4177977104\C,-2.4367047001,1.7900667685,0.1999663
93\C,-1.640823923,0.9094285026,-0.5475594827\C,-1.6992269481,0.9887373
465,-1.9496930894\C,-2.5172144094,1.9151269408,-2.5875114708\H,-2.5669
940453,1.9831298435,-3.6673154469\C,-0.7587251825,-0.1171298972,0.1491
63468\C,-1.207951722,-1.548340418,-0.2072832429\H,-2.4093811115,1.7437
614526,1.285512695\H,-1.0993286306,0.3164080687,-2.5565467684\H,-3.882
7475219,3.4048983653,0.1542769844\H,-0.648650329,-2.290631917,0.369543
1141\H,-1.0516349412,-1.7634116263,-1.2708656971\H,-2.273460382,-1.682
059197,0.0056765376\H,-0.9005208976,0.0171405235,1.2300867742\O,4.8354
367403,-4.4980119629,1.7606761885\N,4.1611540067,-3.7550329334,2.47389
84427\C,3.2925583082,-2.77314842,1.8088765447\O,4.162252011,-3.7762616
396,3.7048195633\C,3.2653641608,-2.7232347867,0.4177977104\C,2.4367047
001,-1.7900667685,-0.199966393\C,1.640823923,-0.9094285026,0.547559482
7\C,1.6992269481,-0.9887373465,1.9496930894\C,2.5172144094,-1.91512694
08,2.5875114708\H,2.5669940453,-1.9831298435,3.6673154469\C,0.75872518
25,0.1171298972,-0.149163468\C,1.207951722,1.548340418,0.2072832429\H,
2.4093811115,-1.7437614526,-1.285512695\H,1.0993286306,-0.3164080687,2
.5565467684\H,3.8827475219,-3.4048983653,-0.1542769844\H,0.648650329,2
.290631917,-0.3695431141\H,1.0516349412,1.7634116263,1.2708656971\H,2.
273460382,1.682059197,-0.0056765376\H,0.9005208976,-0.0171405235,-1.23
00867742\Version=IA32L-G03RevC.02\State=1-AG\HF=-1029.5584154\RMSD=4.
862e-09\RMSF=3.148e-05\Dipole=0.,0.,0.\PG=CI [X(C16H16N2O4)]\@

n.C6H4OCH3-MeHCCHMe-C6H4OCH3

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1\1\GINC-LC119\FOpt\RB3LYP\Gen\C18H22O2\CYL509\28-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C6H4OCH
3-MeHCCHMe-C6H4OCH3.freq\0,1\C,-3.8372390571,0.0537900822,1.438883575
6\C,-3.7736864145,0.3913758461,2.7989280852\C,-2.558964036,0.819833134
9,3.3413082671\C,-1.4288901617,0.9028211185,2.5203858172\C,-1.46891367
49,0.5721428225,1.1640403511\C,-2.7038221301,0.1466585889,0.6420982885
\C,-0.228712591,0.6900968516,0.287494477\O,-4.9429130153,0.2686204151,
3.4974044612\C,-4.9345667797,0.5999264045,4.8754399869\C,-0.4425613762
,1.7348209134,-0.8251602086\H,-2.7840126355,-0.117462591,-0.4097417156
\H,-0.4910346387,1.238176196,2.9584697174\H,-2.4765614298,1.0892875781
,4.388277663\H,-4.787841428,-0.2760384001,1.0307576509\H,-4.2449874928
,-0.0403985807,5.4420756505\H,-5.9534294593,0.4337996062,5.2305824535\
H,-4.661690652,1.6514857671,5.0377521831\H,0.4744264574,1.8947286737,-
1.3999678872\H,-0.7547029916,2.6933024146,-0.3967801472\H,-1.224057945
9,1.4153310953,-1.525488736\H,0.5852268552,1.0549935705,0.9302631475\C
,3.8372390571,-0.0537900822,-1.4388835756\C,3.7736864145,-0.3913758461
,-2.7989280852\C,2.558964036,-0.8198331349,-3.3413082671\C,1.428890161
7,-0.9028211185,-2.5203858172\C,1.4689136749,-0.5721428225,-1.16404035
11\C,2.7038221301,-0.1466585889,-0.6420982885\C,0.228712591,-0.6900968
516,-0.287494477\O,4.9429130153,-0.2686204151,-3.4974044612\C,4.934566
7797,-0.5999264045,-4.8754399869\C,0.4425613762,-1.7348209134,0.825160
2086\H,2.7840126355,0.117462591,0.4097417156\H,0.4910346387,-1.2381761
96,-2.9584697174\H,2.4765614298,-1.0892875781,-4.388277663\H,4.7878414
28,0.2760384001,-1.0307576509\H,4.2449874928,0.0403985807,-5.442075650
5\H,5.9534294593,-0.4337996062,-5.2305824535\H,4.661690652,-1.65148576
71,-5.0377521831\H,-0.4744264574,-1.8947286737,1.3999678872\H,0.754702
9916,-2.6933024146,0.3967801472\H,1.2240579459,-1.4153310953,1.5254887
36\H,-0.5852268552,-1.0549935705,-0.9302631475\Version=IA32L-G03RevC.
02\State=1-AG\HF=-849.5987029\RMSD=6.522e-09\RMSF=2.640e-05\Dipole=0.,
0.,0.\PG=CI [X(C18H22O2)]\@
```

n.C6H4OH-MeHCCHMe-C6H4OH

```
1\1\GINC-LC138\FOpt\RB3LYP\Gen\C16H18O2\CYL509\28-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C6H4OH-
MeHCCHMe-C6H4OH.freq\0,1\C,-3.8713690316,-1.6125013401,0.8709451331\C
,-4.3598268783,-0.587546818,1.6851077662\C,-3.6341359361,0.601814227,1
.8058716669\C,-2.4331060042,0.758387346,1.1149845125\C,-1.9209298065,-
0.2563580694,0.2944909445\C,-2.6679432027,-1.4384273807,0.1912144993\C
,-0.6165288601,-0.0818580156,-0.4736730712\O,-5.5461203368,-0.80224653
49,2.3352211972\C,-0.7257926558,1.0778103153,-1.4826396788\H,-2.300049
709,-2.2450914856,-0.4393263848\H,-1.8905480795,1.6945318957,1.2225063
908\H,-4.0088091261,1.4061597996,2.4373526063\H,-4.4416677773,-2.53194
32479,0.7818282116\H,-5.763921273,-0.01447692,2.8570629236\H,0.1716066
082,1.148336017,-2.1043365876\H,-0.8527805532,2.0395551125,-0.97057471
01\H,-1.5915232095,0.9359039445,-2.1383472507\H,-0.4574474075,-1.00531
06212,-1.0487984926\C,3.8713690316,1.6125013401,-0.8709451331\C,4.3598
268783,0.587546818,-1.6851077662\C,3.6341359361,-0.601814227,-1.805871
6669\C,2.4331060042,-0.758387346,-1.1149845125\C,1.9209298065,0.256358
0694,-0.2944909445\C,2.6679432027,1.4384273807,-0.1912144993\C,0.61652
88601,0.0818580156,0.4736730712\O,5.5461203368,0.8022465349,-2.3352211
972\C,0.7257926558,-1.0778103153,1.4826396788\H,2.300049709,2.24509148
56,0.4393263848\H,1.8905480795,-1.6945318957,-1.2225063908\H,4.0088091
261,-1.4061597996,-2.4373526063\H,4.4416677773,2.5319432479,-0.7818282
116\H,5.763921273,0.01447692,-2.8570629236\H,-0.1716066082,-1.14833601
7,2.1043365876\H,0.8527805532,-2.0395551125,0.9705747101\H,1.591523209
5,-0.9359039445,2.1383472507\H,0.4574474075,1.0053106212,1.0487984926\
\Version=IA32L-G03RevC.02\State=1-AG\HF=-770.9854746\RMSD=6.498e-09\RM
SF=1.657e-05\Dipole=0.,0.,0.\PG=CI [X(C16H18O2)]\@
```

n.CF2CF3-MeHCCHMe-CF2CF3

```
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H8F10\CYL509\21-Aug-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CF2CF3-Me
HCCHMe-CF2CF3.freq\0,1\F,0.5599041227,1.4100860089,-1.9843700405\C,1.
228703975,1.0615558583,-0.8471409891\C,2.7320571878,0.9985264533,-1.20
39753352\C,0.6593136466,-0.2503349498,-0.2400524411\F,1.1144868947,2.1
334437712,-0.0007738948\F,2.9924076621,-0.0051624783,-2.0611475123\F,3
.4520401254,0.7899267454,-0.0848825563\F,3.1338776089,2.1449626547,-1.
7621297382\C,0.1728359889,-1.1506985213,-1.3935086101\H,0.9980470889,-
1.3264921666,-2.087202257\H,-0.6434765897,-0.6940676577,-1.9511026276\
H,-0.1571643548,-2.1150785242,-1.0103746466\H,1.5060291059,-0.76376411
53,0.2296946282\F,-1.7659877345,-0.8120438228,2.5885012505\C,-1.388178
1281,-0.9663840835,1.2800803861\C,-2.7409871312,-0.9074578506,0.523030
7909\C,-0.324535377,0.0982882463,0.9335011109\F,-0.8935634707,-2.23593
94028,1.1671782501\F,-3.2799841041,0.3164919391,0.6762460896\F,-2.6191
926445,-1.1454859811,-0.7921378413\F,-3.5856880174,-1.8139788562,1.029
4656197\C,0.5038535354,0.3735915364,2.2113270394\H,-0.0982315303,0.852
4799422,2.9851486916\H,0.8978637462,-0.5645821297,2.6174447741\H,1.346
2215138,1.0245979873,1.9793642054\H,-0.8823751502,1.0036813259,0.67390
88842\Version=IA64L-G03RevC.02\State=1-A\HF=-1308.0784438\RMSD=7.975e
-09\RMSF=1.398e-06\Dipole=0.2572329,-0.1215819,0.0937438\PG=C01 [X(C8H
8F10)]\@
```

n.CF2H-MeHCCHMe-CF2H

```
1\1\GINC-LC7\FOpt\RB3LYP\Gen\C6H10F4\CYL509\28-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CF2H-MeHCC
HMe-CF2H.freq\0,1\C,1.0883164934,-0.0042059669,-1.6258558211\C,0.7648
730825,0.024440099,-0.1343536529\H,2.1527565243,-0.1850599183,-1.81417
325\F,0.7665963497,1.1763182335,-2.2473569521\F,0.3824481442,-1.000790
9309,-2.2544725353\C,1.5536759876,-1.1102634692,0.5476829181\H,2.61712
20925,-1.042558634,0.2897214057\H,1.1894814674,-2.0914445918,0.2239345
202\H,1.4668802419,-1.0585167503,1.6324489568\H,1.1467366573,0.9842152
351,0.2354184418\C,-1.0883164934,0.0042059669,1.6258558211\C,-0.764873
0825,-0.024440099,0.1343536529\H,-2.1527565243,0.1850599183,1.81417325
\F,-0.7665963497,-1.1763182335,2.2473569521\F,-0.3824481442,1.00079093
09,2.2544725353\C,-1.5536759876,1.1102634692,-0.5476829181\H,-2.617122
0925,1.042558634,-0.2897214057\H,-1.1894814674,2.0914445918,-0.2239345
202\H,-1.4668802419,1.0585167503,-1.6324489568\H,-1.1467366573,-0.9842
152351,-0.2354184418\Version=IA32L-G03RevC.02\State=1-AG\HF=-634.0265
498\RMSD=8.187e-09\RMSF=6.188e-05\Dipole=0.,0.,0.\PG=CI [X(C6H10F4)]\@
```

n.CF3-MeHCCHMe-CF3

```
1\1\GINC-LC38\FOpt\RB3LYP\Gen\C6H8F6\CYL509\28-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CF3-MeHCC
HMe-CF3.freq\0,1\F,0.4223936633,1.9948263833,-1.4567985634\C,0.1729991
717,1.9396065769,-0.1263575044\F,1.3354039401,2.2112594803,0.511536486
7\C,-0.424271776,0.5901964978,0.282260991\F,-0.6602645874,2.9626867979
,0.1651567271\C,-1.9098083651,0.5508089064,-0.1273639224\H,-2.01738094
54,0.5223039501,-1.2168928915\H,-2.425749399,1.4379941773,0.2443520135
\H,-2.4038867028,-0.3277588344,0.2856516506\H,-0.3595820771,0.56485066
82,1.3763872189\F,-0.4223936633,-1.9948263833,1.4567985634\C,-0.172999
1717,-1.9396065769,0.1263575044\F,-1.3354039401,-2.2112594803,-0.51153
64867\C,0.424271776,-0.5901964978,-0.282260991\F,0.6602645874,-2.96268
67979,-0.1651567271\C,1.9098083651,-0.5508089064,0.1273639224\H,2.0173
809454,-0.5223039501,1.2168928915\H,2.425749399,-1.4379941773,-0.24435
20135\H,2.4038867028,0.3277588344,-0.2856516506\H,0.3595820771,-0.5648
506682,-1.3763872189\Version=IA32L-G03RevC.02\State=1-AG\HF=-832.5302
```

336\RMSD=9.571e-09\RMSF=3.450e-05\Dipole=0.,0.,0.\PG=CI [X(C6H8F6)]\@

n.CC12H-MeHCCHMe-CC12H

1\1\GINC-LC49\FOpt\RB3LYP\Gen\C6H10Cl4\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC12H-Me
HCCHMe-CC12H.freq\0,1\C,-0.2098305202,1.1431116991,-1.569604614\C,-0.
1467554538,0.7627706154,-0.0802955089\H,0.6716185294,0.8133248032,-2.1
105250778\C,-1.3886957174,1.2294990771,0.6962881766\H,-1.2000223173,1.
2282291964,1.7735910386\H,-2.2533516232,0.5894521248,0.4914913537\H,-1.
.6540798303,2.2531508353,0.4207349108\H,0.7280793956,1.307447559,0.298
1668256\C,0.2098305202,-1.1431116991,1.569604614\C,0.1467554538,-0.762
7706154,0.0802955089\H,-0.6716185294,-0.8133248032,2.1105250778\C,1.38
86957174,-1.2294990771,-0.6962881766\H,1.2000223173,-1.2282291964,-1.7
735910386\H,2.2533516232,-0.5894521248,-0.4914913537\H,1.6540798303,-2.
.2531508353,-0.4207349108\H,-0.7280793956,-1.307447559,-0.2981668256\C
1,-1.6155157187,0.3838893124,-2.4244258194\Cl,-0.2402304099,2.93921379
11,-1.7947018121\Cl,0.2402304099,-2.9392137911,1.7947018121\Cl,1.61551
57187,-0.3838893124,2.4244258194\Version=IA32L-G03RevC.02\State=1-AG\HF
=-2075.4491696\RMSD=2.692e-09\RMSF=3.064e-05\Dipole=0.,0.,0.\PG=CI [X
(C6H10Cl4)]\@

n.CC13-MeHCCHMe-CC13

1\1\GINC-LC9\FOpt\RB3LYP\Gen\C6H8Cl6\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CC13-MeHCC
HMe-CC13.freq\0,1\C,1.0536160857,-0.0928397163,-1.7288333461\C,0.7704
08652,-0.0687385475,-0.1761139697\C,1.4468071769,-1.2696146511,0.51074
34855\H,2.5050950945,-1.3138121004,0.2595628214\H,0.9809957504,-2.2178
962141,0.2262833443\H,1.3833907156,-1.1677816076,1.5916782039\H,1.2708
916526,0.8431122467,0.1652718851\C,-1.0536157734,0.0928296529,1.728827
7911\C,-0.7703936677,0.0687931711,0.1761122594\C,-1.4467589866,1.26972
4343,-0.5106821818\H,-2.5050517605,1.3139213427,-0.2595205995\H,-0.980
9398226,2.217980018,-0.2261490486\H,-1.3833203167,1.167962288,-1.59162
26307\H,-1.2708962858,-0.8430284615,-0.1653229521\Cl,2.7362034549,-0.6
630783371,-2.1112433179\Cl,0.9707198902,1.5637362069,-2.4687053981\Cl,
-0.087124293,-1.1961298377,-2.5982378699\Cl,0.0873491472,1.1958097101,
2.5983295155\Cl,-0.9710912165,-1.5638177389,2.4685817536\Cl,-2.7360890
975,0.6633986423,2.1112455961\Version=IA32L-G03RevC.02\State=1-A\HF=-
2994.5871418\RMSD=8.635e-09\RMSF=1.648e-05\Dipole=0.0000178,0.0000371,
-0.000003\PG=C01 [X(C6H8Cl6)]\@

n.CH2Cl-MeHCCHMe-CH2Cl

1\1\GINC-LC35\FOpt\RB3LYP\Gen\C6H12Cl2\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Cl-Me
HCCHMe-CH2Cl.freq\0,1\C,0.7709311114,-0.1257501524,0.0394960883\C,1.1
877664429,-0.2818251329,1.5095251107\C,1.5964373905,0.9810432836,-0.63
93433144\H,0.6056343551,-1.0429736757,2.0247802524\H,1.0973578018,0.66
39941786,2.0510011529\H,2.6606933003,0.8470526606,-0.429105349\H,1.301
1477307,1.9720379586,-0.2705457995\H,1.4801605945,0.9769639711,-1.7266
555083\H,0.9806556533,-1.0823856616,-0.4605626871\C,-0.7709311114,0.12
57501524,-0.0394960883\C,-1.1877664429,0.2818251329,-1.5095251107\C,-1.
.5964373905,-0.9810432836,0.6393433144\H,-0.6056343551,1.0429736757,-2.
.0247802524\H,-1.0973578018,-0.6639941786,-2.0510011529\H,-2.660693300
3,-0.8470526606,0.429105349\H,-1.3011477307,-1.9720379586,0.2705457995
\H,-1.4801605945,-0.9769639711,1.7266555083\H,-0.9806556533,1.08238566
16,0.4605626871\Cl,2.9199073415,-0.813070535,1.7011376018\Cl,-2.919907
3415,0.813070535,-1.7011376018\Version=IA32L-G03RevC.02\State=1-AG\HF
=-1156.2704829\RMSD=2.504e-09\RMSF=1.513e-04\Dipole=0.,0.,0.\PG=CI [X(
C6H12Cl2)]\@

n.CH2F-MeHCCHMe-CH2F

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1\1\GINC-LC70\FOpt\RB3LYP\Gen\C6H12F2\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2F-MeHC
CHMe-CH2F.freq\0,1\C,-0.2383214267,0.4690569139,-0.5710862202\C,0.801
8221773,1.5251906868,-0.9499406973\F,1.8943934791,0.9723622418,-1.6224
182784\C,-1.5542014298,1.2037868516,-0.2465783885\H,1.1796121144,2.044
7122336,-0.0588021919\H,0.3566821321,2.2689927333,-1.6215567276\H,-1.4
386588615,1.8503268877,0.632589622\H,-2.3637681527,0.50776448,-0.02771
85602\H,-1.8595552707,1.834445843,-1.0896603722\H,-0.3976884092,-0.146
0800594,-1.4702012235\C,0.2383214267,-0.4690569139,0.5710862202\C,-0.8
018221773,-1.5251906868,0.9499406973\F,-1.8943934791,-0.9723622418,1.6
224182784\C,1.5542014298,-1.2037868516,0.2465783885\H,-1.1796121144,-2
.0447122336,0.0588021919\H,-0.3566821321,-2.2689927333,1.6215567276\H,
1.4386588615,-1.8503268877,-0.632589622\H,2.3637681527,-0.50776448,0.0
277185602\H,1.8595552707,-1.834445843,1.0896603722\H,0.3976884092,0.14
60800594,1.4702012235\Version=IA32L-G03RevC.02\State=1-AG\HF=-435.536
1476\RMSD=3.468e-09\RMSF=5.221e-05\Dipole=0.,0.,0.\PG=CI [X(C6H12F2)]\
\@
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n.CH2OH-MeHCCHMe-CH2OH

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1\1\GINC-LC76\FOpt\RB3LYP\Gen\C6H14O2\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2OH-MeH
CCHMe-CH2OH.freq\0,1\C,-0.1687349737,0.4598467936,-0.6040986551\C,0.9
324228712,1.4899372729,-0.9039769535\O,1.9972459068,0.878728794,-1.633
4083683\C,-1.5004889765,1.2139218444,-0.4311769497\H,1.29722565,1.9275
316624,0.041328457\H,0.499958885,2.3121679206,-1.4955049649\H,2.672445
8917,1.5560831533,-1.7909150877\H,-1.44674171,1.9189271089,0.408441132
2\H,-2.3286199463,0.5364811817,-0.2197765829\H,-1.7357549423,1.7861260
062,-1.3366651329\H,-0.2444310215,-0.1752438568,-1.5000369959\C,0.1687
349737,-0.4598467936,0.6040986551\C,-0.9324228712,-1.4899372729,0.9039
769535\O,-1.9972459068,-0.878728794,1.6334083683\C,1.5004889765,-1.213
9218444,0.4311769497\H,-1.29722565,-1.9275316624,-0.041328457\H,-0.499
958885,-2.3121679206,1.4955049649\H,-2.6724458917,-1.5560831533,1.7909
150877\H,1.44674171,-1.9189271089,-0.4084411322\H,2.3286199463,-0.5364
811817,0.2197765829\H,1.7357549423,-1.7861260062,1.3366651329\H,0.2444
310215,0.1752438568,1.5000369959\Version=IA32L-G03RevC.02\State=1-AG\
HF=-387.4861842\RMSD=8.846e-09\RMSF=2.554e-05\Dipole=0.,0.,0.\PG=CI [X
(C6H14O2)]\@
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n.CH2Ph-MeHCCHMe-CH2Ph

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1\1\GINC-LC51\FOpt\RB3LYP\Gen\C18H22\CYL509\28-Jun-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2Ph-MeHC
CHMe-CH2Ph.freq\0,1\C,0.3528874912,0.4020094443,-0.5658452372\C,1.600
4469323,1.1623352578,-0.0341864805\C,2.246580452,2.0958189738,-1.03877
89142\C,1.621874636,3.3019541367,-1.3909067809\C,3.4766709369,1.791926
2497,-1.6365577495\C,2.2024946346,4.1714176189,-2.3136840178\C,4.06403
81559,2.6592968109,-2.5603429186\C,3.4278965108,3.8524122161,-2.903513
4556\H,3.8834039158,4.530235495,-3.620536374\H,1.7011372078,5.10174210
15,-2.5686482772\H,5.0202292154,2.4020601375,-3.0090525053\H,0.6714817
665,3.5645840137,-0.9303338014\H,3.9820421888,0.8655870529,-1.37192916
98\H,1.3173289724,1.7513088535,0.8440569011\H,2.3398329422,0.425907556
8,0.3101844786\C,0.749749958,-0.4808915139,-1.7618320933\H,1.363837969
1,-1.330808492,-1.4337744256\H,1.3360594658,0.0902078599,-2.4878095277
\H,-0.1190833602,-0.8811140637,-2.2920507145\H,-0.3625270052,1.1591265
72,-0.9247414044\C,-0.3528874912,-0.4020094443,0.5658452372\C,-1.60044
69323,-1.1623352578,0.0341864805\C,-2.246580452,-2.0958189738,1.038778
9142\C,-1.621874636,-3.3019541367,1.3909067809\C,-3.4766709369,-1.7919
262497,1.6365577495\C,-2.2024946346,-4.1714176189,2.3136840178\C,-4.06
40381559,-2.6592968109,2.5603429186\C,-3.4278965108,-3.8524122161,2.90
```

35134556\H,-3.8834039158,-4.530235495,3.620536374\H,-1.7011372078,-5.1
017421015,2.5686482772\H,-5.0202292154,-2.4020601375,3.0090525053\H,-0
.6714817665,-3.5645840137,0.9303338014\H,-3.9820421888,-0.8655870529,1
.3719291698\H,-1.3173289724,-1.7513088535,-0.8440569011\H,-2.339832942
2,-0.4259075568,-0.3101844786\C,-0.749749958,0.4808915139,1.7618320933
\H,-1.3638379691,1.330808492,1.4337744256\H,-1.3360594658,-0.090207859
9,2.4878095277\H,0.1190833602,0.8811140637,2.2920507145\H,0.3625270052
, -1.159126572,0.9247414044\\Version=IA32L-G03RevC.02\State=1-AG\HF=-69
9.1789816\RMSD=4.891e-09\RMSF=8.713e-06\Dipole=0.,0.,0.\PG=CI [X(C18H2
2)]\@

n.CH_CH2_2-MeHCCHMe-CH_CH2_2

1\1\GINC-LC105\FOpt\RB3LYP\Gen\C10H18\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH2_2-
MeHCCHMe-CH_CH2_2.freq\0,1\C,-1.539745118,2.3465279646,-1.1034833801\
C,-1.852705085,2.1510367518,0.3631952287\C,-0.4392440795,1.9660364855,
-0.1400771738\H,-1.9118099513,1.6211137602,-1.8174889552\H,-1.52429886
72,3.3628081147,-1.490077371\H,-2.4220889959,1.2699311591,0.6443960211
\H,-2.0775166336,3.0237783103,0.9710802453\H,0.1982518976,2.8196547905
,0.0864835295\C,0.3954192576,0.6664310252,-0.0929855108\C,1.4544747208
,0.8885342217,1.0112729826\H,0.9948624669,0.8581978558,2.0070309303\H,
1.9216841615,1.8731702699,0.8966875771\H,0.9268254609,0.5944851733,-1.
0546396785\C,1.5397410285,-2.3465219163,1.1034936342\C,1.8527014822,-2
.1510436341,-0.363186718\C,0.4392410701,-1.96603564,0.1400841392\H,1.9
118083721,-1.6211034805,1.8174935262\H,1.5242918266,-3.3627990399,1.49
00954604\H,2.4220871296,-1.2699415179,-0.6443949272\H,2.0775111963,-3.
0237907658,-0.9710644395\H,-0.198257049,-2.8196542906,-0.0864694598\C,
-0.3954195199,-0.6664293922,0.0929786244\C,-1.4544649623,-0.8885355438
, -1.0112893114\H,-0.9948425595,-0.8582049994,-2.0070427488\H,-2.260988
2737,-0.1552198992,-0.9863289263\H,-1.9216784773,-1.8731696764,-0.8967
042988\H,-0.9268343627,-0.5944788305,1.0546276132\H,2.260998922,0.155
2211327,0.9863008134\\Version=IA32L-G03RevC.02\State=1-A\HF=-391.82598
56\RMSD=3.621e-10\RMSF=4.415e-06\Dipole=-0.0000004,0.0000007,-0.000000
2\PG=C01 [X(C10H18)]\@

n.CH2CH=CH2-MeHCCHMe-CH2CH=CH2

1\1\GINC-LC124\FOpt\RB3LYP\Gen\C10H18\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2CH=CH2
-MeHCCHMe-CH2CH=CH2.freq\0,1\C,-0.3476313013,1.1221410406,-1.61329821
15\C,-0.3070658903,0.7046039376,-0.114401155\H,0.6810447777,1.19347976
58,-1.9909907748\H,-0.7655613513,2.1355653191,-1.6715612308\C,-1.14050
19277,0.2127924119,-2.5146795547\C,-1.7073444852,0.8471225967,0.505768
1727\C,-2.256768948,0.5550190595,-3.1606157885\H,-0.7536188156,-0.7988
413319,-2.6451139216\H,-2.7837664719,-0.1427155682,-3.8064301239\H,-2.
6845768531,1.5521097189,-3.0729700417\H,-1.6916884619,0.7364784983,1.5
94632149\H,-2.39952242,0.1003672451,0.099235947\H,-2.1271305161,1.8357
852065,0.2852378638\H,0.3543600438,1.4342343544,0.3762473291\C,0.34763
13013,-1.1221410406,1.6132982115\C,0.3070658903,-0.7046039376,0.114401
155\H,-0.6810447777,-1.1934797658,1.9909907748\H,0.7655613513,-2.13556
53191,1.6715612308\C,1.1405019277,-0.2127924119,2.5146795547\C,1.70734
44852,-0.8471225967,-0.5057681727\C,2.256768948,-0.5550190595,3.160615
7885\H,0.7536188156,0.7988413319,2.6451139216\H,2.7837664719,0.1427155
682,3.8064301239\H,2.6845768531,-1.5521097189,3.0729700417\H,1.6916884
619,-0.7364784983,-1.594632149\H,2.39952242,-0.1003672451,-0.099235947
\H,2.1271305161,-1.8357852065,-0.2852378638\H,-0.3543600438,-1.4342343
544,-0.3762473291\\Version=IA32L-G03RevC.02\State=1-AG\HF=-391.8597977
\RMSD=3.316e-09\RMSF=8.986e-06\Dipole=0.,0.,0.\PG=CI [X(C10H18)]\@

n.CH2CH3-MeHCCHMe-CH2CH3

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1\1\GINC-LC48\FOpt\RB3LYP\Gen\C8H18\CYL509\28-Jun-2008\0\#\B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH2CH3-MeHC
CHMe-CH2CH3.freq\0,1\C,-0.2666194416,-0.6926261403,0.2305845671\C,0.38
42242352,-0.7918320467,1.7627752577\C,-0.5466549024,-1.8856890352,-0.3
320156742\C,-2.0289947201,-1.9378732298,0.0619889675\H,-0.0595172753,-
2.8098794708,0.0089085325\H,-0.4678503794,-1.8977100549,-1.4259431541\
H,-0.5650732708,-0.5553884826,2.2591191478\H,1.140515845,-0.1081450456
,2.1611906672\H,0.6711112213,-1.8065979662,2.0641668925\H,-2.503827471
9,-2.8358231208,-0.3499958164\H,-2.161826505,-1.9675085975,1.14937867\
H,-2.5849872996,-1.0721948263,-0.3158879806\H,1.2810249824,-0.80494979
92,-0.1817605699\C,-0.2666194416,0.6926261403,-0.2305845671\C,-0.38422
42352,0.7918320467,-1.7627752577\C,0.5466549024,1.8856890352,0.3320156
742\C,2.0289947201,1.9378732298,-0.0619889675\H,0.0595172753,2.8098794
708,-0.0089085325\H,0.4678503794,1.8977100549,1.4259431541\H,0.5650732
708,0.5553884826,-2.2591191478\H,-1.140515845,0.1081450456,-2.16119066
72\H,-0.6711112213,1.8065979662,-2.0641668925\H,2.5038274719,2.8358231
208,0.3499958164\H,2.161826505,1.9675085975,-1.14937867\H,2.5849872996
,1.0721948263,0.3158879806\H,-1.2810249824,0.8049497992,0.1817605699\
Version=IA32L-G03RevC.02\State=1-AG\HF=-315.7041972\RMSD=2.091e-09\RMS
F=6.502e-06\Dipole=0.,0.,0.\PG=CI [X(C8H18)]\@
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n.CH_CH3_2-MeHCCHMe-CH_CH3_2

```
1\1\GINC-LC144\FOpt\RB3LYP\Gen\C10H22\CYL509\28-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH_CH3_2-
MeHCCHMe-CH_CH3_2.freq\0,1\C,-0.0642637056,1.485778212,1.3024594107\H
,0.3687964515,1.5998730935,2.3031211381\H,-1.1515068199,1.5977460299,1
.3991624351\H,0.2999520921,2.3202674641,0.7002714231\C,0.3161362314,0.
1152014381,0.7046525337\C,0.0104321046,-0.9855243646,1.7835703254\C,0.
9706225439,-2.1899824073,1.7739142532\C,-1.4594568074,-1.4369650868,1.
8312727142\H,-1.6351422808,-2.0648405921,2.7130614421\H,-1.7435309183,
-2.0258153766,0.9520331438\H,-2.1443942026,-0.5835060529,1.8952389046\
H,2.0159871062,-1.8577845703,1.7674171336\H,0.8288922811,-2.8524266326
,0.9157911515\H,0.8229218512,-2.7942397675,2.6778054842\H,0.202204699,
-0.4864401507,2.7443568952\H,1.4086531057,0.1153976036,0.574277864\C,0
.0642637056,-1.485778212,-1.3024594107\H,-0.3687964515,-1.5998730935,-
2.3031211381\H,1.1515068199,-1.5977460299,-1.3991624351\H,-0.299952092
1,-2.3202674641,-0.7002714231\C,-0.3161362314,-0.1152014381,-0.7046525
337\C,-0.0104321046,0.9855243646,-1.7835703254\C,-0.9706225439,2.18998
24073,-1.7739142532\C,1.4594568074,1.4369650868,-1.8312727142\H,1.6351
422808,2.0648405921,-2.7130614421\H,1.7435309183,2.0258153766,-0.95203
31438\H,2.1443942026,0.5835060529,-1.8952389046\H,-2.0159871062,1.8577
845703,-1.7674171336\H,-0.8288922811,2.8524266326,-0.9157911515\H,-0.8
229218512,2.7942397675,-2.6778054842\H,-0.202204699,0.4864401507,-2.74
43568952\H,-1.4086531057,-0.1153976036,-0.574277864\Version=IA32L-G03
RevC.02\State=1-AG\HF=-394.3188345\RMSD=8.844e-09\RMSF=6.394e-06\Dipol
e=0.,0.,0.\PG=CI [X(C10H22)]\@
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n.C_CH3_3-MeHCCHMe-C_CH3_3

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1\1\GINC-LC114\FOpt\RB3LYP\Gen\C12H26\CYL509\29-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\C_CH3_3-M
eHCCHMe-C_CH3_3.freq\0,1\C,-0.050947671,0.0505318887,3.2903759963\C,0
.4340011561,0.6178434347,1.9297613813\C,-0.1720467914,2.0331924967,1.8
098649791\C,0.0011500604,-0.3335934067,0.7181163772\H,0.3792338272,0.6
479928401,4.1028385034\H,0.2746822584,-0.9858922442,3.4417211469\H,-1.
1383312235,0.087863667,3.4038995043\C,1.9751951741,0.6880244604,2.0806
38254\C,-1.3455485786,-1.0184990807,1.0341116532\H,2.2383546083,1.3210
805592,2.9372857975\H,2.3813906243,-0.3122280722,2.2778666037\H,0.0601
392762,2.619407322,2.7075673613\H,-1.2646890802,1.9883765403,1.7243727
529\H,0.2040678,2.5945104515,0.9502946291\H,-2.1751761135,-0.300436078
```

6,1.0564006915\H,-1.320361774,-1.5260125738,1.999515474\H,0.7593327862
,-1.1306125748,0.6954186468\C,0.0509659539,-0.0505392316,-3.2903692097
\C,-0.4340102115,-0.6178355235,-1.9297581556\C,0.1719921985,-2.0332036
345,-1.8098582247\C,-0.0011303613,0.3335889701,-0.7181141787\H,-0.3792
099543,-0.6480006516,-4.1028342998\H,-0.2746490441,0.9858878127,-3.441
7267091\H,1.1383511197,-0.0878843749,-3.403874477\C,-1.9752057678,-0.6
879663157,-2.0806444719\C,1.3455840181,1.0184573457,-1.0341221158\H,-2
.2383800873,-1.3210082234,-2.9372979549\H,-2.498646933,-1.0855143825,-
1.2122818768\H,-2.3813683711,0.3123003705,-2.2778686274\H,-0.060205167
4,-2.6194100606,-2.7075631531\H,1.2646352173,-1.9884224468,-1.72435692
\H,-0.2041475521,-2.5945105775,-0.950291775\H,2.1751952038,0.300374815
, -1.056398672\H,1.3204077464,1.5259536059,-1.9995355239\H,1.5922301171
,1.7835878401,-0.3006998943\H,-0.7592922289,1.1306277656,-0.6954102725
\H,-1.5921764411,-1.7836225052,0.3006760614\H,2.4986183095,1.085582755
2,1.212269274\Version=IA32L-G03RevC.02\State=1-A\HF=-472.9275236\RMSD
=9.767e-09\RMSF=2.211e-06\Dipole=0.0000002,0.0000008,-0.0000008\PG=C01
[X(C12H26)]\@

n.CCH-MeHCCHMe-CCH

1\1\GINC-LC144\FOpt\RB3LYP\Gen\C8H10\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CCH-MeHCCH
Me-CCH.freq\0,1\C,0.3373254345,-0.662270588,0.2484587861\C,0.60225934
34,-0.6492280156,1.767544436\C,-0.4742676596,-1.829024451,-0.117101162
5\C,-1.1444680556,-2.7970790715,-0.3878259865\H,-1.731925669,-3.653767
7995,-0.6286094439\H,-0.3384819907,-0.5623275975,2.3223232237\H,1.0933
376394,-1.5762856861,2.0781357654\H,1.2428627159,0.1962745372,2.032721
3926\H,1.3047589754,-0.7393106857,-0.2689897637\C,-0.3373254345,0.6622
70588,-0.2484587861\C,-0.6022593434,0.6492280156,-1.767544436\C,0.4742
676596,1.829024451,0.1171011625\C,1.1444680556,2.7970790715,0.38782598
65\H,1.731925669,3.6537677995,0.6286094439\H,0.3384819907,0.5623275975
, -2.3223232237\H,-1.0933376394,1.5762856861,-2.0781357654\H,-1.2428627
159,-0.1962745372,-2.0327213926\H,-1.3047589754,0.7393106857,0.2689897
637\Version=IA32L-G03RevC.02\State=1-AG\HF=-310.7311673\RMSD=4.975e-0
9\RMSF=3.533e-05\Dipole=0.,0.,0.\PG=CI [X(C8H10)]\@

n.CH=C_CH3_2-MeHCCHMe-CH=C_CH3_2

1\1\GINC-LC7\FOpt\RB3LYP\Gen\C12H22\CYL509\28-Jun-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH=C_CH3_2-
MeHCCHMe-CH=C_CH3_2.freq\0,1\H,4.2912100967,-1.8190234714,-1.11195774
65\C,3.3649123443,-2.411202204,-1.1050863455\C,2.2937236496,-1.7405051
75,-0.2742874723\C,2.6920425045,-1.5245776656,1.1669042113\C,1.1213871
833,-1.3951209231,-0.8325653483\C,-0.1150715765,-0.7427067737,-0.22124
66525\C,-0.7415014138,-1.5995953441,0.8986119565\H,1.020775096,-1.6244
478861,-1.8943679113\H,3.0485489685,-2.5573495981,-2.1426030102\H,3.63
01276274,-3.3938993341,-0.6892853672\H,3.6204169902,-0.9389258734,1.22
39036995\H,2.9043952845,-2.4853432951,1.6573199108\H,1.9355942583,-1.0
076555392,1.7578017775\H,-0.1007642298,-1.6547591548,1.784925191\H,-0.
9059603498,-2.6245552267,0.5485259139\H,-1.7049982436,-1.1832619415,1.
209510115\H,-0.8584613648,-0.7117485232,-1.027941053\H,-4.2912100967,1
.8190234714,1.1119577465\C,-3.3649123443,2.411202204,1.1050863455\C,-2
.2937236496,1.740505175,0.2742874723\C,-2.6920425045,1.5245776656,-1.1
669042113\C,-1.1213871833,1.3951209231,0.8325653483\C,0.1150715765,0.7
427067737,0.2212466525\C,0.7415014138,1.5995953441,-0.8986119565\H,-1.
020775096,1.6244478861,1.8943679113\H,-3.0485489685,2.5573495981,2.142
6030102\H,-3.6301276274,3.3938993341,0.6892853672\H,-3.6204169902,0.93
89258734,-1.2239036995\H,-2.9043952845,2.4853432951,-1.6573199108\H,-1
.9355942583,1.0076555392,-1.7578017775\H,0.1007642298,1.6547591548,-1.
784925191\H,0.9059603498,2.6245552267,-0.5485259139\H,1.7049982436,1.1
832619415,-1.209510115\H,0.8584613648,0.7117485232,1.027941053\Version=IA32L-G03RevC.02\State=1-AG\HF=-310.7311673\RMSD=4.975e-09\RMSF=3.533e-05\Dipole=0.,0.,0.\PG=CI [X(C8H10)]\@

n=IA32L-G03RevC.02\State=1-AG\HF=-470.4973952\RMSD=6.856e-09\RMSF=8.60
7e-06\Dipole=0.,0.,0.\PG=CI [X(C12H22)]\@

n.CH=CH2-MeHCCHMe-CH=CH2

1\1\GINC-LC74\FOpt\RB3LYP\Gen\C8H14\CYL509\28-Jun-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH=CH2-MeHC
CHMe-CH=CH2.freq\0,1\H,2.4572650206,1.1148498007,0.4959866975\C,2.523
5432625,0.1551401277,1.0027004358\H,3.4871191147,-0.084593677,1.444630
4784\C,1.4954868702,-0.6911586057,1.0852329853\C,0.0697354457,-0.47723
13487,0.6063669496\H,1.6478540693,-1.6280078635,1.6242406833\C,-0.7578
141374,-0.0099116928,1.8277934518\H,-0.416572113,0.9786379509,2.156560
9375\H,-0.6276634544,-0.6990380497,2.6702218764\H,-1.8238114442,0.0530
479239,1.5972753952\H,-0.3143428438,-1.4617806563,0.2995864121\H,-2.45
72650206,-1.1148498007,-0.4959866975\C,-2.5235432625,-0.1551401277,-1.
0027004358\H,-3.4871191147,0.084593677,-1.4446304784\C,-1.4954868702,0
.6911586057,-1.0852329853\C,-0.0697354457,0.4772313487,-0.6063669496\H
, -1.6478540693,1.6280078635,-1.6242406833\C,0.7578141374,0.0099116928,
-1.8277934518\H,0.416572113,-0.9786379509,-2.1565609375\H,0.6276634544
,0.6990380497,-2.6702218764\H,1.8238114442,-0.0530479239,-1.5972753952
\H,0.3143428438,1.4617806563,-0.2995864121\Version=IA32L-G03RevC.02\S
tate=1-AG\HF=-313.2305959\RMSD=3.042e-09\RMSF=5.911e-05\Dipole=0.,0.,0
.\PG=CI [X(C8H14)]\@

n.CH=CHCH3-MeHCCHMe-CH=CHCH3

1\1\GINC-LC129\FOpt\RB3LYP\Gen\C10H18\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CH=CHCH3-
MeHCCHMe-CH=CHCH3.freq\0,1\H,2.6213091044,0.5481387078,-0.3289942669\
C,2.6133312946,0.2835283641,0.7291229447\C,3.9591109173,0.2393886716,1
.3974340459\C,1.4523318281,0.0252372934,1.337899415\C,0.0502259493,0.1
358537426,0.7618758015\H,1.4824788858,-0.2227590285,2.4016057876\C,-0.
5068272343,1.5254467818,1.151468024\H,0.0634854925,2.3140423632,0.6463
708004\H,-0.4114397453,1.6918100517,2.2307606904\H,-1.5594006717,1.635
4931762,0.878742094\H,3.8734528433,-0.0344620082,2.4547167738\H,4.6253
504272,-0.4871119674,0.9121958888\H,4.4649363264,1.2131639482,1.340309
1326\H,-0.5617322494,-0.6232149822,1.2722358093\H,-2.6213091044,-0.548
1387078,0.3289942669\C,-2.6133312946,-0.2835283641,-0.7291229447\C,-3.
9591109173,-0.2393886716,-1.3974340459\C,-1.4523318281,-0.0252372934,-
1.337899415\C,-0.0502259493,-0.1358537426,-0.7618758015\H,-1.482478885
8,0.2227590285,-2.4016057876\C,0.5068272343,-1.5254467818,-1.151468024
\H,-0.0634854925,-2.3140423632,-0.6463708004\H,0.4114397453,-1.6918100
517,-2.2307606904\H,1.5594006717,-1.6354931762,-0.878742094\H,-3.87345
28433,0.0344620082,-2.4547167738\H,-4.6253504272,0.4871119674,-0.91219
58888\H,-4.4649363264,-1.2131639482,-1.3403091326\H,0.5617322494,0.623
2149822,-1.2722358093\Version=IA32L-G03RevC.02\State=1-AG\HF=-391.868
96\RMSD=4.725e-09\RMSF=2.675e-05\Dipole=0.,0.,0.\PG=CI [X(C10H18)]\@

n.CHO-MeHCCHMe-CHO

1\1\GINC-LC70\FOpt\RB3LYP\Gen\C6H10O2\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CHO-MeHCC
HMe-CHO.freq\0,1\O,0.8139411552,2.1491764301,-1.711013779\C,0.9158009
537,1.553720208,-0.6625444796\H,1.8759024593,1.5594338613,-0.093969331
8\C,-0.1934091305,0.755257566,0.001050421\C,-0.4205384868,1.3023060746
,1.4236433556\H,0.4912622596,1.2201522844,2.027476488\H,-1.2073335307,
0.7475069691,1.9437315838\H,-0.7143622905,2.3568417031,1.3928920438\H,
-1.0940221404,0.8964472971,-0.6095237932\O,-0.8139411552,-2.1491764301
,1.711013779\C,-0.9158009537,-1.553720208,0.6625444796\H,-1.8759024593
, -1.5594338613,0.0939693318\C,0.1934091305,-0.755257566,-0.001050421\C
,0.4205384868,-1.3023060746,-1.4236433556\H,-0.4912622596,-1.220152284
4,-2.027476488\H,1.2073335307,-0.7475069691,-1.9437315838\H,0.71436229

05,-2.3568417031,-1.3928920438\H,1.0940221404,-0.8964472971,0.60952379
32\Version=IA32L-G03RevC.02\State=1-AG\HF=-385.0828195\RMSD=8.750e-09
\RMSF=2.503e-05\Dipole=0.,0.,0.\PG=CI [X(C6H10O2)]\@

n.CN-MeHCCHMe-CN

1\1\GINC-LC124\FOpt\RB3LYP\Gen\C6H8N2\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CN-MeHCCH
Me-CN.freq\0,1\N,-0.963658309,-0.4050876769,-2.7958772097\C,-0.871039
7282,-0.2378508227,-1.6508144631\C,-0.7555465459,-0.0427133997,-0.1976
157285\C,-1.5158309931,-1.154282518,0.5534016227\H,-1.4675414378,-0.97
60108004,1.6311455238\H,-2.5658524656,-1.1717046342,0.2491267982\H,-1.
0811473223,-2.1361913148,0.3401962485\H,-1.2162093422,0.9261123546,0.0
378825475\N,0.963658309,0.4050876769,2.7958772097\C,0.8710397282,0.237
8508227,1.6508144631\C,0.7555465459,0.0427133997,0.1976157285\C,1.5158
309931,1.154282518,-0.5534016227\H,1.4675414378,0.9760108004,-1.631145
5238\H,2.5658524656,1.1717046342,-0.2491267982\H,1.0811473223,2.136191
3148,-0.3401962485\H,1.2162093422,-0.9261123546,-0.0378825475\Version
=IA32L-G03RevC.02\State=1-AG\HF=-342.9314402\RMSD=9.153e-09\RMSF=8.139
e-05\Dipole=0.,0.,0.\PG=CI [X(C6H8N2)]\@

n.COCH3-MeHCCHMe-COCH3

1\1\GINC-LC127\FOpt\RB3LYP\Gen\C8H14O2\CYL509\28-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\COCH3-Me
HCCHMe-COCH3.freq\0,1\C,-2.4211934228,0.488704421,-1.4570157736\C,-1.
7579186241,-0.5794903336,-0.6016673833\C,-0.6638898967,-0.1485352477,0
.3853615081\O,-2.0828057434,-1.7490090514,-0.6924215923\H,-2.995175003
9,0.0079480544,-2.2516244584\H,-1.6910293309,1.1825360464,-1.888568191
1\H,-3.1048453846,1.0873173886,-0.8420416917\C,-1.1142427253,1.0360956
686,1.2597786023\H,-0.3877963857,1.2386150232,2.0524372259\H,-2.077388
621,0.8243574595,1.737679731\H,-1.2153371289,1.955963811,0.6738926041\
H,-0.5031141585,-1.0289666798,1.0189217957\C,2.4211934228,-0.488704421
,1.4570157736\C,1.7579186241,0.5794903336,0.6016673833\C,0.6638898967,
0.1485352477,-0.3853615081\O,2.0828057434,1.7490090514,0.6924215923\H,
2.9951750039,-0.0079480544,2.2516244584\H,1.6910293309,-1.1825360464,1
.8885681911\H,3.1048453846,-1.0873173886,0.8420416917\C,1.1142427253,-
1.0360956686,-1.2597786023\H,0.3877963857,-1.2386150232,-2.0524372259\
H,2.077388621,-0.8243574595,-1.737679731\H,1.2153371289,-1.955963811,-
0.6738926041\H,0.5031141585,1.0289666798,-1.0189217957\Version=IA32L-
G03RevC.02\State=1-AG\HF=-463.7302399\RMSD=4.515e-09\RMSF=7.045e-06\Di
pole=0.,0.,0.\PG=CI [X(C8H14O2)]\@

n.CON_CH2CH3_2-MeHCCHMe-CON_CH2CH3_2

1\1\GINC-LC30\FOpt\RB3LYP\Gen\C14H28N2O2\CYL509\29-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CON_CH
2CH3_2-MeHCCHMe-CON_CH2CH3_2.freq\0,1\H,4.2320301736,-0.5622715421,1.
4386543632\C,3.7113718181,-0.833305886,0.5130892907\C,3.1025381525,0.4
203642746,-0.1271445735\N,2.4271622833,0.1714664775,-1.4028684347\C,3.
3044806104,-0.0385214884,-2.5664585719\C,3.5925908565,1.2536752893,-3.
3356767682\C,1.0778597397,0.2431975539,-1.6621708059\O,0.6613434462,0.
0761458753,-2.8101779368\C,0.0326261591,0.5380587583,-0.5593789857\C,0
.1024188304,1.9820567241,-0.0187392863\H,3.8932894355,1.1630541999,-0.
30158164\H,2.4039083975,0.8798073087,0.5682300688\H,2.8210109144,-0.76
22258159,-3.2252199181\H,4.2368861264,-0.4817098373,-2.2026572249\H,2.
9384541507,-1.5678663556,0.7596858741\H,4.4376423119,-1.316636673,-0.1
487328513\H,2.6632204329,1.662974428,-3.7403892702\H,4.2745088218,1.05
47184383,-4.1707177562\H,4.0595690642,2.0091380573,-2.6925915975\H,0.9
133346323,2.1411831816,0.6976523238\H,-0.8300396503,2.2318197202,0.498
0218981\H,0.2293069648,2.693724886,-0.8417302898\H,-0.8847981179,0.473
8370491,-1.1486568557\H,-4.2320301736,0.5622715421,-1.4386543632\C,-3.

7113718181,0.833305886,-0.5130892907\C,-3.1025381525,-0.4203642746,0.1
271445735\N,-2.4271622833,-0.1714664775,1.4028684347\C,-3.3044806104,0
.0385214884,2.5664585719\C,-3.5925908565,-1.2536752893,3.3356767682\C,
-1.0778597397,-0.2431975539,1.6621708059\O,-0.6613434462,-0.0761458753
,2.8101779368\C,-0.0326261591,-0.5380587583,0.5593789857\C,-0.10241883
04,-1.9820567241,0.0187392863\H,-3.8932894355,-1.1630541999,0.30158164
\H,-2.4039083975,-0.8798073087,-0.5682300688\H,-2.8210109144,0.7622258
159,3.2252199181\H,-4.2368861264,0.4817098373,2.2026572249\H,-2.938454
1507,1.5678663556,-0.7596858741\H,-4.4376423119,1.316636673,0.14873285
13\H,-2.6632204329,-1.662974428,3.7403892702\H,-4.2745088218,-1.054718
4383,4.1707177562\H,-4.0595690642,-2.0091380573,2.6925915975\H,-0.9133
346323,-2.1411831816,-0.6976523238\H,0.8300396503,-2.2318197202,-0.498
0218981\H,-0.2293069648,-2.693724886,0.8417302898\H,0.8847981179,-0.47
38370491,1.1486568557\\Version=IA32L-G03RevC.02\State=1-AG\HF=-810.330
8496\RMSD=6.072e-09\RMSF=1.420e-05\Dipole=0.,0.,0.\PG=CI [X(C14H28N2O2
)]\@

n.CON_CH3_2-MeHCCHMe-CON_CH3_2

1\1\GINC-LC126\FOpt\RB3LYP\Gen\C10H20N2O2\CYL509\29-Jun-2008\0\#\B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CON_C
H3_2-MeHCCHMe-CON_CH3_2.freq\0,1\C,-0.0164341057,0.4120955906,0.66141
86572\C,-1.3971397008,1.055262458,0.9256531007\N,-2.4862057366,0.29628
63695,1.2922551326\O,-1.494857885,2.2744045008,0.7870522402\C,0.598012
4634,-0.3298578676,1.866367809\C,-2.5271709294,-1.1389435708,1.5200415
583\C,-3.7404445979,0.9811775494,1.5830865367\H,-3.3872885864,-1.56933
35092,0.991013499\H,-1.631397958,-1.633314499,1.1572758409\H,-2.642723
4908,-1.3672503157,2.5894672898\H,-4.5442876304,0.5879998353,0.9471298
005\H,-4.0270699767,0.8277174878,2.6325244508\H,-3.6068849819,2.044318
0493,1.3925084165\H,1.6797283107,-0.4262607003,1.7277750539\H,0.205885
3061,-1.3403420142,2.0050404018\H,0.4313135191,0.2338741377,2.79085542
27\H,0.5864116837,1.3112753104,0.5141189365\C,0.0164341057,-0.41209559
06,-0.6614186572\C,1.3971397008,-1.055262458,-0.9256531007\N,2.4862057
366,-0.2962863695,-1.2922551326\O,1.494857885,-2.2744045008,-0.7870522
402\C,-0.5980124634,0.3298578676,-1.866367809\C,2.5271709294,1.1389435
708,-1.5200415583\C,3.7404445979,-0.9811775494,-1.5830865367\H,3.38728
85864,1.5693335092,-0.991013499\H,1.631397958,1.633314499,-1.157275840
9\H,2.6427234908,1.3672503157,-2.5894672898\H,4.5442876304,-0.58799983
53,-0.9471298005\H,4.0270699767,-0.8277174878,-2.6325244508\H,3.606884
9819,-2.0443180493,-1.3925084165\H,-1.6797283107,0.4262607003,-1.72777
50539\H,-0.2058853061,1.3403420142,-2.0050404018\H,-0.4313135191,-0.23
38741377,-2.7908554227\H,-0.5864116837,-1.3112753104,-0.5141189365\\Ve
rsion=IA32L-G03RevC.02\State=1-AG\HF=-653.0695905\RMSD=4.022e-09\RMSF=
4.471e-06\Dipole=0.,0.,0.\PG=CI [X(C10H20N2O2)]\@

n.CONH2-MeHCCHMe-CONH2

1\1\GINC-LC84\FOpt\RB3LYP\Gen\C6H12N2O2\CYL509\28-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\CONH2-M
eHCCHMe-CONH2.freq\0,1\C,-0.0396782996,0.4144527291,-0.6596992605\C,-
1.500997242,0.5483596865,-1.1088188793\N,-2.2693668228,1.4269463172,-0
.3903999145\O,-1.968186818,-0.127555398,-2.0150366724\C,0.6794986558,
1.7705449997,-0.5493651329\H,-1.8612601227,2.1051636991,0.2352567725\H
, -3.2116099891,1.5929093206,-0.7165477346\H,1.7556017617,1.6274299921,
-0.41772182\H,0.335050409,2.3528201371,0.3141436172\H,0.5251677705,2.3
690121547,-1.453669824\H,0.4300932347,-0.168615626,-1.4591772073\C,0.0
396782996,-0.4144527291,0.6596992605\C,1.500997242,-0.5483596865,1.108
8188793\N,2.2693668228,-1.4269463172,0.3903999145\O,1.968186818,0.1275
555398,2.0150366724\C,-0.6794986558,-1.7705449997,0.5493651329\H,1.861
2601227,-2.1051636991,-0.2352567725\H,3.2116099891,-1.5929093206,0.716
5477346\H,-1.7556017617,-1.6274299921,0.41772182\H,-0.335050409,-2.352

8201371,-0.3141436172\H,-0.5251677705,-2.3690121547,1.453669824\H,-0.4
300932347,0.168615626,1.4591772073\\Version=IA32L-G03RevC.02\State=1-A
G\HF=-495.8468728\RMSD=9.908e-09\RMSF=2.116e-05\Dipole=0.,0.,0.\PG=CI
[X(C6H12N2O2)]\\@

n.CONHCH3-MeHCCHMe-CONHCH3

1\1\GINC-LC142\FOpt\RB3LYP\Gen\C8H16N2O2\CYL509\28-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\CONHCH
3-MeHCCHMe-CONHCH3.freq\\0,1\H,-4.3112979947,0.4358876956,-1.397584511
1\C,-3.7560335368,-0.496663004,-1.5521288846\N,-2.5596401351,-0.534046
1855,-0.7299293681\C,-1.3087552397,-0.7219379712,-1.2499327489\C,-0.15
94990065,-0.728067981,-0.2300261672\O,-1.100283438,-0.8415172829,-2.45
29282266\C,-0.406581458,-1.6813235773,0.9528750428\H,-2.6635544234,-0.
4814784653,0.2728891424\H,-3.4357408264,-0.5566584447,-2.5930221298\H,
-4.4197277541,-1.3421600274,-1.3329200524\H,0.5025176254,-1.8023854483
,1.548621031\H,-0.7157565312,-2.6702330922,0.598137408\H,-1.1763883072
, -1.3043245089,1.6371783649\H,0.6955769159,-1.0996811066,-0.8056433871
\H,4.3112979947,-0.4358876956,1.3975845111\C,3.7560335368,0.496663004,
1.5521288846\N,2.5596401351,0.5340461855,0.7299293681\C,1.3087552397,0
.7219379712,1.2499327489\C,0.1594990065,0.728067981,0.2300261672\O,1.1
00283438,0.8415172829,2.4529282266\C,0.406581458,1.6813235773,-0.95287
50428\H,2.6635544234,0.4814784653,-0.2728891424\H,3.4357408264,0.55665
84447,2.5930221298\H,4.4197277541,1.3421600274,1.3329200524\H,-0.50251
76254,1.8023854483,-1.548621031\H,0.7157565312,2.6702330922,-0.5981374
08\H,1.1763883072,1.3043245089,-1.6371783649\H,-0.6955769159,1.0996811
066,0.8056433871\\Version=IA32L-G03RevC.02\State=1-AG\HF=-574.4688622\
RMSD=9.571e-09\RMSF=5.437e-06\Dipole=0.,0.,0.\PG=CI [X(C8H16N2O2)]\\@

n.COOC_CH3_3-MeHCCHMe-COOC_CH3_3

1\1\GINC-LC111\FOpt\RB3LYP\Gen\C14H26O4\CYL509\29-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\COOC_CH
3_3-MeHCCHMe-COOC_CH3_3.freq\\0,1\H,-2.6458501448,-2.5887636806,-4.511
4262572\C,-2.4352360808,-2.183785271,-3.5151622653\C,-0.9829395567,-1.
6991496081,-3.4566826789\C,-0.7204658319,-0.532242344,-4.4142638004\O,
-0.641318578,-1.3059538764,-2.0745126423\C,-1.2824206904,-0.3064100626
, -1.4335912053\O,-2.1678089435,0.3771489583,-1.9057048244\C,-0.7605351
942,-0.1548586652,-0.0059387059\C,-0.0128109428,-2.8521677249,-3.72483
57786\C,-1.1096701222,-1.409828202,0.8165562776\H,-0.1634993623,-3.243
4311044,-4.7365317042\H,-0.1726104706,-3.6664753795,-3.0107380513\H,1.
0246792911,-2.514254704,-3.6348312406\H,-3.1323728209,-1.368969976,-3.
3137554184\H,-2.6000061566,-2.9822145132,-2.7832811138\H,-0.8633097168
, -0.8681153468,-5.4476212905\H,0.3126809328,-0.1810948218,-4.313828024
5\H,-1.3988991311,0.299646881,-4.2192884099\H,-0.8410818544,-1.2692558
629,1.868569761\H,-0.5751618892,-2.2869633375,0.4394868746\H,-2.184644
8127,-1.6165898494,0.7725393353\H,-1.294225672,0.7068673962,0.40510930
23\H,2.6458501448,2.5887636806,4.5114262572\C,2.4352360808,2.183785271
, 3.5151622653\C,0.9829395567,1.6991496081,3.4566826789\C,0.7204658319,
0.532242344,4.4142638004\O,0.641318578,1.3059538764,2.0745126423\C,1.2
824206904,0.3064100626,1.4335912053\O,2.1678089435,-0.3771489583,1.905
7048244\C,0.7605351942,0.1548586652,0.0059387059\C,0.0128109428,2.8521
677249,3.7248357786\C,1.1096701222,1.409828202,-0.8165562776\H,0.16349
93623,3.2434311044,4.7365317042\H,0.1726104706,3.6664753795,3.01073805
13\H,-1.0246792911,2.514254704,3.6348312406\H,3.1323728209,1.368969976
, 3.3137554184\H,2.6000061566,2.9822145132,2.7832811138\H,0.8633097168,
0.8681153468,5.4476212905\H,-0.3126809328,0.1810948218,4.3138280245\H,
1.3988991311,-0.299646881,4.2192884099\H,0.8410818544,1.2692558629,-1.
868569761\H,0.5751618892,2.2869633375,-0.4394868746\H,2.1846448127,1.6
165898494,-0.7725393353\H,1.294225672,-0.7068673962,-0.4051093023\\Ver
sion=IA32L-G03RevC.02\State=1-AG\HF=-850.1010308\RMSD=8.100e-09\RMSF=1

.994e-05\Dipole=0.,0.,0.\PG=CI [X(C14H26O4)]\@

n.COOCH2CH3-MeHCCHMe-COOCH2CH3

1\1\GINC-LC38\FOpt\RB3LYP\Gen\C10H18O4\CYL509\28-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\COOCH2CH
3-MeHCCHMe-COOCH2CH3.freq\0,1\C,0.049818364,-0.2273412556,-0.74067717
71\C,1.3650073731,-0.9507245081,-1.0030222539\O,1.4647760065,-2.080703
434,-1.430453226\O,2.4298750484,-0.1659864494,-0.7169658273\C,3.732408
0866,-0.7484214658,-0.9576160735\C,4.7732824152,0.2867315355,-0.575311
0037\C,-0.1099074977,0.9462420719,-1.7264045104\H,3.8236712957,-1.6639
733991,-0.3643563906\H,3.8003426668,-1.0317694682,-2.012808989\H,4.661
6287608,1.1949619361,-1.1762141512\H,5.7776589245,-0.1168113523,-0.743
9341589\H,4.6848755904,0.560003002,0.4811144145\H,0.6506970821,1.71314
94222,-1.5508136527\H,-1.0962724255,1.4090032819,-1.6180856052\H,-0.01
69528665,0.599611038,-2.7613279723\H,-0.7314742516,-0.9684998278,-0.93
19213328\C,-0.049818364,0.2273412556,0.7406771771\C,-1.3650073731,0.95
07245081,1.0030222539\O,-1.4647760065,2.080703434,1.430453226\O,-2.429
8750484,0.1659864494,0.7169658273\C,-3.7324080866,0.7484214658,0.95761
60735\C,-4.7732824152,-0.2867315355,0.5753110037\C,0.1099074977,-0.946
2420719,1.7264045104\H,-3.8236712957,1.6639733991,0.3643563906\H,-3.80
03426668,1.0317694682,2.012808989\H,-4.6616287608,-1.1949619361,1.1762
141512\H,-5.7776589245,0.1168113523,0.7439341589\H,-4.6848755904,-0.56
0003002,-0.4811144145\H,-0.6506970821,-1.7131494222,1.5508136527\H,1.0
962724255,-1.4090032819,1.6180856052\H,0.0169528665,-0.599611038,2.761
3279723\H,0.7314742516,0.9684998278,0.9319213328\Version=IA32L-G03Rev
C.02\State=1-AG\HF=-692.8377501\RMSD=6.729e-09\RMSF=1.595e-05\Dipole=0
.,0.,0.\PG=CI [X(C10H18O4)]\@

n.COOCH3-MeHCCHMe-COOCH3

1\1\GINC-LC102\FOpt\RB3LYP\Gen\C8H14O4\CYL509\28-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\COOCH3-M
eHCCHMe-COOCH3.freq\0,1\C,-0.0105261788,-0.7729572052,0.0720585338\C,
0.0678337306,-1.1869378565,1.5357332012\O,0.915935117,-1.9080913611,2.
0139015955\O,-0.9525746639,-0.6629227675,2.2564956566\C,-0.976446592,-
1.024652705,3.6471765589\H,-1.8472423599,-0.5196503693,4.0662605201\C,
-1.2511351161,-1.4070169653,-0.5865651959\H,-1.0684857172,-2.108128535
5,3.7598081089\H,-0.0619554646,-0.6936677672,4.1465203186\H,-1.2495430
152,-2.4940126186,-0.4518432235\H,-1.2606094835,-1.2056657572,-1.66270
8405\H,-2.1735150236,-1.0078611721,-0.153672758\H,0.8922789101,-1.1798
430386,-0.3923102868\C,0.0105261788,0.7729572052,-0.0720585338\C,-0.06
78337306,1.1869378565,-1.5357332012\O,-0.915935117,1.9080913611,-2.013
9015955\O,0.9525746639,0.6629227675,-2.2564956566\C,0.976446592,1.0246
52705,-3.6471765589\H,1.8472423599,0.5196503693,-4.0662605201\C,1.2511
351161,1.4070169653,0.5865651959\H,1.0684857172,2.1081285355,-3.759808
1089\H,0.0619554646,0.6936677672,-4.1465203186\H,1.2495430152,2.494012
6186,0.4518432235\H,1.2606094835,1.2056657572,1.662708405\H,2.17351502
36,1.0078611721,0.153672758\H,-0.8922789101,1.1798430386,0.3923102868\
\Version=IA32L-G03RevC.02\State=1-AG\HF=-614.1996142\RMSD=5.802e-09\RM
SF=8.536e-06\Dipole=0.,0.,0.\PG=CI [X(C8H14O4)]\@

n.COOH-MeHCCHMe-COOH

1\1\GINC-LC84\FOpt\RB3LYP\Gen\C6H10O4\CYL509\28-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\COOH-MeHC
CHMe-COOH.freq\0,1\C,-0.5680884762,0.520890646,-0.0212843989\C,-0.849
4928036,1.0619512165,1.3700124255\O,-0.0385712688,1.1911721609,2.26271
45657\O,-2.1399063171,1.4580523156,1.5019508652\C,-0.2433487963,1.7271
4286,-0.9322104673\H,-2.2136028289,1.8436842062,2.3958007\H,0.66938514
37,2.2326680931,-0.5967573598\H,-1.0629317866,2.45200672,-0.9175120988
\H,-0.105362541,1.3915327463,-1.9627921762\H,-1.4785091688,0.043056695

6,-0.3972395557\C,0.5680884762,-0.520890646,0.0212843989\C,0.849492803
6,-1.0619512165,-1.3700124255\O,0.0385712688,-1.1911721609,-2.26271456
57\O,2.1399063171,-1.4580523156,-1.5019508652\C,0.2433487963,-1.727142
86,0.9322104673\H,2.2136028289,-1.8436842062,-2.3958007\H,-0.669385143
7,-2.2326680931,0.5967573598\H,1.0629317866,-2.45200672,0.9175120988\H
,0.105362541,-1.3915327463,1.9627921762\H,1.4785091688,-0.0430566956,0
.3972395557\Version=IA32L-G03RevC.02\State=1-AG\HF=-535.5881404\RMSD=
3.112e-09\RMSF=1.426e-05\Dipole=0.,0.,0.\PG=CI [X(C6H10O4)]\@

n.COPh-MeHCCHMe-COPh

1\1\GINC-LC31\FOpt\RB3LYP\Gen\C18H18O2\CYL509\29-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\COPh-MeH
CCHMe-COPh.freq\0,1\C,-4.9218852977,-2.0176943484,-0.1399812244\C,-5.
0077048706,-1.8250698713,1.2421607179\C,-3.8843839025,-1.403873322,1.9
539840918\C,-2.6773997773,-1.1773234879,1.2915969157\C,-2.577802154,-1
.366213613,-0.0967136017\C,-3.7201707822,-1.7885708027,-0.8007304212\C
, -1.3291334407,-1.1413474401,-0.9057159104\O,-1.3686152983,-1.29349030
04,-2.1200974126\C,0.0172436539,-0.7278645694,-0.2810922762\C,0.567421
7953,-1.7586112595,0.7270212261\H,-3.6339710938,-1.9297071931,-1.87270
33442\H,-1.8223309827,-0.8519670335,1.8703071314\H,-3.9440378443,-1.25
08257333,3.0279507839\H,-5.7936870526,-2.3456442805,-0.6996694037\H,-5
.9461280253,-2.0025061792,1.7608541383\H,1.6333646931,-1.5785661368,0.
9012304999\H,0.4646776754,-2.7758317813,0.3337295428\H,0.0682387346,-1
.719080306,1.6984881835\H,0.6815488264,-0.7426523751,-1.1493642999\C,4
.9218852977,2.0176943484,0.1399812244\C,5.0077048706,1.8250698713,-1.2
421607179\C,3.8843839025,1.403873322,-1.9539840918\C,2.6773997773,1.17
73234879,-1.2915969157\C,2.577802154,1.366213613,0.0967136017\C,3.7201
707822,1.7885708027,0.8007304212\C,1.3291334407,1.1413474401,0.9057159
104\O,1.3686152983,1.2934903004,2.1200974126\C,-0.0172436539,0.7278645
694,0.2810922762\C,-0.5674217953,1.7586112595,-0.7270212261\H,3.633971
0938,1.9297071931,1.8727033442\H,1.8223309827,0.8519670335,-1.87030713
14\H,3.9440378443,1.2508257333,-3.0279507839\H,5.7936870526,2.34564428
05,0.6996694037\H,5.9461280253,2.0025061792,-1.7608541383\H,-1.6333646
931,1.5785661368,-0.9012304999\H,-0.4646776754,2.7758317813,-0.3337295
428\H,-0.0682387346,1.719080306,-1.6984881835\H,-0.6815488264,0.742652
3751,1.1493642999\Version=IA32L-G03RevC.02\State=1-AG\HF=-847.2025505
\RMSD=8.258e-09\RMSF=4.497e-06\Dipole=0.,0.,0.\PG=CI [X(C18H18O2)]\@

n.H-Me2CCMe2-H

1\1\GINC-LC81\FOpt\RB3LYP\Gen\C6H14\CYL509\26-Jun-2008\0\#B3LYP/GEN 6
D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\H-Me2CCMe
2-H.freq\0,1\C,-0.3216998895,0.6238490639,-0.3321064292\H,-0.65659807
25,1.2880820658,0.4813225457\C,0.6799234213,1.4096483736,-1.1962100403
\C,-1.5535263724,0.265568148,-1.1815933603\H,1.5133582918,1.8107486475
, -0.6115884134\H,0.1857368721,2.2571667503,-1.6855892378\H,1.100026521
5,0.772709198,-1.9863124984\H,-1.2903339325,-0.4521610728,-1.970273828
2\H,-1.9574119688,1.1590793718,-1.6719996949\H,-2.3600142988,-0.172840
2324,-0.5861069668\C,0.3216998895,-0.6238490639,0.3321064292\H,0.65659
80725,-1.2880820658,-0.4813225457\C,-0.6799234213,-1.4096483736,1.1962
100403\C,1.5535263724,-0.265568148,1.1815933603\H,-1.5133582918,-1.810
7486475,0.6115884134\H,-0.1857368721,-2.2571667503,1.6855892378\H,-1.1
000265215,-0.772709198,1.9863124984\H,1.2903339325,0.4521610728,1.9702
738282\H,1.9574119688,-1.1590793718,1.6719996949\H,2.3600142988,0.1728
402324,0.5861069668\Version=IA32L-G03RevC.02\State=1-AG\HF=-237.08250
38\RMSD=3.859e-09\RMSF=3.245e-06\Dipole=0.,0.,0.\PG=CI [X(C6H14)]\@

n.BH2-Me2CCMe2-BH2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C6H16B2\CYL509\23-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\BH2-Me2

CCMe2-BH2.freq\0,1\H,-1.8977674032,1.2914547535,-1.1940596203\B,-1.9428149802,0.538924047,-0.2630972356\C,-0.6493670479,0.014297998,0.4522777426\H,-3.0236768741,0.2812577389,0.1874159162\C,-0.89212082,-1.3000948732,1.230878372\C,-0.4853709811,1.1571523679,1.5121598357\H,-1.7776698196,-1.2198072609,1.8714367542\H,-0.037850888,-1.5447128168,1.8776916528\H,-1.055923626,-2.151929848,0.561634895\H,-1.3255764005,1.1619889139,2.2161291083\H,-0.4159232375,2.1564855612,1.0681019451\H,0.4274199952,0.9918190245,2.0973735364\H,2.7858487568,-1.166506993,-0.3686325575\B,1.9246942933,-0.6060765827,0.2493833924\C,0.6167639376,-0.1356446972,-0.4772087473\H,2.1561068625,-0.3289218729,1.3916049146\C,1.1305259361,1.2418607236,-1.0203090232\C,0.2706789568,-1.0109174269,-1.7047438393\H,1.933342199,1.0992297144,-1.7528847625\H,0.3141624005,1.7665654828,-1.531420413\H,1.5088985478,1.9060310504,-0.235194304\H,1.1435015189,-1.139005771,-2.3549261955\H,-0.0643430063,-2.0131778055,-1.4156416054\H,-0.5266054809,-0.5549317462,-2.3083860902\Version=IA64L-G03RevC.02\State=1-A\HF=-287.9254525\RMSD=9.914e-09\RMSF=6.582e-06\Dipole=0.03277,0.1218333,0.0248744\PG=C01 [X(C6H16B2)]\@

n.CH3-Me2CCMe2-CH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H18\CYL509\24-Aug-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.CH3-Me2CCMe2-CH3.freq\0,1\H,1.6021291807,-1.3944530699,-1.241422728\C,1.4129277656,-1.3770328808,-0.1631571043\H,2.3815583621,-1.4896637206,0.3387227223\H,0.8130308713,-2.2587607086,0.0881388452\C,0.7391769957,-0.060362973,0.2872941898\C,1.6291513191,1.1072238892,-0.1976952992\C,0.7460421616,-0.0394875314,1.8332374279\H,2.666775804,0.9384982835,0.1148490021\H,1.3149275529,2.0671187934,0.2249342935\H,1.6308481203,1.2037868638,-1.2890866165\H,1.7790780789,-0.006246629,2.2000464771\H,0.2791224088,-0.9336830706,2.2588705831\H,0.2291519737,0.8368026635,2.2399364036\H,-1.2572299584,1.8076375756,0.9602940084\C,-1.3076445735,1.4838878524,-0.085215007\H,-2.3631507516,1.5083484653,-0.382062987\H,-0.7820813294,2.2270449161,-0.6937047552\C,-0.7391696834,0.0603305894,-0.28734014\C,-1.6988054987,-0.9278042574,0.4148900662\C,-0.7816859604,-0.2467907664,-1.8020446366\H,-2.6789949525,-0.9069615837,-0.0766449213\H,-1.3365801842,-1.9609729085,0.3724009297\H,-1.8577124591,-0.6695269714,1.4669438494\H,-1.785289172,-0.0432082392,-2.1946703459\H,-0.079004614,0.3712477067,-2.3718878233\H,-0.5565340873,-1.2967918977,-2.0154739174\Version=IA64L-G03RevC.02\State=1-A\HF=-315.7013605\RMSD=6.774e-09\RMSF=1.037e-05\Dipole=0.0000123,0.0000144,-0.0000047\PG=C01 [X(C8H18)]\@

n.NH2-Me2CCMe2-NH2

1\1\GINC-LC57\FOpt\RB3LYP\Gen\C6H16N2\CYL509\26-Jun-2008\0\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.NH2-Me2CCMe2-NH2.freq\0,1\H,-1.4629724311,1.6364903346,-0.7545987058\N,-0.4519862389,1.7520659186,-0.7143855252\C,0.1467001308,0.7599071395,0.2029568857\H,-0.1056275557,1.6161494634,-1.662364388\C,-0.4151669177,1.0835539044,1.6016601112\C,1.6601094089,1.0537873195,0.2147562055\H,-0.0025387373,0.4240083191,2.3725919002\H,-1.5070358532,0.9995576011,1.6341974061\H,-0.1581512139,2.11390696,1.8639859219\H,1.8244299506,2.0853357453,0.5394394747\H,2.1060589139,0.9484754412,-0.7804320495\H,2.2017195998,0.3922559447,0.8993147291\H,1.4629724311,-1.6364903346,0.7545987058\N,0.4519862389,-1.7520659186,0.7143855252\C,-0.1467001308,-0.7599071395,-0.2029568857\H,0.1056275557,-1.6161494634,1.662364388\C,0.4151669177,-1.0835539044,-1.6016601112\C,-1.6601094089,-1.0537873195,-0.2147562055\H,0.0025387373,-0.4240083191,-2.3725919002\H,1.5070358532,-0.9995576011,-1.6341974061\H,0.1581512139,-2.11390696,-1.8639859219\H,-1.8244299506,-2.0853357453,-0.5394394747\H,-2.1060589139,-0.9484754412,0.7804320495\H,-2.2017195998,-0.3922559447,-0.8993147291\Version=IA32L-G03RevC.02\State=1-AG\HF=-347.7658985\RMSD=5.026e-09\RMSF=3.868e-05\Dip

ole=0.,0.,0.\PG=CI [X(C6H16N2)]\@

n.OH-Me2CCMe2-OH

1\1\GINC-LC126\FOpt\RB3LYP\Gen\C6H14O2\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.OH-Me2CCMe2-OH.freq\|0,1\C,0.3720517794,-0.6492462288,0.2312601198\O,0.3913143644,-0.5621070566,1.6677693451\C,1.8129253402,-0.7012441572,-0.3035043046\C,-0.3783430504,-1.9202900386,-0.2001717607\H,0.8471764279,-1.3533808135,1.9946531996\H,-0.5221938068,-1.942010496,-1.2837967632\H,-1.3542993263,-1.988537,0.2875070923\H,0.200087105,-2.8085719609,0.0852611734\H,2.4177953323,0.1103495713,0.1093222167\H,1.8289271544,-0.6344479087,-1.3946949958\H,2.283594859,-1.6493790933,-0.012618677\C,-0.3720517794,0.6492462288,-0.2312601198\O,-0.3913143644,0.5621070566,-1.6677693451\C,-1.8129253402,0.7012441572,0.3035043046\C,0.3783430504,1.9202900386,0.2001717607\H,-0.8471764279,1.3533808135,-1.9946531996\H,0.5221938068,1.942010496,1.2837967632\H,1.3542993263,1.988537,-0.2875070923\H,-0.200087105,2.8085719609,-0.0852611734\H,-2.4177953323,-0.1103495713,-0.1093222167\H,-1.8289271544,0.6344479087,1.3946949958\H,-2.283594859,1.6493790933,0.012618677\|Version=IA32L-G03RevC.02\State=1-AG\HF=-387.5061513\RMSD=5.002e-09\RMSF=2.527e-05\Dipole=0.,0.,0.\PG=CI [X(C6H14O2)]\@

n.F-Me2CCMe2-F

1\1\GINC-LC77\FOpt\RB3LYP\Gen\C6H12F2\CYL509\26-Jun-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.F-Me2CCMe2-F.freq\|0,1\C,0.5425484665,0.5715910077,-1.7997297426\C,0.6050246247,0.4019533109,-0.2832594539\C,1.9511307432,-0.1765704713,0.1475604969\F,0.4992508845,1.6924044387,0.2889589092\H,1.4381502145,1.0920559145,-2.1525124044\H,-0.328515567,1.1609216323,-2.0965162644\H,0.4891085825,-0.4059308077,-2.2875370898\H,2.7643968833,0.3881628931,-0.3183864034\H,2.0285952801,-1.2232201599,-0.1604767301\H,2.0783631675,-0.1185284901,1.2313428088\C,-0.5425484665,-0.5715910077,1.7997297426\C,-0.6050246247,-0.4019533109,0.2832594539\C,-1.9511307432,0.1765704713,-0.1475604969\F,-0.4992508845,-1.6924044387,-0.2889589092\H,-1.4381502145,-1.0920559145,2.1525124044\H,0.328515567,-1.1609216323,2.0965162644\H,-0.4891085825,0.4059308077,2.2875370898\H,-2.7643968833,-0.3881628931,0.3183864034\H,-2.0285952801,1.2232201599,0.1604767301\H,-2.0783631675,0.1185284901,-1.2313428088\|Version=IA32L-G03RevC.02\State=1-AG\HF=-435.5600401\RMSD=2.007e-09\RMSF=2.456e-05\Dipole=0.,0.,0.\PG=CI [X(C6H12F2)]\@

n.SiH3-Me2CCMe2-SiH3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C6H18Si2\CYL509\21-Aug-2008\0\#\B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.SiH3-Me2CCMe2-SiH3.freq\|0,1\H,-1.3753586538,-0.6052021293,-3.0939943989\Si,-1.6400562502,-0.3280494707,-1.6542426219\C,0.0642028143,-0.0682934381,-0.7870705006\H,-2.5008660648,0.8846100996,-1.5827135786\H,-2.415238651,-1.4774599417,-1.1092772785\C,0.9886430978,-1.2090531194,-1.282533986\C,0.6250647345,1.2623984128,-1.350363829\H,1.6811213249,1.3953170278,-1.0773502428\H,0.0767741235,2.1389857368,-0.9909567957\H,0.5842948271,1.2771958872,-2.4468665909\H,1.9810802668,-1.1451927603,-0.8178181214\H,1.1341445819,-1.1419324733,-2.3665291174\H,0.588896386,-2.2058487429,-1.0688070854\H,1.4399851719,0.3596288583,3.1028683694\Si,1.5597541052,0.6331880722,1.6432162366\C,-0.0363031144,-0.0377221133,0.790901441\H,2.8094198706,-0.0203821379,1.1634028719\H,1.7142673009,2.1043721827,1.474704633\C,-1.1888288806,0.8798383735,1.2729526579\C,-0.2890943925,-1.4491488396,1.3785899009\H,-1.1762671475,-1.9130014733,0.9283280293\H,0.5527943921,-2.132440557,1.2255740812\H,-0.4680276951,-1.3892325377,2.4579944671\H,-2.1687473784,0.4576040591,1.0103936722\H,-1.180089

1992,0.9867518824,2.3650573125\H,-1.1360589816,1.8861709425,0.84550506
32\Version=IA64L-G03RevC.02\State=1-A\HF=-818.4451518\RMSD=2.050e-09\
RMSF=5.074e-06\Dipole=0.0138587,-0.0526615,0.001903\PG=C01 [X(C6H18Si2
)]\@

n.PH2-Me2CCMe2-PH2

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C6H16P2\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\N.PH2-Me2
CCMe2-PH2.freq\0,1\H,-2.5298526602,0.9366514617,-0.5065592399\p,-1.48
64300686,1.8408070787,-0.1611758416\H,-1.6942655957,1.686624868,1.2392
197418\C,0.0185875461,0.6715136371,-0.4209252626\C,1.2460923705,1.5759
351979,-0.1581564373\C,-0.0211673441,0.3520341745,-1.9333108938\H,0.92
73002031,-0.078861023,-2.2695665295\H,-0.1839908729,1.2675148506,-2.51
42540561\H,-0.8202037758,-0.3497627181,-2.1931251543\H,2.1829009735,1.
0222260765,-0.289380788\H,1.2483702447,2.0009478638,0.8505704851\H,1.2
566922821,2.4117950345,-0.865250187\H,2.4184700697,-1.1073621119,-0.41
89470037\p,1.3517910935,-1.9484448336,0.008666254\H,0.9185452721,-2.22
51762715,-1.3184512139\C,0.0354322004,-0.6282991278,0.4821522723\C,-1.
2991254897,-1.4080291161,0.43812858\C,0.3468353017,-0.3019846869,1.962
133463\H,-0.3536119218,0.4407379895,2.3610810406\H,0.2530066574,-1.204
4614213,2.5749035682\H,1.3606201361,0.0856574844,2.10406701\H,-2.09492
61723,-0.8551311872,0.947374509\H,-1.6325627833,-1.611825469,-0.584499
6756\H,-1.1968349395,-2.3720295753,0.9503309771\Version=IA64L-G03RevC
.02\State=1-A\HF=-920.9460805\RMSD=3.177e-09\RMSF=6.036e-06\Dipole=-0.
0385908,-0.0308621,-0.0436794\PG=C01 [X(C6H16P2)]\@

n.SH-Me2CCMe2-SH

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C6H14S2\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\N.SH-Me2C
CMe2-SH.freq\0,1\C,0.3525620992,-0.6648406313,0.2407201658\S,0.003642
4753,-0.8044089867,2.0965926387\C,1.8789997635,-0.5815388759,0.0528623
626\C,-0.1715663272,-1.9403198698,-0.4428873751\H,0.3729669425,-2.0990
612924,2.1874404479\H,-0.0853266318,-1.8514213878,-1.5312370297\H,-1.2
144467816,-2.1453689701,-0.1916242232\H,0.4251518593,-2.8042938751,-0.
1295877146\H,2.3073429379,0.3040958397,0.5269371255\H,2.1438362038,-0.
5676285182,-1.0112744916\H,2.3558970244,-1.4602582381,0.4985165586\C,-
0.3946537725,0.6351094329,-0.2552318555\S,0.1920214635,0.9426132664,-2
.0291372791\C,-1.9236313251,0.4604129944,-0.2794363787\C,-0.0413171356
,1.8795535809,0.5806830636\H,-0.8125091279,1.7886026626,-2.3389736588\
H,-0.4201391381,1.785129967,1.6055231337\H,1.0353024068,2.0569235287,0
.6254471337\H,-0.5060135958,2.7668915315,0.1392363353\H,-2.2420043372,
-0.2960319378,-0.9999970554\H,-2.2894901903,0.1740053784,0.7125127589\
H,-2.4035504071,1.4068870486,-0.5524649705\Version=IA64L-G03RevC.02\St
ate=1-A\HF=-1033.4411724\RMSD=2.389e-09\RMSF=9.730e-06\Dipole=-0.2412
07,-0.170372,-0.0831562\PG=C01 [X(C6H14S2)]\@

n.Cl-Me2CCMe2-Cl

1\1\GINC-AC11\FOpt\RB3LYP\Gen\C6H12Cl2\CYL509\29-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\N.Cl-Me2
CCMe2-Cl.freq\0,1\C,0.5344146769,0.5685474079,0.0925700715\C,1.874177
058,0.075645739,0.6463685858\C,0.0291873509,1.7690370595,0.8975283342\
H,2.5721473705,0.914329328,0.7140197576\H,2.3269723222,-0.6886875737,0
.011942871\H,1.730327216,-0.3387225141,1.6487833166\H,0.8143635953,2.5
276522141,0.9536437861\H,-0.2223878631,1.4530038293,1.9144042385\H,-0.
8512272462,2.2288300759,0.4445432894\C,-0.5344146769,-0.5685474079,-0.
0925700715\C,-1.874177058,-0.075645739,-0.6463685858\C,-0.0291873509,-
1.7690370595,-0.8975283342\H,-2.5721473705,-0.914329328,-0.7140197576\
H,-2.3269723222,0.6886875737,-0.011942871\H,-1.730327216,0.3387225141,
-1.6487833166\H,-0.8143635953,-2.5276522141,-0.9536437861\H,0.22238786

31,-1.4530038293,-1.9144042385\H,0.8512272462,-2.2288300759,-0.4445432
894\C1,0.9016911858,1.2232187185,-1.6243907802\C1,-0.9016911858,-1.223
2187185,1.6243907802\\Version=IA64L-G03RevC.02\State=1-AG\HF=-1156.277
0142\RMSE=2.703e-09\RMSF=3.428e-05\Dipole=0.,0.,0.\PG=CI [X(C6H12Cl2)]
\\@

n.Br-Me2CCMe2-Br

1\1\GINC-LC32\FOpt\RB3LYP\Gen\C6H12Br2\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Br-Me2
CCMe2-Br.freq\\0,1\Br,0.5761098869,-1.4566141911,-1.8169194651\C,0.228
1084373,-0.7418486221,0.087328359\C,1.5594948435,-0.9187101543,0.82103
66917\C,-0.8384312717,-1.6742426377,0.6664070499\H,2.3754756425,-0.371
9255826,0.3453641435\H,1.8301869567,-1.9771533254,0.8436539921\H,1.456
7084659,-0.5660142061,1.8526164374\H,-0.4565569508,-2.6976548005,0.696
1939061\H,-1.7581017799,-1.6743226813,0.0788114787\H,-1.0769057811,-1.
3642989622,1.6892369818\Br,-0.5761098869,1.4566141911,1.8169194651\C,-
0.2281084373,0.7418486221,-0.087328359\C,-1.5594948435,0.9187101543,-0.
.8210366917\C,0.8384312717,1.6742426377,-0.6664070499\H,-2.3754756425,
0.3719255826,-0.3453641435\H,-1.8301869567,1.9771533254,-0.8436539921\
H,-1.4567084659,0.5660142061,-1.8526164374\H,0.4565569508,2.6976548005
, -0.6961939061\H,1.7581017799,1.6743226813,-0.0788114787\H,1.076905781
1,1.3642989622,-1.6892369818\\Version=IA32L-G03RevC.02\State=1-AG\HF=-
5383.6469501\RMSE=2.457e-09\RMSF=1.037e-04\Dipole=0.,0.,0.\PG=C02H [SG
H(C2Br2),X(C4H12)]\\@

n.N_CH3_2-Me2CCMe2-N_CH3_2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C10H24N2\CYL509\21-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.N_CH3_
2-Me2CCMe2-N_CH3_2.freq\\0,1\C,2.7870489515,-0.1347760967,0.7081981345
\H,3.8149394485,-0.3522628437,0.3841312391\H,2.5238164906,-0.877028698
,1.461897394\H,2.8117618507,0.854760281,1.2003892193\N,1.9112801021,-0.
.209088658,-0.4496170893\C,0.4722192403,-0.5864012034,-0.330378931\C,2
.3497911238,0.7233306412,-1.4700452161\C,0.3680489951,-1.7215560124,0.
7097435389\C,0.0812244265,-1.2298707642,-1.6841519546\H,3.4007360214,0.
.5147620295,-1.7158357149\H,2.3029753849,1.7870816047,-1.1633252894\H,
1.7742548885,0.6154719091,-2.3903670844\H,0.7787233539,-2.0459321853,-
1.8982623928\H,0.118186581,-0.5340425683,-2.5253709548\H,-0.9287222368
, -1.6438354208,-1.6511158628\H,1.1391394299,-2.4733986984,0.5107369181
\H,-0.6050716563,-2.2119876436,0.6348249962\H,0.481904278,-1.380124568
5,1.7418899492\C,-2.8056138524,-0.5137370052,-0.2644296152\H,-3.829582
9501,-0.31755991,0.0839972288\H,-2.7434982923,-0.1697650264,-1.2977204
47\H,-2.678371412,-1.6144836955,-0.2650574446\N,-1.8733943296,0.191618
7638,0.593713922\C,-0.5378341275,0.6165860326,0.0806932732\C,-2.080374
64,-0.1902747502,1.9809226788\C,-0.8156447262,1.5679268591,-1.10985410
47\C,0.124282217,1.4949539858,1.1629684675\H,-3.1217039205,0.033332288
,2.2538916908\H,-1.9211871341,-1.2643619471,2.1883874254\H,-1.44170773
59,0.3793244783,2.6561615455\H,-0.6011703387,2.2250259861,1.5373606963
\H,0.5064995495,0.9255312341,2.0141628441\H,0.9651321215,2.046700639,0.
.7367807871\H,-1.4803572942,2.3686766503,-0.7703556247\H,0.1058184885,
2.022788527,-1.4792606729\H,-1.2966009723,1.076526719,-1.9586159025\\V
ersion=IA64L-G03RevC.02\State=1-A\HF=-504.9645595\RMSE=6.292e-09\RMSF=
5.764e-06\Dipole=0.0125009,-0.0057257,0.0477379\PG=C01 [X(C10H24N2)]\\
@

n.NHCH3-Me2CCMe2-NHCH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H20N2\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCH3-M
e2CCMe2-NHCH3.freq\\0,1\C,2.4292785305,-1.1391877547,0.9149507872\H,3.
4139008439,-1.5348276611,0.6377846241\H,1.9928001124,-1.8415152003,1.6

```
312777559\H,2.5964351628,-0.1842915533,1.4435941687\N,1.6118160288,-1.
0734125773,-0.2878934337\C,0.1571401488,-0.7979401911,-0.2507978557\C,
-0.5246875574,-1.936302195,0.5340736051\C,-0.2816387065,-0.9403724431,
-1.7242287001\H,2.0521284865,-0.4603895107,-0.9681412393\H,0.141720023
3,-0.1528809105,-2.3585931423\H,-1.3687960201,-0.9086689792,-1.8301311
111\H,0.0761472848,-1.9012158832,-2.1061931271\H,-0.1992763944,-1.9904
353705,1.5761219608\H,-0.2925884672,-2.8946964175,0.0590529909\H,-1.61
46306746,-1.8176213022,0.5379961457\C,-2.0145088458,1.7299492892,-1.21
27165364\H,-3.0919318555,1.9284374291,-1.1796326655\H,-1.5160404602,2.
703117876,-1.2616908771\H,-1.8046451933,1.2011397262,-2.1570922692\N,-
1.6527714641,1.0409607036,0.0192214479\C,-0.2587820923,0.6435196177,0.
3343304707\C,0.7005159343,1.7286060473,-0.1848630045\C,-0.2092380464,0.
6650483005,1.8811369625\H,-2.2859794329,0.2679538259,0.1985500635\H,-
1.0035743338,0.0452857358,2.3099831909\H,0.7448119894,0.3177351291,2.2
861419357\H,-0.3809891136,1.6894725639,2.225803494\H,0.7749633735,1.74
64394434,-1.2776543586\H,0.3582312697,2.7157123063,0.1429846674\H,1.70
55252549,1.5784878431,0.2192273203\\Version=IA64L-G03RevC.02\\State=1-A
\\HF=-426.3647156\\RMSD=6.620e-09\\RMSF=7.968e-06\\Dipole=0.0531874,0.0459
063,-0.1324703\\PG=C01 [X(C8H20N2)]\\@
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n.NHCHO-Me2CCMe2-NHCHO

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1\1\GINC-LC70\FOpt\RB3LYP\Gen\C8H16N2O2\CYL509\26-Jun-2008\0\\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHCHO
-Me2CCMe2-NHCHO.freq\\0,1\H,2.3992501489,-0.5237300106,-1.9210493328\C
,1.4753350575,-0.4755966205,-2.5220326671\O,1.4885482097,-0.3523293146
,-3.7355919988\N,0.331880978,-0.5696967108,-1.7811242905\C,0.154538418
,-0.7147573866,-0.3252338561\H,-0.510708753,-0.5391816565,-2.345236368
6\C,1.4013995603,-1.3593303427,0.3110131036\C,-1.0220596975,-1.6905630
207,-0.1235422977\H,-1.2670961959,-1.8012246389,0.9358987048\H,-0.7495
147079,-2.6755675445,-0.5148819216\H,2.2963738664,-0.7348551229,0.2550
097607\H,1.6230786123,-2.3089516534,-0.1856830401\H,1.2053596242,-1.57
24427817,1.3655987185\H,-2.3992501489,0.5237300106,1.9210493328\C,-1.4
753350575,0.4755966205,2.5220326671\O,-1.4885482097,0.3523293146,3.735
5919988\N,-0.331880978,0.5696967108,1.7811242905\C,-0.154538418,0.7147
573866,0.3252338561\H,0.510708753,0.5391816565,2.3452363686\C,-1.40139
95603,1.3593303427,-0.3110131036\C,1.0220596975,1.6905630207,0.1235422
977\H,1.2670961959,1.8012246389,-0.9358987048\H,0.7495147079,2.6755675
445,0.5148819216\H,-2.2963738664,0.7348551229,-0.2550097607\H,-1.62307
86123,2.3089516534,0.1856830401\H,-1.2053596242,1.5724427817,-1.365598
7185\H,1.9249810715,1.3653752565,0.651239389\H,-1.9249810715,-1.365375
2565,-0.651239389\\Version=IA32L-G03RevC.02\\State=1-AG\\HF=-574.4466125
\\RMSD=4.362e-09\\RMSF=1.289e-05\\Dipole=0.,0.,0.\\PG=CI [X(C8H16N2O2)]\\@
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n.NHCOCH3-Me2CCMe2-NHCOCH3

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1\1\GINC-LC141\FOpt\RB3LYP\Gen\C10H20N2O2\CYL509\27-Jun-2008\0\\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NHC
OCH3-Me2CCMe2-NHCOCH3.freq\\0,1\H,-0.9204019895,2.7077553238,-3.321548
9041\C,-0.46037558,3.3527781232,-2.565816109\C,-0.0976400832,2.6371232
319,-1.2660711172\H,-1.1535148537,4.1697612704,-2.3368872425\H,0.44649
58425,3.8004849201,-2.9803725735\N,-0.6523348444,1.3924438573,-1.13201
55643\O,0.6244530664,3.1761990007,-0.4345224786\C,-0.6461879992,0.4679
456888,0.0282527788\H,-1.2102152029,1.0761264192,-1.9124201134\C,-0.72
74753289,1.2537110618,1.3511104752\C,-1.9445944555,-0.3529678051,-0.11
11328322\H,-1.9998683785,-0.880432904,-1.0689968532\H,-2.8054487066,0.
3210632251,-0.0396169572\H,-2.0262515777,-1.1074126442,0.6711787206\H,
0.1100599618,1.936127516,1.4854341501\H,-0.7755209467,0.5517030794,2.1
891983612\H,-1.6438578812,1.8529347913,1.3624195526\H,0.9204019895,-2.
7077553238,3.3215489041\C,-0.46037558,-3.3527781232,2.565816109\C,0.097
6400832,-2.6371232319,1.2660711172\H,1.1535148537,-4.1697612704,2.3368
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872425\H,-0.4464958425,-3.8004849201,2.9803725735\N,0.6523348444,-1.39
24438573,1.1320155643\O,-0.6244530664,-3.1761990007,0.4345224786\C,0.6
461879992,-0.4679456888,-0.0282527788\H,1.2102152029,-1.0761264192,1.9
124201134\C,0.7274753289,-1.2537110618,-1.3511104752\C,1.9445944555,0.
3529678051,0.1111328322\H,1.9998683785,0.880432904,1.0689968532\H,2.80
54487066,-0.3210632251,0.0396169572\H,2.0262515777,1.1074126442,-0.671
1787206\H,-0.1100599618,-1.936127516,-1.4854341501\H,0.7755209467,-0.5
517030794,-2.1891983612\H,1.6438578812,-1.8529347913,-1.3624195526\\Ve
rsion=IA32L-G03RevC.02\State=1-AG\HF=-653.0946699\RMSD=7.709e-09\RMSF=
2.408e-06\Dipole=0.,0.,0.\PG=CI [X(C10H20N2O2)]\@

n.NO2-Me2CCMe2-NO2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C6H12N2O4\CYL509\21-Aug-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.NO2-M
e2CCMe2-NO2.freq\\0,1\O,-2.1436846945,-1.4478063223,-0.8574142969\N,-1
.221840239,-0.7491535223,-1.2592756002\C,0.0785692914,-0.6872467052,-0
.4079622504\O,-1.2540158276,-0.0734415609,-2.2856506206\C,1.2435591552
, -0.911360586,-1.3795899811\C,0.0188424392,-1.8148533055,0.6274167752\
H,2.1876912153,-0.7845681211,-0.8463936643\H,1.2088546309,-0.218072717
9,-2.2196978569\H,1.1995293877,-1.9322495532,-1.7727781372\H,0.9804945
262,-1.8748902958,1.1444073828\H,-0.1556021824,-2.7685872627,0.1247214
452\H,-0.769847877,-1.6739842161,1.367012165\O,0.6027797781,0.62058015
06,2.5839142465\N,1.0547047816,0.6594727305,1.4465204159\C,0.052895549
,0.7577789235,0.2606543097\O,2.2510336806,0.6087339144,1.1685020395\C,
-1.3222651128,1.1160352157,0.8331624966\C,0.5657592661,1.8816915868,-0
.6477703125\H,-2.0081609404,1.3249240503,0.0075966844\H,-1.7468571421,
0.3246147834,1.451445306\H,-1.2438878929,2.0174276624,1.4447860657\H,-
0.0529265798,1.9304540554,-1.5458793895\H,0.4920327038,2.8387712732,-0
.1211650428\H,1.6055613313,1.7271256547,-0.9350458413\\Version=IA64L-G
03RevC.02\State=1-A\HF=-646.0776011\RMSD=4.305e-09\RMSF=6.049e-06\Dipo
le=0.2375992,0.1275682,-0.2662452\PG=C01 [X(C6H12N2O4)]\@

n.OCF3-Me2CCMe2-OCF3

1\1\GINC-IC144\FOpt\RB3LYP\Gen\C8H12F6O2\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCF3
-Me2CCMe2-OCF3.freq\\0,1\C,-0.2480321075,0.1562888195,-0.7332413811\O,
-1.6104237946,-0.4112242165,-0.7067921411\C,-2.5719356715,-0.030109413
4,-1.5607735596\F,-3.0816787056,1.1917761366,-1.2767000886\F,-3.573571
517,-0.9130957802,-1.4724042756\F,-2.1672942628,0.0146259692,-2.853142
3337\C,-0.2516438865,1.6608028828,-1.0269504207\C,0.5666239382,-0.5972
900957,-1.7919071204\H,1.6304839992,-0.3818973246,-1.6652640076\H,0.26
4826956,-0.2844853068,-2.7934391533\H,0.4134244036,-1.6761251589,-1.71
46085278\H,0.763914846,2.0440853121,-0.9045571079\H,-0.9175528169,2.21
17506165,-0.3614719057\H,-0.5665600121,1.8475097897,-2.0562501304\C,0.
2480321075,-0.1562888195,0.7332413811\O,1.6104237946,0.4112242165,0.70
67921411\C,2.5719356715,0.0301094134,1.5607735596\F,3.0816787056,-1.19
17761366,1.2767000886\F,3.573571517,0.9130957802,1.4724042756\F,2.1672
942628,-0.0146259692,2.8531423337\C,0.2516438865,-1.6608028828,1.02695
04207\C,-0.5666239382,0.5972900957,1.7919071204\H,-1.6304839992,0.3818
973246,1.6652640076\H,-0.264826956,0.2844853068,2.7934391533\H,-0.4134
244036,1.6761251589,1.7146085278\H,-0.763914846,-2.0440853121,0.904557
1079\H,0.9175528169,-2.2117506165,0.3614719057\H,0.5665600121,-1.84750
97897,2.0562501304\\Version=IA32L-G03RevC.02\State=1-AG\HF=-1061.59469
07\RMSD=7.714e-09\RMSF=2.129e-05\Dipole=0.,0.,0.\PG=CI [X(C8H12F6O2)]\
\@

n.OCH2CH3-Me2CCMe2-OCH2CH3

1\1\GINC-IC102\FOpt\RB3LYP\Gen\C10H22O2\CYL509\26-Jun-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCH2C

H3-Me2CCMe2-OCH2CH3.freq\0,1\H,-1.7443591287,-4.6964192903,1.02378063
49\C,-0.9412685241,-3.970453238,0.853868611\C,-1.5208512674,-2.5907121
722,0.5777201702\O,-0.431317651,-1.7052827844,0.3679402014\C,-0.716693
8707,-0.3214649866,0.0841530443\C,-1.5349877547,-0.1820732398,-1.21225
90434\C,-1.4776182293,0.3346225427,1.2504086806\H,-2.1749953558,-2.627
1832911,-0.3061194503\H,-2.1363191638,-2.2635998331,1.4289650223\H,-0.
2999024489,-3.947084046,1.7410385953\H,-0.3385421145,-4.3106112262,0.0
053486841\H,-1.1181881271,-0.8018755432,-2.0115708116\H,-1.5336863485,
0.86015748,-1.5398127499\H,-2.5750940026,-0.4865617803,-1.0560348098\H
, -1.0198759706,0.0841598506,2.211895121\H,-2.52076332,0.0027418828,1.2
762506832\H,-1.4715450111,1.4205935713,1.1313768622\H,1.7443591287,4.6
964192903,-1.0237806349\C,0.9412685241,3.970453238,-0.853868611\C,1.52
08512674,2.5907121722,-0.5777201702\O,0.431317651,1.7052827844,-0.3679
402014\C,0.7166938707,0.3214649866,-0.0841530443\C,1.5349877547,0.1820
732398,1.2122590434\C,1.4776182293,-0.3346225427,-1.2504086806\H,2.174
9953558,2.6271832911,0.3061194503\H,2.1363191638,2.2635998331,-1.42896
50223\H,0.2999024489,3.947084046,-1.7410385953\H,0.3385421145,4.310611
2262,-0.0053486841\H,1.1181881271,0.8018755432,2.0115708116\H,1.533686
3485,-0.86015748,1.5398127499\H,2.5750940026,0.4865617803,1.0560348098
\H,1.0198759706,-0.0841598506,-2.211895121\H,2.52076332,-0.0027418828,
-1.2762506832\H,1.4715450111,-1.4205935713,-1.1313768622\\Version=IA32
L-G03RevC.02\State=1-AG\HF=-544.7515573\RMSD=9.655e-09\RMSF=8.256e-06\
Dipole=0.,0.,0.\PG=CI [X(C10H22O2)]\@

n.OCH3-Me2CCMe2-OCH3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C8H18O2\CYL509\28-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCH3-Me
2CCMe2-OCH3.freq\0,1\C,-0.794219465,-0.9017626495,-2.7990878299\O,-0.
6870532085,-0.0755916687,-1.6579987313\C,0.0476414959,-0.5854486437,-0.
.5275227057\H,-1.319428838,-1.8447857927,-2.5911510014\H,-1.3791732504
, -0.3355850375,-3.5296455995\H,0.1826573548,-1.1366926156,-3.244938723
7\C,-0.6029181028,-1.86939858,0.0177091665\C,1.5129503189,-0.866854922
1,-0.9050664027\H,-0.1876987847,-2.1060565278,1.0000996612\H,-0.410217
6464,-2.7200720149,-0.6443941391\H,-1.6866207592,-1.7543492884,0.11291
68698\H,2.1052260973,-1.0192445485,0.0002040271\H,1.9430525002,-0.0346
8798,-1.4700735205\H,1.5950318726,-1.7701454423,-1.5186334559\C,0.7930
744425,0.9012747706,2.7996049601\O,0.6873081564,0.0757337092,1.6579250
383\C,-0.04723303793,0.5856031335,0.5272904986\H,1.3156783778,1.8458174
025,2.592149444\H,1.3799416452,0.335986918,3.5293137424\H,-0.184167582
3,1.1332758012,3.2462543643\C,0.6032849653,1.8695646995,-0.0177516811\
C,-1.5125598337,0.8669960777,0.9047569821\H,0.1878267522,2.1064245712,
-1.0000031956\H,0.4108787814,2.7201346228,0.6445580136\H,1.686944836,1.
.7545099678,-0.1133534132\H,-2.1049206672,1.0196126883,-0.0004306214\H
, -1.9426210898,0.0346994673,1.4696103967\H,-1.5945698331,1.7701781691,
1.5185087678\\Version=IA64L-G03RevC.02\State=1-A\HF=-466.1135992\RMSD=
2.798e-09\RMSF=1.056e-05\Dipole=-0.0003371,-0.0001427,0.0000669\PG=C01
[X(C8H18O2)]\@

n.OCHO-Me2CCMe2-OCHO

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H14O4\CYL509\21-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCHO-Me
2CCMe2-OCHO.freq\0,1\C,-0.024535345,-0.7602968836,-0.0196313652\O,-0.
1021414112,-1.3137735867,1.3525183176\C,0.9469211516,-1.596355981,2.14
19175184\H,0.5502875732,-2.07900839,3.0507754706\O,2.1188886053,-1.383
8831719,1.9534446122\C,1.259728114,-1.1586550077,-0.7593889926\C,-1.22
21787241,-1.4427354409,-0.693524521\H,-1.0137262761,-2.5133073561,-0.7
868915337\H,-2.1289675583,-1.3275006749,-0.0955318946\H,2.1484145154,-
0.6396958975,-0.4058566981\H,1.12711765,-0.9489588684,-1.8245571772\H,
1.4273905171,-2.2337305306,-0.6485888593\C,-0.1830498172,0.8043028883,

0.1333789519\O,0.2392055341,1.4365081647,-1.1364078349\C,-0.5221608931
,1.5908103628,-2.2279858336\H,0.061016028,2.1788614885,-2.9556184833\O
, -1.6391806822,1.183954507,-2.4414351061\C,-1.5958311363,1.2363862248,
0.5406094284\C,0.8264895867,1.4024171699,1.123159245\H,0.7772639596,2.
4928143534,1.0515539688\H,1.8497932269,1.0865137702,0.9153556184\H,-2.
3497135823,0.9652125261,-0.1957642014\H,-1.84319685,0.7676609577,1.498
2916294\H,-1.6217629343,2.3225128655,0.6774515159\H,-1.4077973661,-1.0
266785851,-1.6845050599\H,0.5774071093,1.1176170403,2.1477192065\\Vers
ion=IA64L-G03RevC.02\State=1-A\HF=-614.1787509\RMSD=8.981e-09\RMSF=2.8
82e-06\Dipole=-0.1649652,0.1297242,0.1879762\PG=C01 [X(C8H14O4)]\\@

n.OCOCH3-Me2CCMe2-OCOCH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C10H18O4\CYL509\21-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.OCOCH3
-Me2CCMe2-OCOCH3.freq\\0,1\C,0.1075468402,-0.0415722873,-0.8346490011\
O,1.5122532286,-0.4836675232,-0.9267137141\C,2.5931090041,0.3196365151
, -1.0319692266\C,3.8318344414,-0.5269483823,-1.2417707131\O,2.59847179
25,1.530531887,-0.9690582808\C,-0.2022910132,1.0873949428,-1.824151973
8\C,-0.6382164977,-1.308348688,-1.2796776026\H,4.7101413946,0.11870563
43,-1.2737134606\H,3.7482966203,-1.0869875661,-2.1791042486\H,3.932741
6138,-1.2589893121,-0.4341618103\H,-0.2542356111,-1.6099290035,-2.2587
22297\H,-1.7080912991,-1.1119442029,-1.3796772232\H,-0.5030185815,-2.1
357199051,-0.5817969193\H,0.4007073702,1.9763715957,-1.6512652487\H,-1.
.262057699,1.3481683098,-1.7388056525\H,-0.0199130732,0.7390515633,-2.
8464212182\C,-0.2055942597,0.3389852655,0.6678133001\O,-1.6778657411,0.
.3857126254,0.7841368854\C,-2.4708729495,-0.6244919789,1.2134921445\C,
-3.8975339967,-0.1262704697,1.3294835772\O,-2.1194586297,-1.7543154295
,1.4687831465\C,0.457515352,-0.6182766441,1.6684197113\C,0.1751608439,
1.7799741538,1.0351009328\H,-4.5459032191,-0.9523027797,1.6239217081\H
, -3.9555876416,0.6749503884,2.0737332892\H,-4.2338576448,0.2922001536,
0.3753658625\H,-0.0391558767,1.9433198104,2.0964000033\H,-0.4110234705
,2.5001307145,0.4594739311\H,0.3378669332,-1.6695602039,1.4151522127\H
,1.5248794921,-0.3833885783,1.71781268\H,0.034233516,-0.4588356319,2.6
64232522\H,1.232825386,1.9681719743,0.8478446813\\Version=IA64L-G03Rev
C.02\State=1-A\HF=-692.8283641\RMSD=9.250e-09\RMSF=4.481e-06\Dipole=-0
.170257,0.0177062,-0.2376963\PG=C01 [X(C10H18O4)]\\@

n.Si_CH3_3-Me2CCMe2-Si_CH3_3

1\1\GINC-AC27\FOpt\RB3LYP\Gen\C12H30Si2\CYL509\29-Aug-2008\0\#B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Si_CH
3_3-Me2CCMe2-Si_CH3_3.freq\\0,1\H,3.3844094453,-0.9356777081,-1.217985
2973\C,3.4103768005,-0.5830755333,-0.1802702237\H,4.4389530531,-0.2581
360527,0.0246781182\H,3.2042761102,-1.4404604106,0.4691511995\Si,2.238
588355,0.8875577312,0.11186837\C,0.3645494326,0.6058062885,-0.40300244
56\C,2.4333593025,1.4398874724,1.9221577254\C,2.9364797957,2.309759139
8,-0.9453087721\C,0.3215527159,0.7097692573,-1.9506874224\C,-0.3944943
638,1.8371931887,0.1558949903\H,3.9412703191,2.5660091001,-0.585942207
3\H,2.3313891628,3.2222031451,-0.8899111488\H,3.0284723417,2.036190977
5,-2.0023287679\H,3.4767832413,1.7312752706,2.0984449722\H,2.185682011
1,0.6545731538,2.6429391917\H,1.8115547671,2.3125333347,2.1531229617\H
,0.126324921,2.7735855033,-0.0797258044\H,-0.5153698253,1.7989422573,1.
.2430492412\H,-1.3950219959,1.9233219512,-0.2865045418\H,0.9888832018,
-0.0049190698,-2.4449101054\H,0.6165861957,1.7110258969,-2.2817888503\
H,-0.688072402,0.5316098551,-2.3364608683\H,-2.6841031445,-0.199411647
8,2.4551207985\C,-3.0774284552,0.1232012079,1.4841873866\H,-4.15539688
61,-0.0834703554,1.4877986036\H,-2.9516356188,1.2082642869,1.417979589
2\Si,-2.2677093725,-0.8170408057,0.041796168\C,-0.3057553749,-0.748449
8997,0.0918857997\C,-3.078989871,-0.2217037238,-1.5733153195\C,-2.8025
290508,-2.6344037968,0.237930466\C,0.0686490706,-1.0460579882,1.567097

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6367\C,0.189982506,-1.9513258738,-0.7540402017\H,-3.8942309187,-2.6794
985674,0.3406009925\H,-2.5315624231,-3.2438880285,-0.6313769483\H,-2.3
746691045,-3.1139524349,1.1260253284\H,-4.1558779193,-0.4296661175,-1.
5222887299\H,-2.9628454732,0.8529583463,-1.7491704441\H,-2.69024218,-0
.7484027802,-2.452709263\H,-0.1276254636,-2.8989181777,-0.30642732\H,-
0.1891395982,-1.9351124201,-1.7818610579\H,1.283534796,-1.9772658559,-
0.8117633544\H,-0.1420458622,-0.2031384171,2.2327316229\H,-0.481119545
,-1.9119390074,1.9564361253\H,1.1340179897,-1.289471419,1.6665947138\
Version=IA64L-G03RevC.02\State=1-A\HF=-1054.3912721\RMSD=6.401e-09\RMS
F=6.485e-06\Dipole=0.0018023,-0.0043772,-0.0095104\PG=C01 [X(C12H30Si2
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n.P_CH3_2-Me2CCMe2-P_CH3_2

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1\1\GINC-AC27\FOpt\RB3LYP\Gen\C10H24P2\CYL509\29-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.P_CH3_
2-Me2CCMe2-P_CH3_2.freq\|0,1\C,-0.7879723329,-0.0269234262,3.141618869
7\H,-0.0669368905,0.7754608704,3.3246170468\H,-0.9889000116,-0.5043448
66,4.1078660674\P,-0.0287302157,-1.3391755767,2.0450559251\C,-1.555535
1447,-2.365897583,1.7148111023\C,0.5443681269,-0.4753870151,0.39185574
5\H,-1.3285582468,-3.1728878141,1.0112046884\H,-2.4270448519,-1.811408
4117,1.3520522366\H,-1.8253816683,-2.8368634436,2.6676906603\C,1.51459
42687,0.6103865059,0.9085425735\C,1.399383944,-1.595449023,-0.25525441
56\H,2.2118517862,-1.8856904292,0.4183615365\H,1.8484088243,-1.2656060
733,-1.1958578085\H,0.8167233853,-2.4978328451,-0.4677018681\H,2.13112
87485,0.2217169533,1.7286299191\H,0.9938140239,1.4988742823,1.27693655
92\H,2.2007333624,0.9278623781,0.1179409186\C,1.6721335478,0.765003190
5,-2.7523640452\H,1.5759065787,-0.2233666342,-3.2124496506\H,1.9250824
862,1.4693156143,-3.5539686917\P,0.0298761775,1.3232296987,-2.05543939
41\C,0.5769395009,2.9269039131,-1.2617935259\C,-0.5177572985,0.1092459
103,-0.6292505589\H,-0.2329217519,3.3432721639,-0.6551994218\H,0.76156
23334,3.6336755157,-2.0793022055\C,-1.2092327406,-1.0179918957,-1.4389
239219\C,-1.6258279427,0.9176508516,0.0819733085\H,-2.2523872133,1.443
9288129,-0.6489075784\H,-2.2869513161,0.2564879219,0.6497602567\H,-1.2
240249163,1.6639307748,0.7733242545\H,-2.0303820002,-0.6052243669,-2.0
334281979\H,-0.5246106958,-1.5156288674,-2.133604183\H,-1.7201413797,0
.4112560518,2.7754499955\H,1.4814602534,2.8655682405,-0.6509887678\H,2
.5044736916,0.74763377,-2.0413836039\H,-1.6266575327,-1.7861900006,-0.
7825809159\Version=IA64L-G03RevC.02\State=1-A\HF=-1078.2024597\RMSD=3
.777e-09\RMSF=3.109e-06\Dipole=-0.0132143,0.1809762,0.1173481\PG=C01 [
X(C10H24P2)]\@
```

n.SC_CH3_2CN-Me2CCMe2-SC_CH3_2CN

```
1\1\GINC-LC132\FOpt\RB3LYP\Gen\C14H24N2S2\CYL509\27-Jun-2008\0\#B3LYP
/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.SC_
CH3_2CN-Me2CCMe2-SC_CH3_2CN.freq\|0,1\N,-1.0232968653,-3.6407515391,-1
.9724207965\C,-0.9898446184,-3.5259519255,-0.8162560841\C,-0.969141731
3,-3.4237070798,0.6475832462\S,-0.0185515985,-1.9176625248,1.253726564
1\C,-0.5826499595,-0.259402724,0.4754805285\C,-1.9257662997,-0.3985136
693,-0.2551398627\C,-0.7805182898,0.6476043726,1.7039770801\C,-0.13015
26529,-4.6005796551,1.2052584518\C,-2.404244523,-3.501848257,1.2063459
809\H,0.8826078516,-4.5977574619,0.7958012818\H,-0.0713973173,-4.52577
00304,2.2955036691\H,-0.6136538751,-5.5484807357,0.9463937767\H,-2.370
4050579,-3.4102720518,2.2955538741\H,-2.8510100787,-4.4686913953,0.945
6563206\H,-3.0449061354,-2.7148822352,0.8077864597\H,-2.7122715829,-0.
6686232818,0.4540001544\H,-1.9114645318,-1.1350496015,-1.0603860113\H,
-1.5975512205,0.2616724629,2.3196158101\H,0.1095688799,0.710086262,2.3
348625979\N,1.0232968653,3.6407515391,1.9724207965\C,0.9898446184,3.52
59519255,0.8162560841\C,0.9691417313,3.4237070798,-0.6475832462\S,0.01
85515985,1.9176625248,-1.2537265641\C,0.5826499595,0.259402724,-0.4754
```

805285\C,1.9257662997,0.3985136693,0.2551398627\C,0.7805182898,-0.6476
043726,-1.7039770801\C,0.1301526529,4.6005796551,-1.2052584518\C,2.404
244523,3.501848257,-1.2063459809\H,0.0713973173,4.5257700304,-2.295503
6691\H,0.6136538751,5.5484807357,-0.9463937767\H,2.3704050579,3.410272
0518,-2.2955538741\H,2.8510100787,4.4686913953,-0.9456563206\H,3.04490
61354,2.7148822352,-0.8077864597\H,2.7122715829,0.6686232818,-0.454000
1544\H,1.9114645318,1.1350496015,1.0603860113\H,1.5975512205,-0.261672
4629,-2.3196158101\H,-0.1095688799,-0.710086262,-2.3348625979\H,1.0372
960377,-1.6617608364,-1.3847632747\H,2.2013009054,-0.5692201839,0.6859
992232\H,-1.0372960377,1.6617608364,1.3847632747\H,-2.2013009054,0.569
2201839,-0.6859992232\H,-0.8826078516,4.5977574619,-0.7958012818\\Vers
ion=IA32L-G03RevC.02\State=1-AG\HF=-1453.7792775\RMSD=6.915e-09\RMSF=1
.868e-05\Dipole=0.,0.,0.\PG=CI [X(C14H24N2S2)]\@

n.SCH2COOCH3-Me2CCMe2-SCH2COOCH3

1\1\GINC-LC34\FOpt\RB3LYP\Gen\C12H22O4S2\CYL509\27-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2
COOCH3-Me2CCMe2-SCH2COOCH3.freq\\0,1\S,1.1082851277,0.9636880317,-1.76
57815687\C,0.3721311809,-0.3510045797,-0.6060433156\C,1.6264964734,-1.
1226638469,-0.149306156\C,-0.5229509457,-1.3188504936,-1.3941421035\C,
-0.1476664185,1.3269564635,-3.0725578623\C,0.0850418613,0.5058487114,-
4.3247464634\O,-0.4905255595,-0.5233470589,-4.6072730305\O,1.041518180
8,1.0672871863,-5.0928220129\C,1.3924653843,0.3308842816,-6.2760607961
\H,-0.0315881159,2.3900841381,-3.2976839769\H,-1.1579120848,1.14683184
15,-2.707804286\H,0.5227237255,0.2143437488,-6.9279976974\H,1.77363665
64,-0.6587593606,-6.0106294733\H,2.1660503938,0.9206881885,-6.76823910
5\H,2.0992569192,-1.6043438333,-1.0091334755\H,2.3740800033,-0.4779490
091,0.3228413053\H,-0.8464901932,-2.1309800065,-0.7359631167\H,-1.4175
244419,-0.8484298521,-1.8069678249\H,0.0291664022,-1.748686439,-2.2330
070834\S,-1.1082851277,-0.9636880317,1.7657815687\C,-0.3721311809,0.35
10045797,0.6060433156\C,-1.6264964734,1.1226638469,0.149306156\C,0.522
9509457,1.3188504936,1.3941421035\C,0.1476664185,-1.3269564635,3.07255
78623\C,-0.0850418613,-0.5058487114,4.3247464634\O,0.4905255595,0.5233
470589,4.6072730305\O,-1.0415181808,-1.0672871863,5.0928220129\C,-1.39
24653843,-0.3308842816,6.2760607961\H,0.0315881159,-2.3900841381,3.297
6839769\H,1.1579120848,-1.1468318415,2.707804286\H,-0.5227237255,-0.21
43437488,6.9279976974\H,-1.7736366564,0.6587593606,6.0106294733\H,-2.1
660503938,-0.9206881885,6.768239105\H,-2.0992569192,1.6043438333,1.009
1334755\H,-2.3740800033,0.4779490091,-0.3228413053\H,0.8464901932,2.13
09800065,0.7359631167\H,1.4175244419,0.8484298521,1.8069678249\H,-0.02
91664022,1.748686439,2.2330070834\H,-1.3417684776,1.9061278706,-0.5604
309257\H,1.3417684776,-1.9061278706,0.5604309257\\Version=IA32L-G03Rev
C.02\State=1-AG\HF=-1567.8017744\RMSD=4.579e-09\RMSF=3.570e-06\Dipole=
0.,0.,0.\PG=CI [X(C12H22O4S2)]\@

n.SCH2Ph-Me2CCMe2-SCH2Ph

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C20H26S2\CYL509\30-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SCH2Ph
-Me2CCMe2-SCH2Ph.freq\\0,1\C,0.2530468179,-0.2115214078,0.7269972089\S
,1.3199256225,1.2433858628,1.3131929506\C,1.6904292743,0.8181544847,3.
0756422958\C,1.1715774004,-1.4357972459,0.5493447424\C,-0.8146981855,-
0.5310181662,1.7891583983\C,2.6732080547,1.8258487595,3.6207098827\H,2
.1121571494,-0.1908310093,3.1218522922\H,0.7661672573,0.8339760408,3.6
587845897\C,4.0528965012,1.6396553696,3.4605068114\C,2.221646113,2.971
9007478,4.2876791593\C,4.9601207698,2.5712581374,3.9641317852\C,3.1269
075805,3.9063304525,4.7918816454\C,4.4992423887,3.7078190164,4.6321335
088\H,5.2056647364,4.4333272898,5.0265978543\H,2.7599230656,4.78792801
06,5.3108607651\H,6.0271820668,2.4092939077,3.8361799121\H,1.15299954,
3.1299985802,4.4133474314\H,4.4149094985,0.7581111162,2.9366869904\H,-

```
1.5349598482,-1.2530198316,1.3903157443\H,-1.3600454367,0.3606669726,2
.1090778607\H,0.5925309952,-2.3298279411,0.2914176692\H,1.6971710888,-
1.6514892985,1.4853085107\H,1.9241697635,-1.2784664095,-0.2262050957\C
,-0.4004541444,0.2629458932,-0.6385037614\S,-1.1879151435,-1.289539083
5,-1.3923231499\C,-2.285067426,-0.6105625672,-2.7187861378\C,-1.483146
1506,1.3335403996,-0.4104979842\C,0.6416155342,0.8024729162,-1.6370736
062\C,-2.8577571692,-1.7614262239,-3.5099652467\H,-3.0878730887,-0.023
3118013,-2.2657947119\H,-1.6995105773,0.0467162142,-3.3692997084\C,-4.
0971311971,-2.3156008708,-3.1650129617\C,-2.1566265839,-2.3031835914,-
4.595700793\C,-4.6293315527,-3.380246307,-3.8931663976\C,-2.6863242333
,-3.36654587,-5.3259255644\C,-3.9253362327,-3.9081132533,-4.9766534666
\H,-4.3396978495,-4.735555641,-5.5464259955\H,-2.1323133475,-3.7717107
946,-6.1686222733\H,-5.5943835738,-3.7956032178,-3.6149864148\H,-1.189
4162456,-1.8869023908,-4.867308361\H,-4.6480436576,-1.9071134988,-2.32
09583691\H,0.1692377178,0.9994566622,-2.604983696\H,1.4585827232,0.097
0215334,-1.8030230632\H,-1.0716768597,2.1633598489,0.173649201\H,-1.82
63008104,1.742197743,-1.3658446541\H,-2.3531576381,0.9361680967,0.1186
82246\H,1.0693548006,1.7493746978,-1.2884783304\H,-0.3537444873,-0.980
777389,2.6738556844\Version=IA64L-G03RevC.02\State=1-A\HF=-1574.16465
71\RMSD=7.969e-09\RMSF=2.193e-06\Dipole=-0.2423463,0.0846878,0.1454061
\PG=C01 [X(C20H26S2)]\@
```

n.SCH3-Me2CCMe2-SCH3

```
1\1\GINC-LC114\FOpt\RB3LYP\Gen\C8H18S2\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.SCH3-M
e2CCMe2-SCH3.freq\0,1\S,0.3914806184,-0.1867573112,-2.2555740654\C,0.
1081504321,-0.6511631954,-0.4388666551\C,1.4027196308,-1.3960882189,-0.
0578401573\C,-1.0606696209,-1.6429383675,-0.3350415741\C,-1.236515098
7,-0.2949007473,-3.0828804615\H,-1.036742831,-0.0427699855,-4.12859237
94\H,-1.9639940156,0.4185382123,-2.6878277718\H,-1.6510107549,-1.30488
61732,-3.0441129835\H,1.3656949023,-1.6957245888,0.9943041754\H,1.5042
049535,-2.2994819076,-0.6652945444\H,2.300155243,-0.7906306962,-0.2170
806718\H,-1.1637965337,-1.982155908,0.7001225009\H,-2.0170702453,-1.21
30588505,-0.6425490156\H,-0.8661686246,-2.5177940268,-0.9637184461\S,-
0.3914806184,0.1867573112,2.2555740654\C,-0.1081504321,0.6511631954,0.
4388666551\C,-1.4027196308,1.3960882189,0.0578401573\C,1.0606696209,1.
6429383675,0.3350415741\C,1.2365150987,0.2949007473,3.0828804615\H,1.0
36742831,0.0427699855,4.1285923794\H,1.6510107549,1.3048861732,3.04411
29835\H,-1.5042049535,2.2994819076,0.6652945444\H,-2.300155243,0.79063
06962,0.2170806718\H,1.1637965337,1.982155908,-0.7001225009\H,2.017070
2453,1.2130588505,0.6425490156\H,0.8661686246,2.5177940268,0.963718446
1\H,-1.3656949023,1.6957245888,-0.9943041754\H,1.9639940156,-0.4185382
123,2.6878277718\Version=IA32L-G03RevC.02\State=1-AG\HF=-1112.0645354
\RMSD=3.722e-09\RMSF=1.898e-05\Dipole=0.,0.,0.\PG=CI [X(C8H18S2)]\@
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n.SO2CH3-Me2CCMe2-SO2CH3

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1\1\GINC-LC146\FOpt\RB3LYP\Gen\C8H18O4S2\CYL509\26-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.SO2C
H3-Me2CCMe2-SO2CH3.freq\0,1\C,-0.634492594,-0.3234567205,0.3379097302
\S,-0.5039165766,-0.2827743268,2.2721367831\C,0.3958074751,-1.76853978
21,2.81401649\O,0.2922932014,0.8723663522,2.7325344038\O,-1.8822386071
,-0.4538655545,2.7676309393\H,-0.1751346221,-2.6636648603,2.5711360313
\H,0.4599695855,-1.6463535331,3.8980576844\H,1.39571591,-1.8026950229,
2.3826030799\C,-0.8656091865,-1.8127884592,0.0100393848\C,-1.938156535
5,0.4429632547,0.0510015641\H,-2.192617723,0.3193583302,-1.0055928637\
H,-1.8696492082,1.5078398526,0.2863870256\H,-2.7546390977,0.0255175471
,0.6418764696\H,0.0139977265,-2.4352289008,0.1867964382\H,-1.132403232
3,-1.9144679725,-1.0415635779\H,-1.6913660508,-2.1947662575,0.61833157
99\C,0.634492594,0.3234567205,-0.3379097302\S,0.5039165766,0.282774326
```

8,-2.2721367831\C,-0.3958074751,1.7685397821,-2.81401649\O,-0.29229320
14,-0.8723663522,-2.7325344038\O,1.8822386071,0.4538655545,-2.76763093
93\H,0.1751346221,2.6636648603,-2.5711360313\H,-0.4599695855,1.6463535
331,-3.8980576844\H,-1.39571591,1.8026950229,-2.3826030799\C,0.8656091
865,1.8127884592,-0.0100393848\C,1.9381565355,-0.4429632547,-0.0510015
641\H,2.192617723,-0.3193583302,1.0055928637\H,1.8696492082,-1.5078398
526,-0.2863870256\H,2.7546390977,-0.0255175471,-0.6418764696\H,-0.0139
977265,2.4352289008,-0.1867964382\H,1.1324032323,1.9144679725,1.041563
5779\H,1.6913660508,2.1947662575,-0.6183315799\\Version=IA32L-G03RevC.
02\State=1-AG\HF=-1412.8346473\RMSD=2.764e-09\RMSF=1.743e-05\Dipole=0.
0.,0.0.\PG=CI [X(C8H18O4S2)]\@

n.SOCH3-Me2CCMe2-SOCH3

1\1\GINC-LC143\FOpt\RB3LYP\Gen\C8H18O2S2\CYL509\26-Jun-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.SOCH
3-Me2CCMe2-SOCH3.freq\\0,1\C,-0.558593339,-0.2280872989,0.5086543081\S
, -0.2799011404,0.4435898508,2.2433053399\O,0.8592744292,-0.6371890612,
2.9163837404\C,1.9700827241,0.0185711224,3.5292971251\C,-0.6912683949,
-1.75519028,0.6184954064\H,2.6151876548,-0.7835437563,3.9005105846\H,1.
.6548210041,0.6423385235,4.375325814\H,2.5288516507,0.6414427883,2.818
6278973\C,-1.9278397432,0.4012968384,0.1794881285\H,-1.9250183681,1.49
14325465,0.2869669987\H,-2.6997439497,-0.003113016,0.8397881614\H,-2.2
001189164,0.1787890596,-0.8535567147\H,0.2019429124,-2.2096652408,1.05
2601059\H,-0.8631217818,-2.1903520825,-0.3708785428\H,-1.5375295848,-2.
0088540086,1.2635833525\C,0.558593339,0.2280872989,-0.5086543081\S,0.
2799011404,-0.4435898508,-2.2433053399\O,-0.8592744292,0.6371890612,-2.
9163837404\C,-1.9700827241,-0.0185711224,-3.5292971251\C,0.6912683949
,1.75519028,-0.6184954064\H,-2.6151876548,0.7835437563,-3.9005105846\H
, -1.6548210041,-0.6423385235,-4.375325814\H,-2.5288516507,-0.641442788
3,-2.8186278973\C,1.9278397432,-0.4012968384,-0.1794881285\H,1.9250183
681,-1.4914325465,-0.2869669987\H,2.6997439497,0.003113016,-0.83978816
14\H,2.2001189164,-0.1787890596,0.8535567147\H,-0.2019429124,2.2096652
408,-1.052601059\H,0.8631217818,2.1903520825,0.3708785428\H,1.53752958
48,2.0088540086,-1.2635833525\\Version=IA32L-G03RevC.02\State=1-AG\HF=
-1262.4363919\RMSD=2.429e-09\RMSF=8.128e-06\Dipole=0.,0.,0.\PG=CI [X(C
8H18O2S2)]\@

n.Ph-Me2CCMe2-Ph

1\1\GINC-LC80\FOpt\RB3LYP\Gen\C18H22\CYL509\26-Jun-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.Ph-Me2CC
Me2-Ph.freq\\0,1\H,-5.2448288222,-2.7764884138,-0.2814900336\C,-4.2430
610549,-2.3583252046,-0.2337068058\C,-3.1220780713,-3.1880895085,-0.25
04607878\C,-1.8417658707,-2.6427899111,-0.1888492693\C,-1.6111667005,-
1.2534789402,-0.107958275\C,-2.759745099,-0.443250391,-0.0928410152\C,
-4.048748868,-0.9832507447,-0.1543780203\H,-3.239569777,-4.267177497,-
0.3118044883\C,-0.1154569546,-0.7878607792,-0.0453970465\C,0.464288293
, -1.4771178749,1.2287418313\C,0.5290478609,-1.3378133391,-1.3556776225
\H,-2.6837299158,0.6329321921,-0.0326504304\H,-1.0008642249,-3.3280441
731,-0.2048442463\H,-4.902245918,-0.3099683074,-0.1393047157\H,1.43798
9682,-1.0851200886,1.5228153908\H,0.5743376602,-2.5552244229,1.0776438
645\H,-0.2113293277,-1.3383190266,2.0779292188\H,1.5152037018,-0.91926
78289,-1.5570662258\H,-0.1036864831,-1.1067491373,-2.2177215555\H,0.63
43052281,-2.4261984181,-1.3159171908\H,5.2448288222,2.7764884138,0.281
4900336\C,4.2430610549,2.3583252046,0.2337068058\C,3.1220780713,3.1880
895085,0.2504607878\C,1.8417658707,2.6427899111,0.1888492693\C,1.61116
67005,1.2534789402,0.107958275\C,2.759745099,0.443250391,0.0928410152\
C,4.048748868,0.9832507447,0.1543780203\H,3.239569777,4.267177497,0.31
18044883\C,0.1154569546,0.7878607792,0.0453970465\C,-0.464288293,1.477
1178749,-1.2287418313\C,-0.5290478609,1.3378133391,1.3556776225\H,2.68

37299158,-0.6329321921,0.0326504304\H,1.0008642249,3.3280441731,0.2048
442463\H,4.902245918,0.3099683074,0.1393047157\H,-1.437989682,1.085120
0886,-1.5228153908\H,-0.5743376602,2.5552244229,-1.0776438645\H,0.2113
293277,1.3383190266,-2.0779292188\H,-1.5152037018,0.9192678289,1.55706
62258\H,0.1036864831,1.1067491373,2.2177215555\H,-0.6343052281,2.42619
84181,1.3159171908\\Version=IA32L-G03RevC.02\State=1-AG\HF=-699.140387
1\RMSD=8.696e-09\RMSF=1.557e-05\Dipole=0.,0.,0.\PG=CI [X(C18H22)]\@

n.C6H4CN-Me2CCMe2-C6H4CN

1\1\GINC-LC48\FOpt\RB3LYP\Gen\C20H20N2\CYL509\27-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4CN
-Me2CCMe2-C6H4CN.freq\\0,1\N,-7.4134831701,0.458354376,0.4168755381\C,
-6.2513991503,0.4708295302,0.3615622492\C,-4.8200396338,0.4870054553,0
.293490801\C,-4.0990221192,-0.6999683721,0.1215142936\C,-2.7064298206,
-0.6799837354,0.055545859\C,-1.9680613762,0.5128547264,0.156531544\C,-
2.7240463568,1.6924680305,0.3297195503\C,-4.1107829689,1.6933081093,0.
3978284294\H,-4.6282227414,-1.6439959021,0.0387431547\C,-0.4124032611,
0.6751021304,0.0983970067\C,-0.0315064612,1.332580554,1.4619376339\C,-
0.1586936273,1.6295937698,-1.1104952374\H,-2.2206140345,2.6486783551,0
.4152491494\H,-2.2159133123,-1.6327222843,-0.0781083548\H,-4.649492568
7,2.6259939749,0.5317467592\H,0.8873386189,1.6672415881,-1.4143832341\
H,-0.4697222676,2.6522881372,-0.8781938833\H,-0.7354261353,1.306287341
, -1.981965966\H,1.0397123463,1.3137291065,1.6622813351\H,-0.5228529076
,0.8120084042,2.2890938668\H,-0.3539581052,2.3771681199,1.5001343349\N
,7.4134831701,-0.458354376,-0.4168755381\C,6.2513991503,-0.4708295302,
-0.3615622492\C,4.8200396338,-0.4870054553,-0.293490801\C,4.0990221192
,0.6999683721,-0.1215142936\C,2.7064298206,0.6799837354,-0.055545859\C
,1.9680613762,-0.5128547264,-0.156531544\C,2.7240463568,-1.6924680305,
-0.3297195503\C,4.1107829689,-1.6933081093,-0.3978284294\H,4.628222741
4,1.6439959021,-0.0387431547\C,0.4124032611,-0.6751021304,-0.098397006
7\C,0.0315064612,-1.332580554,-1.4619376339\C,0.1586936273,-1.62959376
98,1.1104952374\H,2.2206140345,-2.6486783551,-0.4152491494\H,2.2159133
123,1.6327222843,0.0781083548\H,4.6494925687,-2.6259939749,-0.53174675
92\H,-0.8873386189,-1.6672415881,1.4143832341\H,0.4697222676,-2.652288
1372,0.8781938833\H,0.7354261353,-1.306287341,1.981965966\H,-1.0397123
463,-1.3137291065,-1.6622813351\H,0.5228529076,-0.8120084042,-2.289093
8668\H,0.3539581052,-2.3771681199,-1.5001343349\\Version=IA32L-G03RevC
.02\State=1-AG\HF=-883.6284354\RMSD=5.594e-09\RMSF=9.360e-06\Dipole=0.
,0.,0.\PG=CI [X(C20H20N2)]\@

n.C6H4NO2-Me2CCMe2-C6H4NO2

1\1\GINC-LC49\FOpt\RB3LYP\Gen\C18H20N2O4\CYL509\27-Jun-2008\0\#B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C6H4
NO2-Me2CCMe2-C6H4NO2.freq\\0,1\O,-5.4349330887,4.3214583005,-1.0563556
122\N,-4.4910930174,4.0148775856,-1.7850201122\C,-3.5037159414,3.06516
45081,-1.2569872167\O,-4.3164094062,4.4477568996,-2.9242652069\C,-3.66
32575111,2.5505359146,0.0265497523\C,-2.7195291088,1.6534272078,0.5099
779832\C,-1.6007281873,1.2390282208,-0.2465843304\C,-1.4877668709,1.78
97893921,-1.5369996691\C,-2.4226462965,2.6920461134,-2.0441265343\H,-2
.3171935879,3.1043793802,-3.0401898784\C,-0.6272847623,0.2232861051,0.
4383704227\C,-0.1376053986,0.9541360927,1.7282821624\C,-1.5155041104,-
1.0192843675,0.7609312802\H,-2.86677558,1.2677845247,1.5120315026\H,-0
.6652611764,1.5312144201,-2.1868703052\H,-4.513146319,2.8537135175,0.6
256926017\H,-0.935674011,-1.8976172318,1.0442534811\H,-2.1162475953,-1
.297774584,-0.1097787798\H,-2.210081277,-0.8069215984,1.5788158533\H,0
.7166232153,0.4668662278,2.1981077312\H,-0.9339389906,1.0123820648,2.4
758815461\H,0.1648109139,1.9796429334,1.4969456625\O,5.4349330887,-4.3
214583005,1.0563556122\N,4.4910930174,-4.0148775856,1.7850201122\C,3.5
037159414,-3.0651645081,1.2569872167\O,4.3164094062,-4.4477568996,2.92

42652069\C,3.6632575111,-2.5505359146,-0.0265497523\C,2.7195291088,-1.6534272078,-0.5099779832\C,1.6007281873,-1.2390282208,0.2465843304\C,1.4877668709,-1.7897893921,1.5369996691\C,2.4226462965,-2.6920461134,2.0441265343\H,2.3171935879,-3.1043793802,3.0401898784\C,0.6272847623,-0.2232861051,-0.4383704227\C,0.1376053986,-0.9541360927,-1.7282821624\C,1.5155041104,1.0192843675,-0.7609312802\H,2.86677558,-1.2677845247,-1.5120315026\H,0.6652611764,-1.5312144201,2.1868703052\H,4.513146319,-2.8537135175,-0.6256926017\H,0.935674011,1.8976172318,-1.0442534811\H,2.1162475953,1.297774584,0.1097787798\H,2.210081277,0.8069215984,-1.5788158533\H,-0.7166232153,-0.4668662278,-2.1981077312\H,0.9339389906,-1.0123820648,-2.4758815461\H,-0.1648109139,-1.9796429334,-1.4969456625\Version=IA32L-G03RevC.02\State=1-AG\HF=-1108.1451235\RMSD=5.832e-09\RM SF=4.778e-06\Dipole=0.,0.,0.\PG=CI [X(C18H20N2O4)]\@

n.C6H4OCH3-Me2CCMe2-C6H4OCH3

1\1\GINC-LC51\FOpt\RB3LYP\Gen\C20H26O2\CYL509\27-Jun-2008\0\#B3LYP/GE N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C6H4OCH3-Me2CCMe2-C6H4OCH3.freq\0,1\C,-3.4934474084,-0.4097352829,2.2415400024\C,-3.4473320249,0.3421526336,3.4178991008\C,-2.3003901829,1.0955637701,3.6817579469\C,-1.2390789671,1.0806420281,2.7753088929\C,-1.2488175643,0.3370909198,1.5818632901\C,-2.4215861206,-0.408555741,1.3524002695\C,0.0242273923,0.4291740863,0.671957365\O,-4.5482852187,0.2753107496,4.225111248\C,-4.5382093801,1.0255542644,5.4277807111\C,1.1983359296,-0.0692301372,1.5700947596\C,0.1609573271,1.9431507673,0.3219466201\H,-2.5342636076,-1.0155500035,0.4655406589\H,-0.3724530058,1.6827727476,3.0278443753\H,-2.2160845313,1.6955469059,4.5811315328\H,-4.3826784319,-0.9967649446,2.0324192847\H,-3.7259618507,0.7092249217,6.0961515388\H,-5.4975958524,0.8313588861,5.911280459\H,-4.4428986167,2.1023658523,5.2330443336\H,2.1194907735,-0.2480670203,1.0150397813\H,0.9285627976,-1.0076685961,2.0633403664\H,1.4241590212,0.6552900836,2.3586291058\H,0.8905407581,2.1393607452,-0.4640709072\H,0.4588383624,2.5237264442,1.2005249689\H,-0.7987592407,2.343475894,-0.0178063129\C,3.4934474084,0.4097352829,-2.2415400024\C,3.4473320249,-0.3421526336,-3.4178991008\C,2.3003901829,-1.0955637701,-3.6817579469\C,1.2390789671,-1.0806420281,-2.7753088929\C,1.2488175643,-0.3370909198,-1.5818632901\C,2.4215861206,0.408555741,-1.3524002695\C,-0.0242273923,-0.4291740863,-0.671957365\O,4.5482852187,-0.2753107496,-4.225111248\C,4.5382093801,-1.0255542644,-5.4277807111\C,-1.1983359296,0.0692301372,-1.5700947596\C,-0.1609573271,-1.9431507673,-0.3219466201\H,2.5342636076,1.0155500035,-0.4655406589\H,0.3724530058,-1.6827727476,-3.0278443753\H,2.2160845313,-1.6955469059,-4.5811315328\H,4.3826784319,0.9967649446,-2.0324192847\H,3.7259618507,-0.7092249217,-6.0961515388\H,5.4975958524,-0.8313588861,-5.911280459\H,4.4428986167,-2.1023658523,-5.2330443336\H,-2.1194907735,0.2480670203,-1.0150397813\H,-0.9285627976,1.0076685961,-2.0633403664\H,-1.4241590212,-0.6552900836,-2.3586291058\H,-0.8905407581,-2.1393607452,0.4640709072\H,-0.4588383624,-2.5237264442,-1.2005249689\H,0.7987592407,-2.343475894,0.0178063129\Version=IA32L-G03RevC.02\State=1-AG\HF=-928.1850988\RMSD=9.658e-09\RMSF=6.659e-06\Dipole=0.,0.,0.\PG=CI [X(C20H26O2)]\@

n.C6H4OH-Me2CCMe2-C6H4OH

1\1\GINC-LC52\FOpt\RB3LYP\Gen\C18H22O2\CYL509\26-Jun-2008\0\#B3LYP/GE N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.C6H4OH-Me2CCMe2-C6H4OH.freq\0,1\C,-3.9775390608,-2.0063340001,0.4113184164\C,-4.4240575913,-1.3072783929,1.535343229\C,-3.5946286958,-0.33709801,2.0926314733\C,-2.3397562021,-0.0702951625,1.5356055896\C,-1.8560615454,-0.7510217468,0.4075037458\C,-2.7272132355,-1.7256234356,-0.1262876726\C,-0.4793465051,-0.5545029777,-0.3150116779\O,-5.661589625,-1.6151937247,2.0326017903\C,0.2148699495,-1.9497337971,-0.2436720811\C,-0.846

```
1360446,-0.160240063,-1.7791299142\H,-2.426375284,-2.2957232963,-0.998
9224386\H,-1.7537288141,0.69556741,2.0231081237\H,-3.9190905806,0.2220
594543,2.9690597124\H,-4.6175683164,-2.764376027,-0.0297309043\H,-5.83
55338267,-1.0557130074,2.8053987008\H,0.0068976188,0.2003918069,-2.354
3376793\H,-1.5989632071,0.6334378726,-1.7824984816\H,-1.2728400902,-1.
010601639,-2.3198786245\H,1.2661103068,-1.9225844645,-0.5312995962\H,-
0.2868213179,-2.6720621695,-0.89496414\H,0.1670241862,-2.3472479915,0.
7743611823\C,3.9775390608,2.0063340001,-0.4113184164\C,4.4240575913,1.
3072783929,-1.535343229\C,3.5946286958,0.33709801,-2.0926314733\C,2.33
97562021,0.0702951625,-1.5356055896\C,1.8560615454,0.7510217468,-0.407
5037458\C,2.7272132355,1.7256234356,0.1262876726\C,0.4793465051,0.5545
029777,0.3150116779\O,5.661589625,1.6151937247,-2.0326017903\C,-0.2148
699495,1.9497337971,0.2436720811\C,0.8461360446,0.160240063,1.77912991
42\H,2.426375284,2.2957232963,0.9989224386\H,1.7537288141,-0.69556741,
-2.0231081237\H,3.9190905806,-0.2220594543,-2.9690597124\H,4.617568316
4,2.764376027,0.0297309043\H,5.8355338267,1.0557130074,-2.8053987008\H
,-0.0068976188,-0.2003918069,2.3543376793\H,1.5989632071,-0.6334378726
,1.7824984816\H,1.2728400902,1.010601639,2.3198786245\H,-1.2661103068,
1.9225844645,0.5312995962\H,0.2868213179,2.6720621695,0.89496414\H,-0.
1670241862,2.3472479915,-0.7743611823\Version=IA32L-G03RevC.02\State=
1-AG\HF=-849.5723548\RMSD=4.495e-09\RMSF=6.097e-06\Dipole=0.,0.,0.\PG=
CI [X(C18H22O2)]\@
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n.CF2CF3-Me2CCMe2-CF2CF3

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1\1\GINC-LC56\FOpt\RB3LYP\Gen\C10H12F10\CYL509\26-Jun-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CF2CF
3-Me2CCMe2-CF2CF3.freq\0,1\F,0.0268256657,1.900078947,-2.4342712547\C
,0.5930724449,1.5220556063,-1.2408262977\C,2.1104532157,1.4196978476,-
1.5939698858\C,-0.2882677962,0.3379196699,-0.6703859215\F,0.5156826893
,2.6160053418,-0.4197358249\F,2.4180401351,0.2511039288,-2.1824425929\F
,2.8819251517,1.5685520299,-0.4986946861\F,2.4367103736,2.4059808509,
-2.4381929337\C,-1.6589536189,1.0440264406,-0.4440513115\C,-0.48150176
84,-0.6988162313,-1.806904849\H,-0.8864296702,-0.2056146897,-2.6924677
63\H,-1.1925243967,-1.464172033,-1.496799481\H,0.4466855537,-1.1944251
08,-2.0949260227\H,-1.9045263517,1.6499454237,-1.3176953842\H,-1.65782
11961,1.7021466384,0.4247288404\F,-0.0268256657,-1.900078947,2.4342712
547\C,-0.5930724449,-1.5220556063,1.2408262977\C,-2.1104532157,-1.4196
978476,1.5939698858\C,0.2882677962,-0.3379196699,0.6703859215\F,-0.515
6826893,-2.6160053418,0.4197358249\F,-2.4180401351,-0.2511039288,2.182
4425929\F,-2.8819251517,-1.5685520299,0.4986946861\F,-2.4367103736,-2.
4059808509,2.4381929337\C,1.6589536189,-1.0440264406,0.4440513115\C,0.
4815017684,0.6988162313,1.806904849\H,0.8864296702,0.2056146897,2.6924
67763\H,1.1925243967,1.464172033,1.496799481\H,-0.4466855537,1.1944251
08,2.0949260227\H,1.9045263517,-1.6499454237,1.3176953842\H,1.65782119
61,-1.7021466384,-0.4247288404\H,2.4547552666,-0.3148990151,0.33272680
16\H,-2.4547552666,0.3148990151,-0.3327268016\Version=IA32L-G03RevC.0
2\State=1-AG\HF=-1386.6843495\RMSD=5.054e-09\RMSF=6.841e-06\Dipole=0.,
0.,0.\PG=CI [X(C10H12F10)]\@
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n.CF2H-Me2CCMe2-CF2H

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1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H14F4\CYL509\23-Aug-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CF2H-Me
2CCMe2-CF2H.freq\0,1\C,1.1389427481,0.3477791839,-1.577036952\C,0.790
9583874,0.1499710862,-0.0898700088\C,1.4897604832,1.3194650744,0.64889
47135\H,2.2125985965,0.5371839748,-1.6963012242\F,0.4771509809,1.41386
632,-2.1409719391\F,0.8395900713,-0.7496168887,-2.3419705816\C,1.49307
14284,-1.1659996986,0.3252705948\H,2.5442765803,-1.1368219399,0.012764
3825\H,1.0344158115,-2.0451522366,-0.1304206839\H,1.4727559379,-1.2894
478159,1.4090506273\H,2.5762027105,1.2415437011,0.5215334588\H,1.27619
```

83551,1.2866063422,1.7172016144\H,1.1809140177,2.2938081758,0.26037476
24\C,-1.1439328725,-0.4984206667,1.532398972\C,-0.7812505341,0.1265962
48,0.1722944902\C,-1.5580791421,-0.7008232449,-0.8807445506\H,-2.20475
73431,-0.3347054053,1.7575032444\F,-0.9325629326,-1.8523509714,1.56654
35114\F,-0.4241043743,0.0393223924,2.5741512764\C,-1.3901053156,1.5513
481713,0.2054252007\H,-2.4813842514,1.485733732,0.2917822636\H,-1.0261
782062,2.1340028338,1.0561358908\H,-1.160333688,2.0931844381,-0.711970
8062\H,-2.6110960398,-0.7794432934,-0.583239627\H,-1.5246924457,-0.213
4847029,-1.8562325891\H,-1.1657748416,-1.7134923963,-0.9877464771\\Ver
sion=IA64L-G03RevC.02\State=1-A\HF=-712.6452311\RMSD=3.205e-09\RMSF=9.
749e-06\Dipole=0.0123083,0.3489482,0.1041752\PG=C01 [X(C8H14F4)]\@

n.CF3-Me2CCMe2-CF3

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H12F6\CYL509\23-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CF3-Me2
CCMe2-CF3.freq\0,1\F,0.0587478186,1.9376010222,-1.7272892583\C,-0.059
4586339,1.9324648091,-0.3756811446\F,1.1338926343,2.3294645218,0.12169
9649\C,-0.537275967,0.576725162,0.1979786904\F,-0.9373143772,2.9184459
273,-0.070808445\C,-2.0311391659,0.4400109988,-0.1932860431\C,-0.44972
57028,0.7206569627,1.7385785777\H,-2.186196975,0.553542029,-1.26926495
45\H,-2.6180128327,1.2118956743,0.3099012272\H,-2.4161975971,-0.532619
3022,0.1116517011\H,0.5799030959,0.7547192503,2.099127418\H,-0.9595424
682,-0.1098992914,2.2290060902\H,-0.9467453651,1.6459200472,2.04329042
24\F,0.8362723912,-1.7621749368,1.7094833196\C,0.21128568,-1.888736588
2,0.5168153579\F,-1.0745686695,-2.2300216457,0.7831769137\C,0.34500425
1,-0.6321016881,-0.3767261466\F,0.7700137711,-2.966624322,-0.084613792
9\C,1.8610287559,-0.3143093427,-0.4267898081\C,-0.1097717988,-1.056505
6593,-1.7967495534\H,2.2434679467,0.0582171101,0.5251838361\H,2.412106
6068,-1.2240124817,-0.6812402894\H,2.0697494221,0.4295381785,-1.197102
5883\H,-1.1078324721,-1.50206295,-1.7926077879\H,-0.1167920415,-0.1967
810809,-2.4661461631\H,0.5830160524,-1.7979002092,-2.2014739685\\Versi
on=IA64L-G03RevC.02\State=1-A\HF=-911.1483169\RMSD=3.785e-09\RMSF=3.96
1e-06\Dipole=-0.1578054,-0.0454677,-0.1467068\PG=C01 [X(C8H12F6)]\@

n.CC12H-Me2CCMe2-CC12H

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H14Cl4\CYL509\23-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC12H-
Me2CCMe2-CC12H.freq\0,1\C,-0.4554653349,1.203392575,-1.4867874188\C,-
0.264529356,0.8257642844,0.023137466\H,0.4081070104,0.8952349719,-2.06
9058414\C,0.9633037581,1.6533908569,0.4888461103\C,-1.4786368886,1.288
603475,0.8535114119\H,1.8691223303,1.4229733876,-0.0781210938\H,1.1776
224344,1.4776797396,1.5440374924\H,0.7571204616,2.718588271,0.38110808
25\H,-1.3603256251,1.0071702418,1.9054832692\H,-2.4191314657,0.8668169
321,0.4939388456\H,-1.5638531361,2.3780265614,0.8154524696\C,0.7433011
352,-1.0595392002,1.5316655782\C,-0.0175795611,-0.7782672528,0.1804011
618\H,0.4000764637,-0.3976250623,2.323428979\C,-1.3748132869,-1.528127
4436,0.2649134337\C,0.7868930182,-1.3792337419,-0.9909866648\H,-1.8887
561523,-1.3561840267,1.2142970851\H,-2.0351904879,-1.2182208757,-0.541
6817277\H,-1.2127400394,-2.6028224361,0.1677845106\H,0.1780367818,-1.4
180223743,-1.8980456322\H,1.7052921938,-0.8250786536,-1.2035605676\H,1
.0759608104,-2.4067539693,-0.7484280942\Cl,-1.8838255041,0.4714287978,
-2.3374179845\Cl,-0.5763363784,3.0000236297,-1.7659507718\Cl,0.4697978
714,-2.7316216805,2.1989078967\Cl,2.5488238651,-0.851459219,1.46358782
\\Version=IA64L-G03RevC.02\State=1-A\HF=-2154.0457237\RMSD=2.033e-09\R
MSF=6.268e-06\Dipole=-0.1083529,0.1481877,0.154958\PG=C01 [X(C8H14Cl4)
]\@

n.CC13-Me2CCMe2-CC13

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C8H12Cl6\CYL509\29-Jun-2008\0\#B3LYP/GE

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N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CC13-Me2CCMe2-CC13.freq\\0,1\C,1.1399852095,-0.1621849796,-1.7088751683\C,0.8289394578,0.2053986043,-0.172197068\C,1.5431085177,1.5586476356,0.1029536006\C,1.5535962028,-0.8813926655,0.6596121626\H,2.6232225534,1.41380268,0.136799345\H,1.2386040689,1.9563851089,1.0683625556\H,1.3288859093,2.3102986721,-0.6595167127\H,2.5981776985,-0.944980464,0.3476684998\H,1.1076895562,-1.8681919803,0.5511365788\H,1.5499707123,-0.6123547984,1.7155315082\C,-1.1501398461,0.0409915306,1.7092747695\C,-0.7831085214,0.3415956288,0.1703883631\C,-1.6789593355,-0.6148998513,-0.6546679019\C,-1.262292401,1.7929800449,-0.114031126\H,-2.7193879061,-0.5017343406,-0.342891745\H,-1.6311942252,-0.3571560544,-1.7123287959\H,-1.4034121724,-1.6614063838,-0.5394687617\H,-2.3514687615,1.8296663718,-0.1475139493\H,-0.9255588238,2.5034942064,0.6436044336\H,-0.8963855132,2.1281565269,-1.0818643972\C1,2.930001759,0.008278084,-2.0547757595\C1,0.3333868706,0.9170755262,-2.9275685418\C1,0.7465430867,-1.8738294933,-2.1553145808\C1,-0.1744181755,0.9788483038,2.9213016765\C1,-1.0469137934,-1.7093094371,2.1671207515\C1,-2.8865949709,0.5093608263,2.0531032571\\Version=IA64L-G03RevC.02\State=1-A\HF=-3073.1871716\RMSE=7.888e-09\RMSF=1.500e-05\Dipole=0.028761,0.3433295,-0.0011335\PG=C01 [X(C8H12Cl6)]\\@
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n.CH2Cl-Me2CCMe2-CH2Cl

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C8H16Cl2\CYL509\23-Aug-2008\0\\#B3LYP/GEN N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Cl-Me2CCMe2-CH2Cl.freq\\0,1\C,0.7679202734,-0.2423045639,-0.0031446786\C,1.1441950454,-0.5859542526,1.4579086331\C,1.7079831472,0.8797699912,-0.5005466252\C,0.9780607549,-1.4847239281,-0.8967597043\H,0.4642122192,-1.3190668843,1.8920886166\H,1.158701181,0.3029358326,2.0869335397\H,2.0447109347,-1.7070912002,-0.9833952821\H,0.5942936476,-1.3240336542,-1.9093675632\H,0.4902891884,-2.3748631336,-0.4885623735\H,2.7489659825,0.5937350559,-0.3240616163\H,1.5346834725,1.8302770606,0.0161020405\H,1.5997821575,1.0522035908,-1.5758201129\C,-0.7739544618,0.2222733065,-0.0027560075\C,-1.0476338693,0.9062393374,-1.3635073682\C,-1.7223732221,-0.9849438983,0.1688361755\C,-1.0697798515,1.2379031285,1.1247011896\H,-0.5098769475,1.8490415366,-1.4526810441\H,-0.782447557,0.2635935443,-2.2031650449\H,-2.0699229057,1.6593826586,0.9880295934\H,-1.0523473602,0.7646991622,2.1113249013\H,-0.3587373379,2.0714228721,1.1339630377\H,-2.7513690063,-0.6376459726,0.2923100156\H,-1.7038569681,-1.6517730358,-0.6982796085\H,-1.4683056372,-1.5760250801,1.0545823702\C1,2.8071481688,-1.3171291514,1.6579626651\C1,-2.7980471077,1.3473440292,-1.6490444978\\Version=IA64L-G03RevC.02\State=1-A\HF=-1234.8866824\RMSE=4.101e-09\RMSF=7.188e-06\Dipole=0.0246548,0.081746,0.0240837\PG=C01 [X(C8H16Cl2)]\\@
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n.CH2F-Me2CCMe2-CH2F

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1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H16F2\CYL509\23-Aug-2008\0\\#B3LYP/GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2F-Me2CCMe2-CH2F.freq\\0,1\C,-0.2615317683,0.5267500212,-0.5004373068\C,0.6679412179,1.7400604844,-0.6715535794\F,1.8690432539,1.4062950167,-1.3026752482\C,-0.3487109822,-0.2006163382,-1.8597441899\C,-1.6573706075,1.1204260438,-0.1862373609\H,0.9155696066,2.2068385203,0.2893295183\H,0.1746472538,2.4902940194,-1.3020536432\H,-1.6321814615,1.8131548968,0.662435489\H,-2.3730110207,0.3304504177,0.0424373587\H,-2.0283283651,1.6784754423,-1.0541784398\H,0.590488325,-0.6900050127,-2.1319916202\H,-0.5810113673,0.51846209,-2.6540541181\H,-1.1470054129,-0.9490462617,-1.8520765509\C,0.2465242691,-0.4395609503,0.656785572\C,-0.4228841251,-1.8214034437,0.583730606\F,-1.8182223261,-1.7537900024,0.6674169254\C,-0.0354099949,0.1475748839,2.0574919174\C,1.7639336914,-0.7295052408,0.5491653582\H,-0.1744851463,-2.3407842654,-0.3474078039\H,-0.080976766
```

, -2.4368973301, 1.4252002332\H, 2.0480532584, -1.1171355556, -0.4334057586
\H, 2.3583726989, 0.1690654394, 0.7277090601\H, 2.054682201, -1.4726623346,
1.3021423748\H, -1.1055596955, 0.1710228381, 2.278854315\H, 0.4480078559, -
0.4695063529, 2.8243730876\H, 0.3603994835, 1.1633755593, 2.1648053047\\Ve
rsion=IA64L-G03RevC.02\State=1-A\HF=-514.1574972\RMSD=2.028e-09\RMSF=3
.075e-06\Dipole=0.049426, 0.0845184, 0.2305209\PG=C01 [X(C8H16F2)]\@

n.CH2OH-Me2CCMe2-CH2OH

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C8H18O2\CYL509\23-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2OH-M
e2CCMe2-CH2OH.freq\0,1\C, -0.2483906234, 0.4156166137, -0.6799078587\C, 0
.8926851879, 1.3649327881, -1.1088974812\O, 2.0579339748, 0.6477091458, -1.
5176064104\C, -0.6711790184, -0.409241206, -1.9161784412\C, -1.4235115655,
1.3528213862, -0.3099581722\H, 1.1324869605, 2.0530408158, -0.2854083998\H
, 0.517930626, 1.9773284306, -1.9448762103\H, 2.7107169098, 1.2967581762, -1.
.8195909353\H, -1.2170694337, 1.9484339835, 0.5836410933\H, -2.3398954625,
0.7917126469, -0.1152330337\H, -1.6235157323, 2.0416328505, -1.1408921157\H
, 0.1731899066, -0.944096063, -2.3571213313\H, -1.0793746815, 0.2579766816
, -2.6854393653\H, -1.4534352647, -1.1370679221, -1.6726746444\C, 0.1699547
525, -0.5233976651, 0.5394151059\C, -1.0588337322, -1.1594551473, 1.2315993
491\O, -1.7218102106, -0.2291223208, 2.0871741391\C, 0.980640064, 0.2491109
253, 1.602179697\C, 1.03411409, -1.7191737786, 0.0648095584\H, -1.753868245
, -1.5589089067, 0.4757168067\H, -0.7005161169, -2.0165950964, 1.8238252562
\H, -2.4368014921, -0.7045325992, 2.5358182872\H, 0.4556162366, -2.43224738
57, -0.5339263098\H, 1.8806394393, -1.3786952346, -0.5322593919\H, 1.421150
4116, -2.2627423742, 0.9355225638\H, 0.4628635412, 1.1465667711, 1.95101341
39\H, 1.1467426812, -0.3873045913, 2.4794330077\H, 1.9612746722, 0.53276171
84, 1.2075389355\\Version=IA64L-G03RevC.02\State=1-A\HF=-466.1056027\RM
SD=6.886e-09\RMSF=1.733e-05\Dipole=-0.12483, 0.077464, -0.058589\PG=C01
[X(C8H18O2)]\@

n.CH2Ph-Me2CCMe2-CH2Ph

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C20H26\CYL509\24-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2Ph-Me
2CCMe2-CH2Ph.freq\0,1\C, -0.2249026269, -0.0670053485, -0.8696151649\C, 1
.0905587626, 0.2648758395, -1.6813178337\C, 1.6344723085, 1.6774624596, -1.
8190114619\C, 1.0206906153, 2.6214210073, -2.6589111766\C, 2.8262667078, 2.
0555485139, -1.1813858503\C, 1.5504728724, 3.9021741544, -2.8186095037\C, 3
.3635646037, 3.334064616, -1.3393361918\C, 2.7222411629, 4.2677277443, -2.1
537825766\H, 3.1376731538, 5.2638843974, -2.2803994686\H, 1.0519128666, 4.6
120702369, -3.4738880616\H, 4.2879071395, 3.5963337089, -0.8308200138\H, 0.
1243476699, 2.3466294775, -3.2076120951\H, 3.3481184142, 1.3341907488, -0.5
56968965\H, 1.892778422, -0.3772800756, -1.3018775468\H, 0.8886697303, -0.0
965742911, -2.6984340594\C, -0.4517139607, -1.5748666288, -1.1403041139\C,
-1.4144410878, 0.6875473399, -1.5020329612\H, 0.3114732373, -2.2047698687,
-0.6719228659\H, -0.4169623092, -1.7677940547, -2.2193999688\H, -1.4233488
501, -1.9148525159, -0.7814729877\H, -1.3097685047, 1.7732550926, -1.438611
996\H, -2.3627136947, 0.4142531858, -1.0269318342\H, -1.5030965796, 0.42439
93177, -2.5635075107\C, -0.115046777, 0.2344245691, 0.6944030812\C, -1.3458
751514, -0.2888056033, 1.536129691\C, -1.6048393718, -1.7622389322, 1.81639
10824\C, -0.7780182237, -2.5227185527, 2.6584769667\C, -2.7627963052, -2.38
01955451, 1.3183808039\C, -1.0740418192, -3.854298322, 2.9544506343\C, -3.0
679282037, -3.709112136, 1.613950505\C, -2.2180780904, -4.4568444412, 2.429
6567604\H, -2.45066445, -5.49225034, 2.6638156913\H, -0.4125782694, -4.4181
326316, 3.6075865145\H, -3.9726244499, -4.1569919048, 1.2105383938\H, 0.101
2618766, -2.0679526635, 3.1036791874\H, -3.4404577981, -1.8060852632, 0.689
5474838\H, -2.2573354161, 0.134797649, 1.1000229789\H, -1.2430338296, 0.203
0977766, 2.5132710121\C, -0.1129531016, 1.7614711385, 0.9682624681\C, 1.194
074997, -0.3326248204, 1.2832088769\H, -1.0852019547, 2.2168145903, 0.75219

09879\H,0.1007978626,1.9461341123,2.0281510381\H,0.6426837303,2.287904
0403,0.3840986685\H,1.320303133,-1.4024236744,1.0938495047\H,2.0673645
526,0.1879980033,0.8815019228\H,1.2122504523,-0.1846973675,2.369569777
6\\Version=IA64L-G03RevC.02\State=1-A\HF=-777.7823512\RMSD=3.914e-09\R
MSF=2.905e-06\Dipole=0.0185797,0.0422435,-0.0250986\PG=C01 [X(C20H26)]
\\@

n.CH_CH2_2-Me2CCMe2-CH_CH2_2

1\1\GINC-LC47\FOpt\RB3LYP\Gen\C12H22\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH_CH2_2
-Me2CCMe2-CH_CH2_2.freq\\0,1\C,-1.9025889371,2.180566124,-0.6754300001
\C,-1.4217228862,2.6671887454,0.6683061992\C,-0.4555137506,1.979054882
7,-0.2723671809\H,-2.1063967387,2.9105556694,-1.455593046\H,-1.3057412
147,3.7354301925,0.8350983591\H,0.1859145492,2.7084790718,-0.765918255
6\C,0.3893490113,0.6946505049,0.0291667422\C,1.0160875042,0.9415119127
,1.4243200463\C,1.5262189808,0.726365432,-1.0268524113\H,2.1057294816,
1.650962848,-0.9198882173\H,1.1294041336,0.7093160232,-2.0471241678\H,
2.2294033219,-0.1020820285,-0.9253492855\H,0.251669126,1.0254246773,2.
2015032226\H,1.5665532214,1.8898673041,1.4157503386\C,1.9025889371,-2.
180566124,0.6754300001\C,1.4217228862,-2.6671887454,-0.6683061992\C,0.
4555137506,-1.9790548827,0.2723671809\H,2.5944896756,-1.3467681655,0.6
807500751\H,2.1063967387,-2.9105556694,1.455593046\H,1.3057412147,-3.7
354301925,-0.8350983591\H,-0.1859145492,-2.7084790718,0.7659182556\C,-
0.3893490113,-0.6946505049,-0.0291667422\C,-1.0160875042,-0.9415119127
, -1.4243200463\C,-1.5262189808,-0.726365432,1.0268524113\H,-2.10572948
16,-1.650962848,0.9198882173\H,-1.1294041336,-0.7093160232,2.047124167
8\H,-2.2294033219,0.1020820285,0.9253492855\H,-0.251669126,-1.02542467
73,-2.2015032226\H,-1.7094812388,-0.15454538,-1.7243426684\H,-1.566553
2214,-1.8898673041,-1.4157503386\H,-2.5944896756,1.3467681655,-0.68075
00751\H,-1.7709988155,2.1277146587,1.5438729853\H,1.7094812388,0.15454
538,1.7243426684\H,1.7709988155,-2.1277146587,-1.5438729853\\Version=I
A32L-G03RevC.02\State=1-AG\HF=-470.4367667\RMSD=6.598e-09\RMSF=1.321e-
05\Dipole=0.,0.,0.\PG=CI [X(C12H22)]\\@

n.CH2CH=CH2-Me2CCMe2-CH2CH=CH2

1\1\GINC-AC16\FOpt\RB3LYP\Gen\C12H22\CYL509\23-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH2CH=CH
2-Me2CCMe2-CH2CH=CH2.freq\\0,1\C,-0.6828135079,1.1148132176,-1.5524060
188\C,-0.4297274147,0.8037685626,-0.0308803698\H,0.2900666195,1.157938
9264,-2.0596125908\H,-1.0866480058,2.13502589,-1.5880539368\C,-1.60453
59522,0.2316207981,-2.3530792265\C,0.5132196354,1.9329840044,0.4472809
953\C,-1.766943631,0.9741458337,0.7218883662\C,-2.8468390857,0.5588612
402,-2.7173093254\H,-1.2053891585,-0.7256625499,-2.6871363986\H,-3.462
7635987,-0.105940695,-3.3174236737\H,-3.2948956846,1.50891096,-2.43188
34743\H,1.5059169915,1.8680558213,-0.0114892768\H,0.6368513764,1.92921
16281,1.5343845865\H,0.0937722482,2.9092204707,0.1768657037\H,-1.66670
63615,0.7517022192,1.7903486509\H,-2.5547310181,0.3353287699,0.3141918
407\H,-2.1119090531,2.012210271,0.6393880588\C,0.8267321344,-0.7660277
684,1.6747280073\C,0.2062243812,-0.634804594,0.2302339292\H,0.17885970
88,-0.2352035761,2.3863249963\H,0.7649372081,-1.8254080075,1.954093649
9\C,2.2576497032,-0.339556269,1.890072126\C,-0.8761505826,-1.742036738
2,0.1600575209\C,1.2964838156,-0.9725688328,-0.8087702921\C,3.23818401
31,-1.1696115358,2.2523458943\H,2.4971837296,0.7137534293,1.7609289563
\H,4.2539328932,-0.8193389572,2.4174661055\H,3.0624371268,-2.233354245
4,2.4035896609\H,-1.5540481105,-1.6994407347,1.0191967155\H,-1.4858645
918,-1.6808610125,-0.7440452278\H,-0.3958739221,-2.7279447327,0.172775
2162\H,0.8728226965,-1.1252350945,-1.8066524105\H,2.063062976,-0.19415
45595,-0.8819170591\H,1.8100848758,-1.8983417317,-0.5263097326\\Versio
n=IA64L-G03RevC.02\State=1-A\HF=-470.4706231\RMSD=8.393e-09\RMSF=2.161

e-06\Dipole=-0.0300686,0.0575787,-0.0220224\PG=C01 [X(C12H22)]\@

n.CH2CH3-Me2CCMe2-CH2CH3

1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H22\CYL509\23-Aug-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.CH2CH3-M
e2CCMe2-CH2CH3.freq\0,1\C,0.2521070737,-0.7018219402,0.1455276417\C,0
.0283049246,-0.8555635475,1.6655445433\C,1.7588316237,-0.9453663381,-0
.1311320241\C,-0.4915159609,-1.8627971233,-0.6079387775\C,-1.832216536
5,-2.3840579895,-0.0637136273\H,0.1927413109,-2.7220396976,-0.61952851
33\H,-0.6152864252,-1.5851805914,-1.6624373747\H,2.3990779743,-0.14207
69886,0.2385237252\H,1.9582511094,-1.0652809949,-1.2014519917\H,2.0768
739157,-1.8722345594,0.3617382729\H,-1.0005996359,-0.6298057882,1.9651
46837\H,0.6933534473,-0.2034528657,2.2401179386\H,0.240804867,-1.88544
80161,1.9770581089\H,-2.1905042299,-3.2010691122,-0.7017458064\H,-1.72
76531589,-2.7892593561,0.9481927549\H,-2.6170688551,-1.624550552,-0.03
59936522\C,-0.1989024611,0.745459674,-0.3618820881\C,0.3907634692,1.05
96220308,-1.7558885255\C,-1.7384747218,0.8333242585,-0.5004494732\C,0.
1763146098,1.9105560623,0.6131574613\C,1.6450303372,2.2192835231,0.939
3186909\H,-0.2518701093,2.8191282825,0.1672517627\H,-0.3677584061,1.77
08698619,1.5558356377\H,-2.1218505536,0.1603143507,-1.2727974923\H,-2.
2527456934,0.6036622413,0.4392423192\H,-2.0285907764,1.8511318301,-0.7
876826815\H,1.480456968,1.1500155649,-1.7448918882\H,0.1310735545,0.28
99080159,-2.4914988661\H,-0.0132479145,2.0099781067,-2.1259263592\H,1.
7045504415,3.1706249429,1.4818020102\H,2.2593702827,2.3231295562,0.038
1628166\H,2.1091677396,1.4598041101,1.5756195122\@Version=IA64L-G03Rev
C.02\State=1-A\HF=-394.3132525\RMSD=3.158e-09\RMSF=2.477e-06\Dipole=0.
0042219,0.0306381,0.0065226\PG=C01 [X(C10H22)]\@

n.CH_CH3_2-Me2CCMe2-CH_CH3_2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C12H26\CYL509\24-Aug-2008\0\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.CH_CH3_2
-Me2CCMe2-CH_CH3_2.freq\0,1\C,-0.4478265857,1.6284518582,1.2376399132
\H,-0.0340135715,1.8765530162,2.2227375653\H,-1.5367701194,1.635583980
6,1.3331572141\H,-0.1734358031,2.4387307317,0.5606862001\C,0.107801104
7,0.2561948176,0.7693024767\C,1.6470974061,0.3592607016,0.8878182669\C
, -0.3484090366,-0.7818661348,1.894842764\C,0.4179343165,-2.1197165287,
2.0006267102\C,-1.8553075712,-1.0755732177,2.0328803693\H,2.1680046324
, -0.5012681361,0.460251671\H,1.9383201784,0.4284791664,1.9434059892\H,
2.0262391936,1.2574745035,0.3939082257\H,-2.0351659742,-1.5881711836,2
.9860780858\H,-2.2278198195,-1.7372161044,1.2436924653\H,-2.4697088072
, -0.1704671859,2.0342747463\H,1.5024101666,-1.9941776596,1.9410086663\H,
0.1203390075,-2.8454556858,1.239829517\H,0.2009774167,-2.573414244,2
.9757186924\H,-0.0782261841,-0.2395068964,2.8134152053\C,-0.223107708,
-1.571118229,-1.054852723\H,-0.3891939571,-1.7466751652,-2.125115561\H
,0.7558289659,-1.9869251881,-0.8029517362\H,-0.9790078412,-2.148801423
6,-0.5169174605\C,-0.3384107312,-0.0600919567,-0.742419036\C,-1.829202
3273,0.3091983906,-0.9711616489\C,0.457771484,0.6888352356,-1.90761635
49\C,0.4996952399,2.2293372464,-1.8736974903\C,1.8692857487,0.17331215
21,-2.2684108818\H,-2.0132785696,1.385397849,-0.9174651668\H,-2.142451
176,-0.0242720876,-1.9680999143\H,-2.4901878323,-0.1722373367,-0.24906
98401\H,2.1496191655,0.5734042296,-3.2507831962\H,2.6376201051,0.49818
36558,-1.5625788666\H,1.9178491299,-0.9164900218,-2.3417308162\H,-0.47
95208299,2.6804643995,-1.6884187915\H,1.1978215158,2.6136035817,-1.122
4858742\H,0.8462265518,2.6004052041,-2.8462794307\H,-0.1564035835,0.43
9451989,-2.7859817822\@Version=IA64L-G03RevC.02\State=1-A\HF=-472.9204
892\RMSD=3.062e-09\RMSF=2.930e-06\Dipole=-0.0120293,0.0102643,0.001390
7\PG=C01 [X(C12H26)]\@

n.C_CH3_3-Me2CCMe2-C_CH3_3

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C14H30\CYL509\28-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.C_CH3_3-
Me2CCMe2-C_CH3_3.freq\\0,1\C,-0.1900611363,0.0695149072,3.3475065802\C
,0.4473041076,0.5915845145,2.0255287157\C,0.0769032683,2.0930879014,1.
9947570127\C,-0.0678602089,-0.3260368707,0.7549426835\H,0.3042242131,0
.5617240787,4.1930566479\H,-0.0708500499,-1.0086838786,3.4934395344\H,
-1.2560114769,0.3057272616,3.4178455363\C,1.9811143345,0.5149441923,2.
27516277\C,0.7388603045,-1.6490701793,0.879902747\C,-1.5457570191,-0.7
112791436,1.008129967\H,2.2386699309,1.2005279245,3.0917025547\H,2.587
8010632,0.8005023147,1.4152808014\H,2.3017324787,-0.4828142083,2.58736
64961\H,0.2547180018,2.5189782038,2.9900888895\H,-0.9764337919,2.26394
20639,1.7549444394\H,0.6907381563,2.6692527154,1.2978425567\H,1.754842
9461,-1.5732265442,0.4845769858\H,0.8262384496,-1.9428678729,1.9290398
07\H,-2.2193886161,0.1513358225,1.046532567\H,-1.6582818773,-1.2560603
229,1.9474316152\H,-1.9045671643,-1.3824121645,0.2284182081\C,0.190061
1363,-0.0695149072,-3.3475065802\C,-0.4473041076,-0.5915845145,-2.0255
287157\C,-0.0769032683,-2.0930879014,-1.9947570127\C,0.0678602089,0.32
60368707,-0.7549426835\H,-0.3042242131,-0.5617240787,-4.1930566479\H,0
.0708500499,1.0086838786,-3.4934395344\H,1.2560114769,-0.3057272616,-3
.4178455363\C,-1.9811143345,-0.5149441923,-2.27516277\C,-0.7388603045,
1.6490701793,-0.879902747\C,1.5457570191,0.7112791436,-1.008129967\H,-
2.2386699309,-1.2005279245,-3.0917025547\H,-2.3017324787,0.4828142083,
-2.5873664961\H,-0.2547180018,-2.5189782038,-2.9900888895\H,0.97643379
19,-2.2639420639,-1.7549444394\H,-0.6907381563,-2.6692527154,-1.297842
5567\H,-1.7548429461,1.5732265442,-0.4845769858\H,-0.8262384496,1.9428
678729,-1.929039807\H,2.2193886161,-0.1513358225,-1.046532567\H,1.6582
818773,1.2560603229,-1.9474316152\H,0.2463314795,-2.4790474027,0.37999
79788\H,-0.2463314795,2.4790474027,-0.3799979788\H,1.9045671643,1.3824
121645,-0.2284182081\H,-2.5878010632,-0.8005023147,-1.4152808014\\Vers
ion=IA64L-G03RevC.02\State=1-AG\HF=-551.5122858\RMSD=6.324e-09\RMSF=1.
112e-05\Dipole=0.,0.,0.\PG=CI [X(C14H30)]\\@
```

n.CCH-Me2CCMe2-CCH

```
1\1\GINC-IC54\FOpt\RB3LYP\Gen\C10H14\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CCH-Me2C
CMe2-CCH.freq\\0,1\C,0.369088533,-0.6720882852,0.2282290397\C,0.615707
547,-0.6797620591,1.7581291431\C,1.7370511567,-0.8253892698,-0.4837040
882\C,-0.4705006757,-1.8321196619,-0.1163342575\C,-1.1315967526,-2.808
1678309,-0.3828137922\H,-1.7123057081,-3.6713468415,-0.6167635639\H,-0
.319893036,-0.6824739432,2.3228008091\H,1.174562879,-1.5782741567,2.03
76594796\H,1.199983895,0.19891648,2.0487691609\H,1.6249667369,-0.93520
85256,-1.5652045222\H,2.365537685,0.0475900368,-0.2816241008\H,2.24940
66987,-1.7177828917,-0.1110022592\C,-0.369088533,0.6720882852,-0.22822
90397\C,-0.615707547,0.6797620591,-1.7581291431\C,-1.7370511567,0.8253
892698,0.4837040882\C,0.4705006757,1.8321196619,0.1163342575\C,1.13159
67526,2.8081678309,0.3828137922\H,1.7123057081,3.6713468415,0.61676356
39\H,0.319893036,0.6824739432,-2.3228008091\H,-1.174562879,1.578274156
7,-2.0376594796\H,-1.199983895,-0.19891648,-2.0487691609\H,-1.62496673
69,0.9352085256,1.5652045222\H,-2.365537685,-0.0475900368,0.2816241008
\H,-2.2494066987,1.7177828917,0.1110022592\\Version=IA32L-G03RevC.02\S
tate=1-AG\HF=-389.3536212\RMSD=8.111e-09\RMSF=3.065e-05\Dipole=0.,0.,0
.\PG=CI [X(C10H14)]\\@
```

n.CH=C_CH3_2-Me2CCMe2-CH=C_CH3_2

```
1\1\GINC-LC110\FOpt\RB3LYP\Gen\C14H26\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CH=C_CH
3_2-Me2CCMe2-CH=C_CH3_2.freq\\0,1\H,3.8545449043,-2.0953808987,-2.4634
858683\C,3.1066352716,-2.5474745513,-1.7963207896\C,2.4156731861,-1.48
69243012,-0.9543073551\C,3.4235940615,-0.729006531,-0.1179805093\C,1.0
```

```
775195962,-1.3735195997,-1.0620806582\C,-0.125871049,-0.5668584281,-0.
5277145539\C,-0.7443344999,0.042995544,-1.8217023254\C,-1.0429770372,-
1.6669680381,0.0869018295\H,0.6633856268,-2.0941484936,-1.7723635177\H
,2.4028326652,-3.1138643358,-2.4134153197\H,3.6514606845,-3.2612501456
,-1.161843281\H,4.176060562,-0.266454891,-0.772796716\H,3.9735589621,-
1.4302314518,0.5260275245\H,3.0159222315,0.0511463668,0.5174861197\H,-
0.4670217385,-2.3095816698,0.7598745493\H,-1.4591301276,-2.3092264931,
-0.6980911921\H,-1.8707132148,-1.2522686922,0.6634649991\H,-1.51530428
51,0.785226334,-1.6113089813\H,-1.1846669817,-0.7412188163,-2.44858059
45\H,0.0298000971,0.5370857056,-2.4168169922\H,-3.8545449043,2.0953808
987,2.4634858683\C,-3.1066352716,2.5474745513,1.7963207896\C,-2.415673
1861,1.4869243012,0.9543073551\C,-3.4235940615,0.729006531,0.117980509
3\C,-1.0775195962,1.3735195997,1.0620806582\C,-0.125871049,0.5668584281
,0.5277145539\C,-0.7443344999,-0.042995544,1.8217023254\C,1.0429770372,
1.6669680381,-0.0869018295\H,-0.6633856268,2.0941484936,1.7723635177\H
,-2.4028326652,3.1138643358,2.4134153197\H,-3.6514606845,3.2612501456,
1.161843281\H,-4.176060562,0.266454891,0.772796716\H,-3.9735589621,1.4
302314518,-0.5260275245\H,-3.0159222315,-0.0511463668,-0.5174861197\H,
0.4670217385,2.3095816698,-0.7598745493\H,1.4591301276,2.3092264931,0.
6980911921\H,1.8707132148,1.2522686922,-0.6634649991\H,1.5153042851,-0
.785226334,1.6113089813\H,1.1846669817,0.7412188163,2.4485805945\H,-0.
0298000971,-0.5370857056,2.4168169922\Version=IA32L-G03RevC.02\State=
1-AG\HF=-549.0867171\RMSD=8.778e-09\RMSF=7.457e-06\Dipole=0.,0.,0.\PG=
CI [X(C14H26)]\@
```

n.CH=CH2-Me2CCMe2-CH=CH2

```
1\1\GINC-LC106\FOpt\RB3LYP\Gen\C10H18\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.CH=CH2-
Me2CCMe2-CH=CH2.freq\0,1\H,2.8485793714,0.6147720038,0.239081722\C,2.
6629910724,-0.1987011556,0.9306773265\H,3.5290479282,-0.5442091097,1.4
90143907\C,1.4753369718,-0.7764461712,1.1247909733\C,0.0727709548,-0.5
714841272,0.5428318954\H,1.4606522156,-1.585218138,1.8600108883\C,-0.3
024689916,-1.9611896141,-0.0468357323\C,-0.8180960901,-0.2860079965,1.
7856763585\H,0.4162527888,-2.2735433636,-0.8102937009\H,-1.2955010912,
-1.9706715752,-0.4989198315\H,-0.286234641,-2.7200015486,0.7442172688\
H,-0.4675198497,0.5966485893,2.3288120782\H,-0.7741389403,-1.133230864
6,2.4800247382\H,-1.8645355779,-0.122995686,1.5229941025\H,-2.84857937
14,-0.6147720038,-0.239081722\C,-2.6629910724,0.1987011556,-0.93067732
65\H,-3.5290479282,0.5442091097,-1.490143907\C,-1.4753369718,0.7764461
712,-1.1247909733\C,-0.0727709548,0.5714841272,-0.5428318954\H,-1.4606
522156,1.585218138,-1.8600108883\C,0.3024689916,1.9611896141,0.0468357
323\C,0.8180960901,0.2860079965,-1.7856763585\H,-0.4162527888,2.273543
3636,0.8102937009\H,1.2955010912,1.9706715752,0.4989198315\H,0.2862346
41,2.7200015486,-0.7442172688\H,0.4675198497,-0.5966485893,-2.32881207
82\H,0.7741389403,1.1332308646,-2.4800247382\H,1.8645355779,0.12299568
6,-1.5229941025\Version=IA32L-G03RevC.02\State=1-AG\HF=-391.839859\RM
SD=4.324e-09\RMSF=9.765e-06\Dipole=0.,0.,0.\PG=CI [X(C10H18)]\@
```

n.CH=CHCH3-Me2CCMe2-CH=CHCH3

```
1\1\GINC-LC108\FOpt\RB3LYP\Gen\C12H22\CYL509\26-Jun-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.CH=CHCH
3-Me2CCMe2-CH=CHCH3.freq\0,1\H,2.8724852074,0.0002919417,-0.182566686
8\C,2.6948333519,0.0001595888,0.8893795044\C,3.9390488054,0.0001934463
,1.7369145575\C,1.4562302647,-0.0000202304,1.3922119048\C,0.0454092323
,-0.0000969577,0.7908202934\H,1.3973291197,-0.0001465607,2.484949028\C
,-0.625716616,-1.2679876955,1.3925646647\C,-0.6259982312,1.2674900903,
1.3928896834\H,-0.0692653965,-2.1719131156,1.127490983\H,-1.6559504535
,-1.3994593477,1.0574493363\H,-0.6348257267,-1.2021134325,2.486905139\
H,-0.06974249,2.1716059102,1.1280556285\H,-0.6351019472,1.2013292353,2
```

```
.4872129249\H,-1.6562581763,1.3988224979,1.0577991051\H,3.6988503782,0
.0000537163,2.8057554111\H,4.563310432,-0.8800798203,1.53027821\H,4.56
31329669,0.880637184,1.530468526\H,-2.8724852074,-0.0002919417,0.18256
66868\C,-2.6948333519,-0.0001595888,-0.8893795044\C,-3.9390488054,-0.0
001934463,-1.7369145575\C,-1.4562302647,0.0000202304,-1.3922119048\C,-
0.0454092323,0.0000969577,-0.7908202934\H,-1.3973291197,0.0001465607,-
2.484949028\C,0.625716616,1.2679876955,-1.3925646647\C,0.6259982312,-1
.2674900903,-1.3928896834\H,0.0692653965,2.1719131156,-1.127490983\H,1
.6559504535,1.3994593477,-1.0574493363\H,0.6348257267,1.2021134325,-2.
486905139\H,0.06974249,-2.1716059102,-1.1280556285\H,0.6351019472,-1.2
013292353,-2.4872129249\H,1.6562581763,-1.3988224979,-1.0577991051\H,-
3.6988503782,-0.0000537163,-2.8057554111\H,-4.563310432,0.8800798203,-
1.53027821\H,-4.5631329669,-0.880637184,-1.530468526\Version=IA32L-G0
3RevC.02\State=1-AG\HF=-470.4773669\RMSD=2.481e-09\RMSF=1.331e-06\Dipo
le=0.,0.,0.\PG=CI [X(C12H22)]\@
```

n.CHO-Me2CCMe2-CHO

```
1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H14O2\CYL509\24-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.CHO-Me2
CCMe2-CHO.freq\|0,1\O,0.2846961465,1.6344413348,-2.233472531\C,0.60653
82776,1.47681425,-1.0759503879\H,1.5971981604,1.8351461619,-0.71747104
82\C,-0.2624598049,0.7986444264,-0.0119564933\C,-1.7432738319,0.988215
39,-0.3974018149\C,0.0185387191,1.499534212,1.3356685986\H,-1.93953127
77,0.6561140766,-1.4180321498\H,-2.0007497547,2.0518859552,-0.34816822
44\H,-2.4138396992,0.4570671021,0.2849706259\H,1.0664254226,1.41550150
87,1.6400438188\H,-0.5941910853,1.0791485561,2.1395955584\H,-0.2221776
371,2.5667214183,1.2642947441\O,0.1052413245,-1.8701200498,2.188245239
1\C,-0.4869076581,-1.3856697148,1.2494539818\H,-1.5989709746,-1.409544
6817,1.2193760784\C,0.1771553253,-0.7410988692,0.0326163444\C,1.704167
1988,-0.9172981009,0.1416343848\C,-0.3340120141,-1.5053632093,-1.21199
50097\H,2.1314319675,-0.3692643765,0.9850889163\H,1.9400100662,-1.9734
90769,0.2990835337\H,2.206148222,-0.5949707298,-0.7766308531\H,-1.4248
253912,-1.5966391005,-1.224366703\H,-0.0298875341,-0.9973698356,-2.132
3573509\H,0.0849824751,-2.5175458711,-1.2260262335\Version=IA64L-G03R
evC.02\State=1-A\HF=-463.704585\RMSD=8.111e-09\RMSF=3.010e-06\Dipole=-
0.2046686,0.2047122,0.0786602\PG=C01 [X(C8H14O2)]\@
```

n.CN-Me2CCMe2-CN

```
1\1\GINC-LC118\FOpt\RB3LYP\Gen\C8H12N2\CYL509\26-Jun-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|n.CN-Me2
CCMe2-CN.freq\|0,1\N,-0.954114979,-0.4203520631,-2.7930862632\C,-0.869
1658,-0.2367498093,-1.649432073\C,-0.7735866583,-0.0029942363,-0.19476
13607\C,-1.544862323,-1.1329168582,0.5317343742\C,-1.4523876306,1.3518
066759,0.1264089089\H,-1.449437366,-1.0085853276,1.6149510349\H,-2.606
0150054,-1.0823561363,0.2714706366\H,-1.180521248,-2.1252060383,0.2567
932928\H,-1.0200047527,2.176487319,-0.4444999268\H,-2.517298032,1.2984
260019,-0.1174130779\H,-1.3539391758,1.5708519924,1.1942310274\N,0.954
114979,0.4203520631,2.7930862632\C,0.8691658,0.2367498093,1.649432073\
C,0.7735866583,0.0029942363,0.1947613607\C,1.544862323,1.1329168582,-0
.5317343742\C,1.4523876306,-1.3518066759,-0.1264089089\H,1.449437366,1
.0085853276,-1.6149510349\H,2.6060150054,1.0823561363,-0.2714706366\H,
1.180521248,2.1252060383,-0.2567932928\H,1.0200047527,-2.176487319,0.4
444999268\H,2.517298032,-1.2984260019,0.1174130779\H,1.3539391758,-1.5
708519924,-1.1942310274\Version=IA32L-G03RevC.02\State=1-AG\HF=-421.5
55775\RMSD=2.221e-09\RMSF=9.459e-06\Dipole=0.,0.,0.\PG=CI [X(C8H12N2)]
\@
```

n.COCH3-Me2CCMe2-COCH3

```
1\1\GINC-AC25\FOpt\RB3LYP\Gen\C10H18O2\CYL509\29-Aug-2008\0\#B3LYP/GE
```

```
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COCH3-  
Me2CCMe2-COCH3.freq\\0,1\\C,-1.9705857617,-1.0303736612,-2.1000907205\\C  
, -1.7783221686,-0.3637054895,-0.7448996465\\C,-0.4907811432,-0.63104109  
65,0.0852232222\\O,-2.6574968335,0.3527226722,-0.2996995119\\H,-2.130269  
2126,-2.1075620236,-1.9666546217\\H,-1.1000498038,-0.9201638184,-2.7535  
454541\\H,-2.8533064611,-0.5997943795,-2.5771037658\\C,0.1043211809,-2.0  
134228673,-0.2590578001\\C,-0.9216940145,-0.6598990488,1.571217147\\H,-0  
.0773117633,-0.9215297518,2.2173206624\\H,-1.6940052562,-1.4222559245,1  
.7187555012\\H,-1.3467614913,0.2906055171,1.8983291198\\H,1.0214562247,-  
2.1885173199,0.3073896566\\H,0.3478433916,-2.1231927217,-1.3183964866\\H  
, -0.6116352636,-2.8021411642,0.0013678929\\C,1.7435273695,1.3717149805,  
2.0679402276\\C,1.6941641716,0.4247950332,0.8779337311\\C,0.5632153901,0  
.5601963041,-0.1831110784\\O,2.5587411326,-0.4247926511,0.7486016722\\H,  
2.0273454479,2.3781722823,1.7365195041\\H,0.7747778049,1.4627443777,2.5  
675777366\\H,2.4959695591,1.0085163041,2.7708862093\\C,-0.1076715242,1.9  
495812279,-0.1071438307\\C,1.2451669305,0.441008246,-1.5655554432\\H,0.5  
124263745,0.4815677362,-2.377322057\\H,1.9315145448,1.2835410756,-1.710  
4893703\\H,1.8319844776,-0.4739904206,-1.6526599682\\H,-0.7943404409,2.0  
956081791,-0.9447714105\\H,-0.6851622622,2.1046762902,0.8068767781\\H,0.  
6515271549,2.7371538238,-0.1700320606\\Version=IA64L-G03RevC.02\\State=  
1-A\\HF=-542.3452703\\RMSD=4.725e-09\\RMSF=2.622e-06\\Dipole=0.0345357,0.0  
998307,-0.2372009\\PG=C01 [X(C10H18O2)]\\@
```

n.CON_CH2CH3_2-Me2CCMe2-CON_CH2CH3_2

```
1\\1\\GINC-AC29\\FOpt\\RB3LYP\\Gen\\C16H32N2O2\\CYL509\\28-Aug-2008\\0\\#B3LYP/  
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CON_  
CH2CH3_2-Me2CCMe2-CON_CH2CH3_2.freq\\0,1\\H,0.068195147,3.2356558942,-4  
.0330083766\\C,-0.5298279778,2.7924025465,-3.2279930331\\C,0.0235251606,  
3.2299271837,-1.8680107959\\N,-0.7894122165,2.8113927834,-0.7156255359\\  
C,-1.8888166924,3.7480639351,-0.4049939358\\C,-1.4740672344,4.890439183  
1,0.5262098867\\C,-0.5616497749,1.838025312,0.2392935788\\O,-1.236302169  
3,1.8751872152,1.2729219466\\C,0.4304627135,0.626351049,0.1039753322\\C,  
1.1114676118,0.5222741893,1.4915896283\\C,1.5871006242,0.7659282999,-0.  
9101994959\\H,0.0672311444,4.3259513081,-1.8355781473\\H,1.0475843595,2.  
8925505864,-1.7503316026\\H,-2.7007661558,3.178847471,0.0491866666\\H,-2  
.248467937,4.1466603667,-1.3600687788\\H,-0.5037545339,1.7054047812,-3.  
3408891884\\H,-1.5667195263,3.1202924032,-3.3616308667\\H,-1.1648407586,  
4.4894478518,1.4942828208\\H,-2.3175498139,5.5724674958,0.6858527986\\H,  
-0.6470531632,5.4753972021,0.1059461473\\H,1.7049814223,1.4246630558,1.  
6798361186\\H,1.7967450641,-0.3306983421,1.5197918414\\H,0.3859840281,0.  
4436529948,2.3007798628\\H,1.2666174191,0.8261416499,-1.9504928261\\H,2.  
2409068142,-0.1053498435,-0.8414186604\\H,2.1948385121,1.6458253031,-0.  
6719725719\\H,-0.9091980184,-3.6268219022,3.6583794354\\C,-0.7447304904,  
-3.7285337088,2.5792775377\\C,0.3427487783,-2.7465114346,2.1279325231\\N  
,0.692561381,-2.8440814138,0.7063842623\\C,1.5609362455,-3.9896606855,0  
.3741541067\\C,3.0551519334,-3.6692782802,0.4710234299\\C,0.4881716041,-  
1.9390883059,-0.3167793077\\O,1.0481606148,-2.1487717651,-1.3967140778\\  
C,-0.4580859134,-0.6847295341,-0.2209821375\\C,-1.0862282168,-0.5650057  
3,-1.6342167213\\C,-1.6650496074,-0.8769984885,0.7309935837\\H,1.2596743  
924,-2.9356923761,2.703056395\\H,0.0500242722,-1.7294422272,2.363806852  
9\\H,1.3175494432,-4.3154495643,-0.6381617927\\H,1.3042033049,-4.8018849  
701,1.0617073012\\H,-1.6929500461,-3.5356853543,2.0699961733\\H,-0.46127  
61853,-4.7681176905,2.3837928807\\H,3.3231329594,-2.9022628562,-0.25973  
12375\\H,3.6483782214,-4.567257262,0.2615400328\\H,3.3281314086,-3.31478  
10055,1.4722909697\\H,-0.335464397,-0.5524161604,-2.422646586\\H,-1.7037  
1834,0.335907382,-1.6941562701\\H,-1.7359833305,-1.4270261273,-1.822485  
8791\\H,-2.0546966404,-1.8944070101,0.6195124048\\H,-2.4655661212,-0.186  
8941576,0.457113203\\H,-1.4597372443,-0.6888152715,1.7830817656\\Versio  
n=IA64L-G03RevC.02\\State=1-A\\HF=-888.9323297\\RMSD=4.823e-09\\RMSF=5.780
```

e-06\Dipole=0.152156,0.230946,0.1208006\PG=C01 [X(C16H32N2O2)]\@

n.CON_CH3_2-Me2CCMe2-CON_CH3_2

1\1\GINC-AC24\FOpt\RB3LYP\Gen\C12H24N2O2\CYL509\28-Aug-2008\0\#\B3LYP/
GEN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CON_
CH3_2-Me2CCMe2-CON_CH3_2.freq\0,1\C,-0.1408616373,0.4542855004,0.6452
827372\C,-1.6094577696,1.0018088142,0.5692651775\N,-2.6471123685,0.500
6257561,1.3278134125\O,-1.8208577473,1.9773540104,-0.1538106128\C,0.22
75058089,-0.2583509736,1.9726283038\C,0.739212703,1.7328181599,0.62846
81484\C,-2.7534430102,-0.7798907886,2.0150898863\C,-3.9044875639,1.246
0728065,1.2972091822\H,-3.6933747036,-1.2638621916,1.720319359\H,-1.94
54289364,-1.4507878574,1.75020765\H,-2.7673924179,-0.6499482541,3.1058
426203\H,-4.5980441046,0.8329286022,0.5513499398\H,-4.3779382361,1.183
7598769,2.2834640722\H,-3.704467427,2.2853643101,1.0438271807\H,3.6933
367413,1.2638513802,-1.7198947073\H,0.5578818416,2.3149355212,1.539119
3716\H,0.5145861586,2.384205559,-0.2151345713\H,1.3081885367,-0.207711
4441,2.1270299492\H,-0.0255789924,-1.316237713,2.0108232518\H,-0.25163
81894,0.2507087304,2.8163360165\C,0.1408640437,-0.454232951,-0.6451798
542\C,1.6094886158,-1.0016386755,-0.5692322881\N,2.646922476,-0.500823
4715,-1.3283001676\O,1.8211549338,-1.9769598738,0.1540694529\C,-0.2275
696654,0.2583998939,-1.972503563\C,-0.7390818723,-1.73285421,-0.628362
5052\C,2.7535133186,0.7799380905,-2.015110654\C,3.904195195,-1.2464615
439,-1.2974266182\H,2.767766907,0.6503426937,-3.1058949002\H,1.9453997
874,1.4507292587,-1.7502540984\H,4.5966039204,-0.8353399202,-0.5493889
965\H,4.3791647504,-1.1817367191,-2.282768685\H,3.703763775,-2.2863977
207,-1.0469596238\H,-0.5576607176,-2.3149678178,-1.5389994707\H,-0.514
3939832,-2.3841953245,0.2152628985\H,-1.3082549939,0.2077139,-2.126885
7045\H,0.0254721735,1.3162990112,-2.0106859434\H,0.2515890287,-0.25062
94662,-2.8162190986\H,-1.7993549452,-1.4606297209,-0.6212954279\H,1.79
94567858,1.4604714834,0.621367767\#Version=IA64L-G03RevC.02\State=1-A\
HF=-731.6735952\RMSD=3.488e-09\RMSF=1.595e-06\Dipole=-0.0000446,-0.000
1033,-0.0001377\PG=C01 [X(C12H24N2O2)]\@

n.CONH2-Me2CCMe2-CONH2

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H16N2O2\CYL509\28-Aug-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\#n.CONH2
-Me2CCMe2-CONH2.freq\0,1\C,-0.1597399704,0.1355866669,-0.7836085726\C
,-1.6191433797,0.656046461,-0.8613391812\N,-1.8052574647,1.9970816285,
-1.0607425341\O,-2.5826858427,-0.0916755251,-0.73326157\C,-0.062358575
7,-1.0220805526,-1.8044089023\C,0.872581849,1.2115303707,-1.1900167339
\H,-1.058149556,2.62802677,-1.3001282426\H,-2.7577502161,2.3097172541,
-1.1902268609\H,1.8710336625,0.7699869018,-1.2451605193\H,0.9243878907
,2.0511820456,-0.4869161803\H,0.646690809,1.6066203539,-2.1876150563\H
,0.8979481025,-1.5319762057,-1.7068331896\H,-0.1495483377,-0.623597467
6,-2.8228126361\H,-0.8710320307,-1.7400249271,-1.6603079292\C,0.108056
5634,-0.3561588656,0.7206792045\C,1.6319420411,-0.6014168271,0.8768809
278\N,2.3296393437,0.2410026686,1.6992691869\O,2.2090906533,-1.5028144
693,0.2783093096\C,-0.4285412399,0.6835342081,1.7304394452\C,-0.577432
947,-1.7084872746,1.0256746252\H,1.8867402379,0.9084472923,2.309125862
8\H,3.3037932299,0.0208159642,1.8551271568\H,-1.6437687313,-1.65105925
27,0.7991083054\H,-0.1260890324,-2.5154516477,0.4466596093\H,-0.454060
0531,-1.9527581741,2.0880528626\H,-1.5191092077,0.7318740543,1.6735975
85\H,-0.1787200052,0.3900173286,2.7569684037\H,-0.0464644449,1.6961844
648,1.5554874659\#Version=IA64L-G03RevC.02\State=1-A\HF=-574.4654918\R
MSD=4.925e-09\RMSF=3.235e-06\Dipole=0.4559183,1.9457957,0.5551994\PG=C
01 [X(C8H16N2O2)]\@

n.CONHCH3-Me2CCMe2-CONHCH3

1\1\GINC-AC26\FOpt\RB3LYP\Gen\C10H20N2O2\CYL509\30-Aug-2008\0\#\B3LYP/

```
GEN 6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.CONH
CH3-Me2CCMe2-CONHCH3.freq\\0,1\\H,-4.2541682083,-0.715255201,-1.6122261
406\\C,-3.3876756869,-0.8502018321,-2.2712315023\\N,-2.1634603436,-1.007
381372,-1.5055308632\\C,-1.1197489813,-0.1294671923,-1.601689894\\C,0.14
20880482,-0.4219296892,-0.7442916974\\O,-1.1754629031,0.8527649731,-2.3
39429372\\C,1.3327348047,-0.4379034548,-1.7315084231\\C,0.0909498888,-1.
8029774395,-0.0518814006\\H,-2.0792208172,-1.8083041382,-0.9005540734\\H
,-3.2706152871,0.0370476417,-2.8942826508\\H,-3.5662684245,-1.721223452
7,-2.9129576984\\H,2.2757085691,-0.4975866872,-1.1849452801\\H,1.3319762
38,0.4545622288,-2.3588398301\\H,1.2503076495,-1.309160032,-2.393200733
2\\H,1.0534059759,-2.01661982,0.420403309\\H,-0.0855291314,-2.5992557712
,-0.7843973692\\H,-0.677481654,-1.8725418254,0.7281970322\\H,1.817787142
5,0.3770736676,4.5517827493\\C,1.8396802092,-0.3400375969,3.7225358256\\
N,0.9275290889,0.0568814732,2.6641657495\\C,1.3484345763,0.3053109593,1
.3872797541\\C,0.2753484126,0.7429435692,0.3529422734\\O,2.530526321,0.1
891496642,1.0689923399\\C,-1.1002074083,1.0271743727,0.998234886\\C,0.78
82582018,2.0685635742,-0.2570841467\\H,-0.0462407869,0.1743388385,2.893
3977154\\H,2.8428206072,-0.3651516287,3.2957013781\\H,1.5890581483,-1.33
48017791,4.1110560974\\H,-1.7749073745,1.4620599309,0.2561655424\\H,-1.5
894644928,0.1298510168,1.3973455208\\H,-1.0061701268,1.7600411035,1.808
0805458\\H,0.1566958827,2.3676858827,-1.0956209777\\H,0.7639808119,2.857
7548521,0.504695776\\H,1.8201643275,1.9688157427,-0.5965829103\\Version
=IA64L-G03RevC.02\\State=1-A\\HF=-653.0869953\\RMSD=3.091e-09\\RMSF=3.094e
-06\\Dipole=-1.3738812,-1.0560329,1.2882341\\PG=C01 [X(C10H20N2O2)]\\@
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n.COOC_CH3_3-Me2CCMe2-COOC_CH3_3

```
1\\1\\GINC-AC24\\FOpt\\RB3LYP\\Gen\\C16H30O4\\CYL509\\27-Aug-2008\\0\\#B3LYP/GE
N 6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\n.COOC_C
H3_3-Me2CCMe2-COOC_CH3_3.freq\\0,1\\H,-2.5331002822,-2.9505197704,-4.49
12024563\\C,-2.3513342067,-2.5467000609,-3.4887937164\\C,-0.8758361047,-
2.1541776446,-3.3570919532\\C,-0.4896355049,-1.0175775199,-4.3092320165
\\O,-0.580685135,-1.7748271831,-1.9590949922\\C,-1.1979203605,-0.7372342
621,-1.3550853106\\O,-2.0029568646,-0.0088116774,-1.8999241693\\C,-0.773
513336,-0.588193129,0.1238462886\\C,0.0279018758,-3.3713835241,-3.56975
99977\\C,-1.8051548814,0.3454147628,0.7935682851\\C,-0.8440974487,-1.966
681722,0.8188739395\\H,-0.1048925926,-3.765329758,-4.5829621167\\H,-0.21
56827737,-4.1640728392,-2.8550857451\\H,1.0811399826,-3.1016729704,-3.4
398479481\\H,-3.0056887327,-1.687783835,-3.3335276773\\H,-2.6048606202,-
3.3238994527,-2.7594643209\\H,-0.6043927318,-1.3557849086,-5.3454307668
\\H,0.5585716512,-0.7342640007,-4.1620624471\\H,-1.1195949382,-0.1405349
048,-4.154940498\\H,-1.6344848491,0.3818921727,1.873741586\\H,-2.8168955
604,-0.034461895,0.6257833043\\H,-1.7697834726,1.3616731639,0.396072045
\\H,-0.5139606207,-1.8806756465,1.8569311669\\H,-0.2281860982,-2.7135987
597,0.3162774193\\H,-1.8790358634,-2.3290486055,0.814920967\\H,2.6962032
563,2.9512316173,4.3952081848\\C,2.4966842607,2.3254981113,3.5179521909
\\C,1.0791624217,2.6016942368,3.0061745686\\C,0.0051285516,2.2024614053,
4.0232348097\\O,0.8615147356,1.8934453499,1.7266791312\\C,0.9186723973,0
.5529536342,1.6320151279\\O,1.1251126396,-0.195367298,2.5695541479\\C,0
.6974179116,0.0529568329,0.1856224399\\C,0.9237118721,4.0695543093,2.600
7613253\\C,1.8119598954,-0.9845583417,-0.0818929794\\C,0.8410321474,1.19
90448934,-0.8376491211\\H,1.0663339047,4.7174798124,3.4720895835\\H,1.66
35289299,4.3420004247,1.84116692\\H,-0.0745006359,4.2542031859,2.190931
3376\\H,2.6194137623,1.2785951634,3.7993070411\\H,3.2352286516,2.5761573
589,2.7484689936\\H,0.1041980506,2.8253381049,4.919541163\\H,-0.99480636
53,2.3661176121,3.607066125\\H,0.1028756492,1.1550886537,4.3122256049\\H
,1.6577024992,-1.4742414017,-1.045560777\\H,2.7851483695,-0.4797856617,
-0.105507145\\H,1.8512179482,-1.7419752291,0.7023038577\\H,0.8352221787,
0.79524461,-1.8552487824\\H,0.0420409654,1.9390025515,-0.7614627822\\H,1
.7920803879,1.7196797872,-0.6927080614\\Version=IA64L-G03RevC.02\\State
```

=1-A\HF=-928.7179424\RMSD=4.294e-09\RMSF=2.699e-06\Dipole=0.3274736,0.1109795,-0.2602727\PG=C01 [X(C16H30O4)]\@

n.COOCH2CH3-Me2CCMe2-COOCH2CH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C12H22O4\CYL509\26-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.COOCH2
CH3-Me2CCMe2-COOCH2CH3.freq\0,1\C,-0.0133632658,-0.0079325062,-0.9491
90559\C,1.420081085,-0.4976004411,-1.2262256618\O,1.7310735101,-1.6537
56058,-1.4212359727\O,2.3257473874,0.5093270467,-1.2403057446\C,3.6949
634009,0.1234645846,-1.507225\C,4.5337547719,1.3875129829,-1.513554428
2\C,-0.3322733896,1.1920124138,-1.8694636933\C,-0.9639598213,-1.168829
3575,-1.3139069575\H,4.0190698153,-0.5834142771,-0.7365626744\H,3.7301
014244,-0.3992542663,-2.4681014846\H,4.186746643,2.0837408398,-2.28376
71095\H,5.5797822776,1.1371013852,-1.7216291085\H,4.4887212936,1.89520
76282,-0.5445325969\H,-0.7685705019,-1.5034880702,-2.3365236497\H,-2.0
049511124,-0.8344206812,-1.2627674755\H,-0.8384910065,-2.0335349671,-0
.6591749031\H,0.3892692309,2.0023667912,-1.7554133294\H,-1.3308479794,
1.5776526146,-1.6492141647\H,-0.3107814446,0.8695770499,-2.9171208357\
C,-0.1404834432,0.3676346561,0.6074099961\C,-1.6453336665,0.4446242217
,0.9258504215\O,-2.3702230203,1.360699579,0.5898879616\O,-2.0961957483
, -0.6214579761,1.6194010091\C,-3.5089076856,-0.6231005344,1.9334151771
\C,-3.797550403,-1.8838349035,2.7261528805\C,0.5672434738,-0.684683746
1,1.4870827975\C,0.4447607498,1.7597106408,0.9368113081\H,-4.076445846
5,-0.5847056326,0.9979433855\H,-3.7441165779,0.2843601812,2.4983057581
\H,-3.2167872855,-1.90473165,3.6539086096\H,-4.861366235,-1.9242476485
,2.9845660211\H,-3.5500584171,-2.7776820134,2.1446840197\H,0.404296413
1,1.927237061,2.0196051878\H,1.4879010763,1.8232678318,0.6202298493\H,
-0.1247153149,2.5574286975,0.4575405425\H,0.2610000988,-1.7067858232,1
.2558949647\H,1.6517800693,-0.6151383464,1.3530999444\H,0.3516555095,-
0.5029055044,2.5441133361\@Version=IA64L-G03RevC.02\State=1-A\HF=-771.
4559024\RMSD=5.543e-09\RMSF=3.231e-06\Dipole=0.2568086,0.0465037,0.368
2191\PG=C01 [X(C12H22O4)]\@

n.COOCH3-Me2CCMe2-COOCH3

1\1\GINC-AC23\FOpt\RB3LYP\Gen\C10H18O4\CYL509\27-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\@n.COOCH3
-Me2CCMe2-COOCH3.freq\0,1\C,-0.1197949642,-0.848771644,0.0293475261\C
, -0.138171889,-1.1759088419,1.5330577039\O,0.8123790987,-1.5772969847,
2.1696408562\O,-1.3541332235,-0.9765234433,2.0981502808\C,-1.435359003
5,-1.2735054596,3.5024492975\H,-2.4679015341,-1.0661808403,3.785106686
7\C,-1.3111255494,-1.5514533478,-0.660714127\C,1.1900165636,-1.4328941
496,-0.5426210028\H,-1.1883019097,-2.3221636617,3.6865924469\H,-0.7458
820206,-0.6432339433,4.0704007331\H,2.0779816778,-0.9383992039,-0.1436
211354\H,1.1969742865,-1.3460667101,-1.6337004053\H,1.2667096738,-2.49
40179786,-0.2897813402\H,-1.1978206588,-2.6385852936,-0.5759104367\H,-
1.335931561,-1.2906179566,-1.7217263638\H,-2.2672935758,-1.2798510056,
-0.210849614\C,-0.1634086213,0.7463816681,-0.1543359856\C,0.2685923529
,1.0390286603,-1.6023965858\O,-0.4288266684,0.851426372,-2.5793848124\
O,1.5241797112,1.5287100664,-1.6930511555\C,1.9851946289,1.8003879674,
-3.0271208035\H,2.9942302869,2.1970571585,-2.9114705685\C,0.76665763,1
.4428992592,0.8615960197\C,-1.5868996762,1.3288287748,-0.0003534491\H,
1.3358101728,2.5310437705,-3.5160672612\H,1.9975816349,0.8837477565,-3
.6228800517\H,-2.2495438159,0.9833308097,-0.7952943228\H,-2.0126453923
,1.0537795376,0.9668501205\H,-1.5428969205,2.4228718363,-0.0567899238\
H,0.8435212494,2.5106443463,0.6363629366\H,0.3550794232,1.3462365392,1
.8716775461\H,1.7773288094,1.0299194355,0.8648080406\@Version=IA64L-G0
3RevC.02\State=1-A\HF=-692.8178796\RMSD=4.764e-09\RMSF=1.790e-06\Dipol
e=-0.0605048,0.3500923,0.2100893\PG=C01 [X(C10H18O4)]\@

n.COOH-Me2CCMe2-COOH

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1\1\GINC-AC23\FOpt\RB3LYP\Gen\C8H14O4\CYL509\27-Aug-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.COOH-Me
2CCMe2-COOH.freq\ \0,1\C,-0.3896823365,0.6936344997,-0.1304049247\C,-0.
4342221089,1.4176327705,1.2235372558\O,0.4736708483,2.0737892759,1.691
5079944\O,-1.6059138102,1.262197474,1.8873157442\C,0.1995151936,1.7025
736236,-1.1426993157\C,-1.8055713354,0.2931387317,-0.5966467595\H,-1.5
007552331,1.7544920991,2.7241107292\H,1.1366130977,2.130643823,-0.7836
30733\H,-0.5074054933,2.5274538358,-1.2894938508\H,0.3699224446,1.2239
548262,-2.1092384307\H,-1.7666988023,-0.0867412953,-1.6226276999\H,-2.
4676285255,1.1639265563,-0.5910346718\H,-2.2591929808,-0.4735866788,0.
0347673118\C,0.5372351681,-0.6031485205,0.0716049826\C,0.298901754,-1.
5623466606,-1.1029634227\O,-0.2997446677,-2.6138052658,-1.043076812\O,
0.842890258,-1.1287242932,-2.2722413724\C,0.1561925729,-1.3617435647,1.
3609083589\C,2.040100756,-0.246108383,0.1359469718\H,0.6253246225,-1.
815470744,-2.9312246852\H,-0.9090360032,-1.5968817511,1.4085419247\H,0.
7016335867,-2.3081002609,1.4105800872\H,0.4266339114,-0.7709540209,2.
2413899974\H,2.2180159499,0.4757348109,0.9369402621\H,2.6248126413,-1.
1482979676,0.3494035028\H,2.4057217735,0.1743742615,-0.8022270573\ \Ver
sion=IA64L-G03RevC.02\State=1-A\HF=-614.2044763\RMSD=5.499e-09\RMSF=5.
636e-06\Dipole=-0.1639508,0.1799646,-0.2414586\PG=C01 [X(C8H14O4)]\ \@
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n.COPh-Me2CCMe2-COPh

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1\1\GINC-AC23\FOpt\RB3LYP\Gen\C20H22O2\CYL509\27-Aug-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\ \n.COPh-M
e2CCMe2-COPh.freq\ \0,1\C,-4.5520591091,-1.5438914832,0.6565949648\C,-5.
632934863,-0.8708888206,0.086455589\C,-5.4262606297,0.3552532598,-0.5
506549447\C,-4.1478743941,0.9013442166,-0.6109852524\C,-3.0445785193,0.
2211801442,-0.0637670799\C,-3.2660140669,-1.0094058267,0.5735264227\C
,-1.717404044,0.9351117309,-0.1597484102\O,-1.7385684663,2.1590474967,
-0.1502737085\C,-0.3429462725,0.2201527558,-0.3771199688\C,-0.48000574
05,-1.2645683029,-0.7869643823\C,0.291837537,0.9558042015,-1.586831402
3\H,-2.4467582822,-1.5441638097,1.0353966009\H,-3.9797640426,1.8647294
052,-1.0805283624\H,-6.263268163,0.8888487303,-0.9928369177\H,-4.70658
64459,-2.4896678768,1.168724501\H,-6.6313268218,-1.2965393294,0.142124
9843\H,1.3178301313,0.6182763213,-1.7547836553\H,0.2848974935,2.037476
3453,-1.4535757199\H,-0.2834800301,0.7300363556,-2.4928128145\H,0.4390
083048,-1.5974198955,-1.2799730478\H,-1.2961828384,-1.3905514772,-1.50
48937213\H,-0.6511669129,-1.9420571462,0.0505505146\C,4.9634924955,0.9
564922609,-0.5945926081\C,5.4151034991,-0.110042373,-1.371078502\C,4.6
77030526,-1.2955625067,-1.4104659228\C,3.4990940186,-1.4068910212,-0.6
778282735\C,3.0096169045,-0.3247932759,0.0775738551\C,3.7666447568,0.8
56921819,0.1176884378\C,1.7454144614,-0.5940476103,0.8650586748\O,1.64
80059863,-1.6977850151,1.3830510446\C,0.537230971,0.3885396582,0.96576
05908\C,0.960380341,1.8554930458,1.1938153766\C,-0.2765462088,-0.04239
16422,2.2075872913\H,3.4546573508,1.6925185398,0.7294487066\H,2.939924
6589,-2.3368400701,-0.6754617046\H,5.0261431855,-2.1372899774,-2.00246
73277\H,5.5438575803,1.8733789955,-0.5373225514\H,6.3404134488,-0.0226
7194,-1.9341526734\H,-1.1528559412,0.600710598,2.3358456953\H,-0.59659
88389,-1.0835671291,2.1570387029\H,0.3403796655,0.0531774514,3.1072968
031\H,0.076109744,2.4731347033,1.3629246453\H,1.597072772,1.9276971617
,2.08389778\H,1.4968638422,2.2878228106,0.3491941375\ \Version=IA64L-G0
3RevC.02\State=1-A\HF=-925.808014\RMSD=4.463e-09\RMSF=2.830e-06\Dipole
=0.0234829,-0.140303,-0.5541983\PG=C01 [X(C20H22O2)]\ \@
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