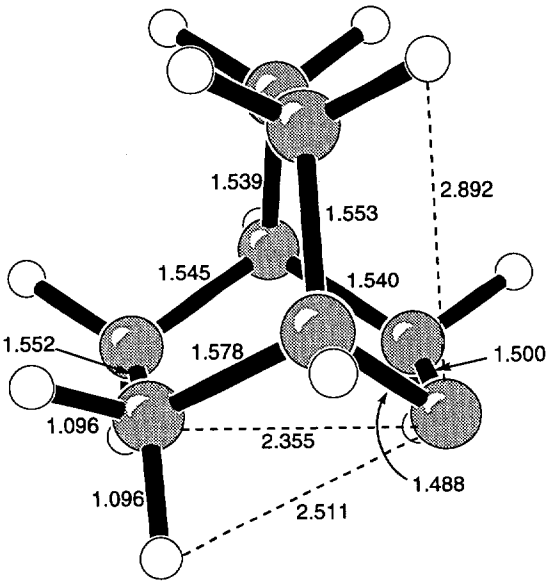
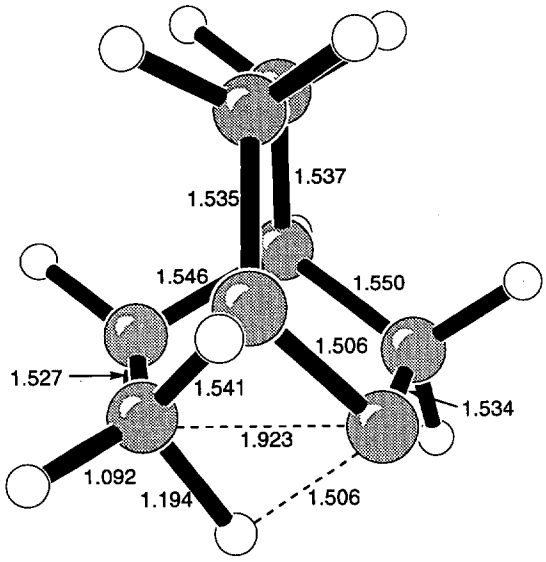
B3LYP/6-31G* Optimized Structures



7

E(RB+HF-LYP) = -311.948272 au

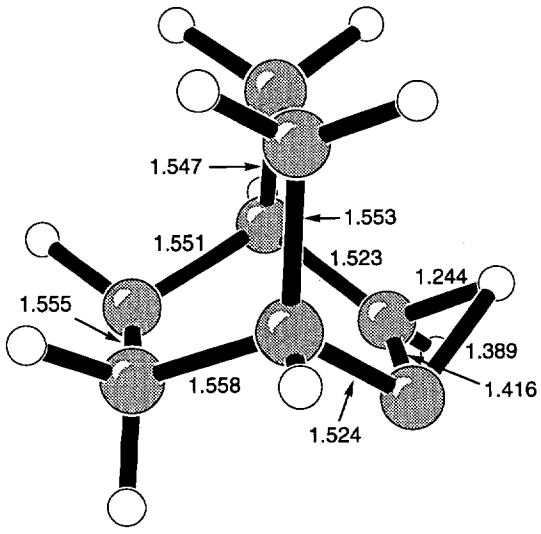
Zero Point Correction = 0.180148 au



50

E(RB+HF-LYP) = -311.939731 au

Zero Point Correction = 0.178968 au

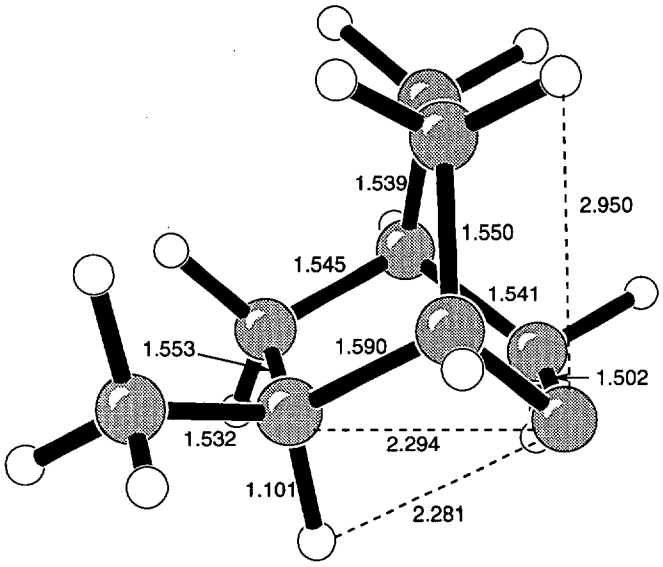


i

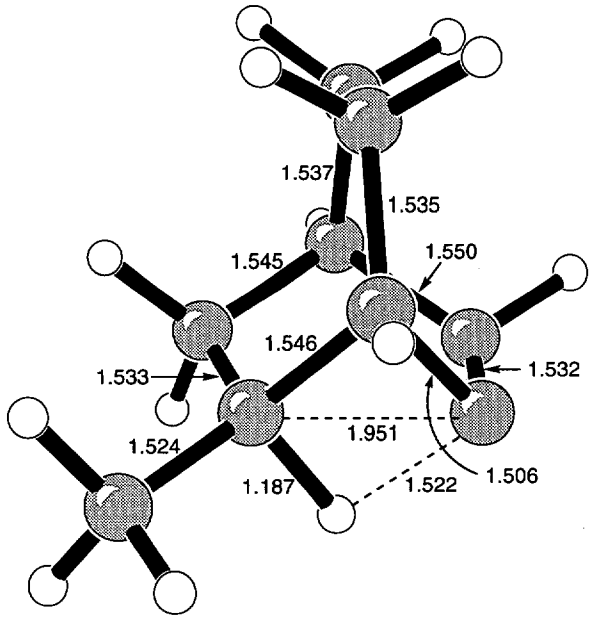
E(RB+HF-LYP) = -311.936337 au

Zero Point Correction = 0.178379 au

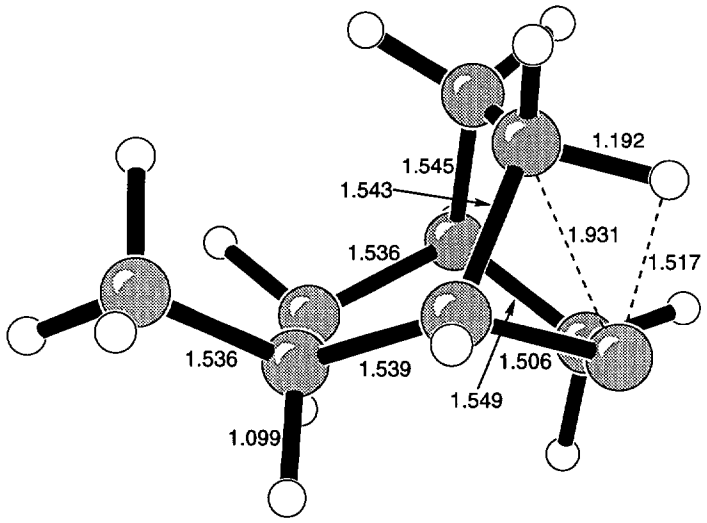
B3LYP/6-31G* Optimized Structures



10b (R = CH_3)
E(RB+HF-LYP) = -351.262263 au
Zero Point Correction = 0.208547 au

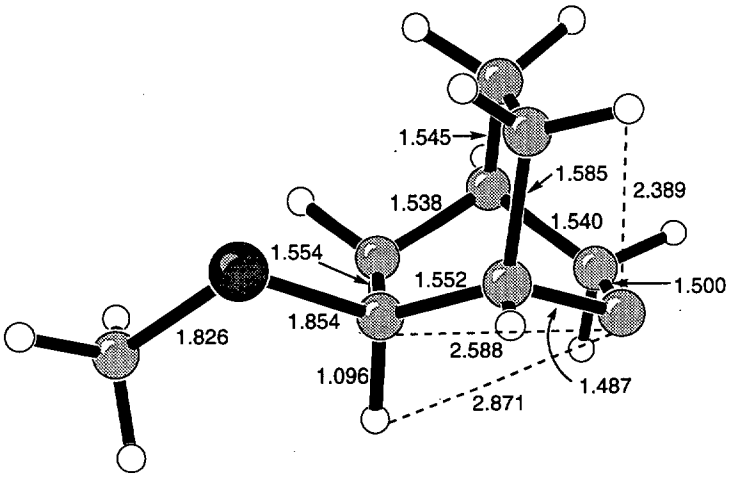


53 (R = CH_3)
E(RB+HF-LYP) = -351.256458 au
Zero Point Correction = 0.207303 au

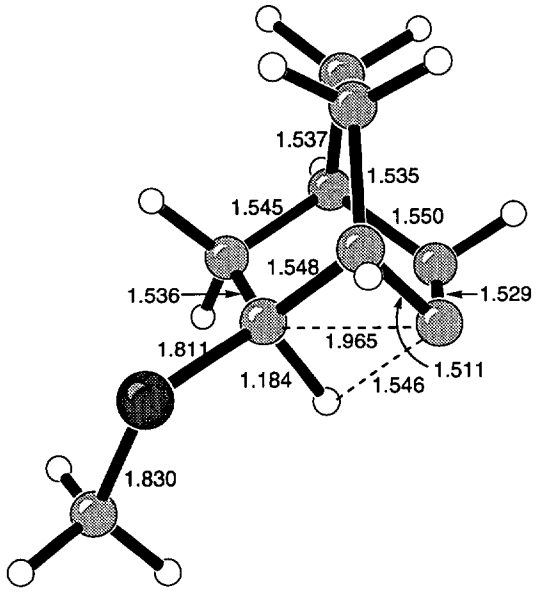


54 (R = CH_3)
E(RB+HF-LYP) = -351.253747 au
Zero Point Correction = 0.207005 au

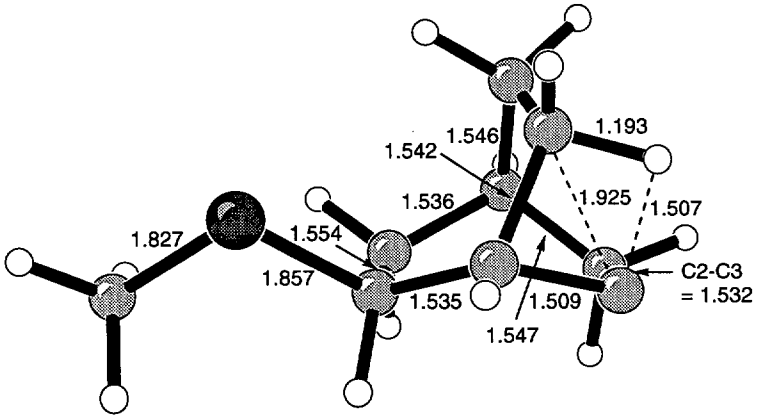
B3LYP/6-31G* Optimized Structures



10c (R = SCH_3)
E(RB+HF-LYP) = -749.445790 au
Zero Point Correction = 0.209336 au

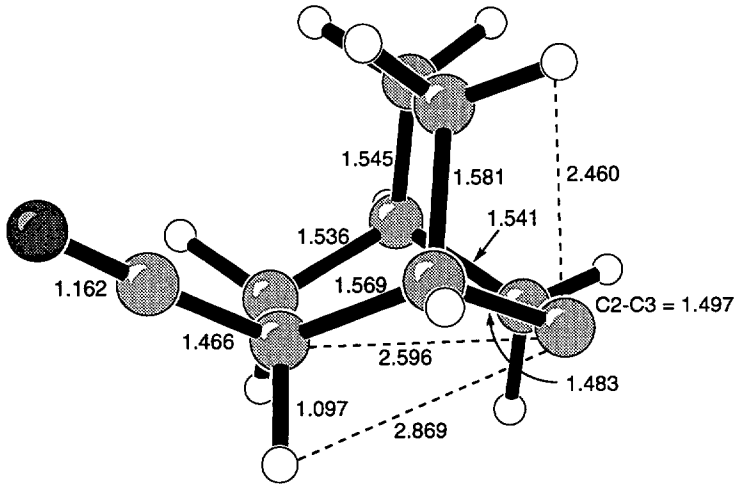


53 (R = SCH_3)
E(RB+HF-LYP) = -749.439552 au
Zero Point Correction = 0.207947 au

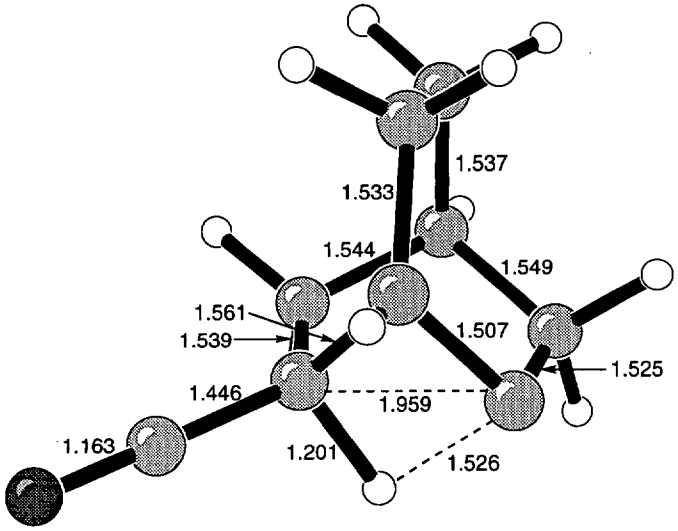


54 (R = SCH_3)
E(RB+HF-LYP) = -749.438262 au
Zero Point Correction = 0.207953 au

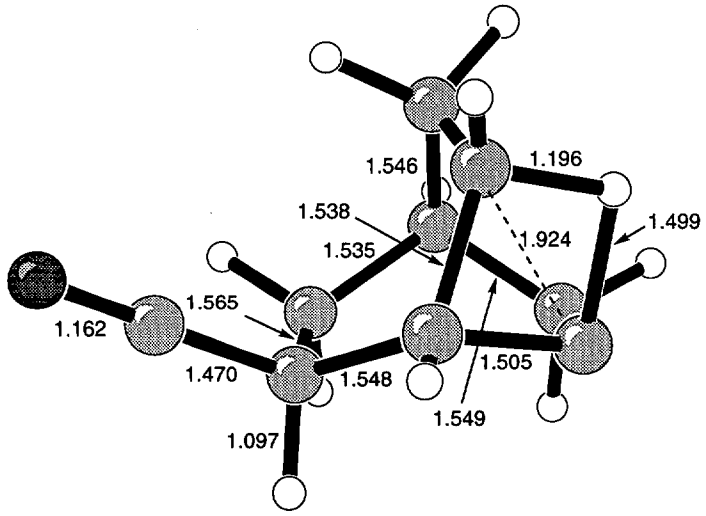
B3LYP/6-31G* Optimized Structures



10e (R = CN)
E(RB+HF-LYP) = -404.187049 au
Zero Point Correction = 0.178983 au

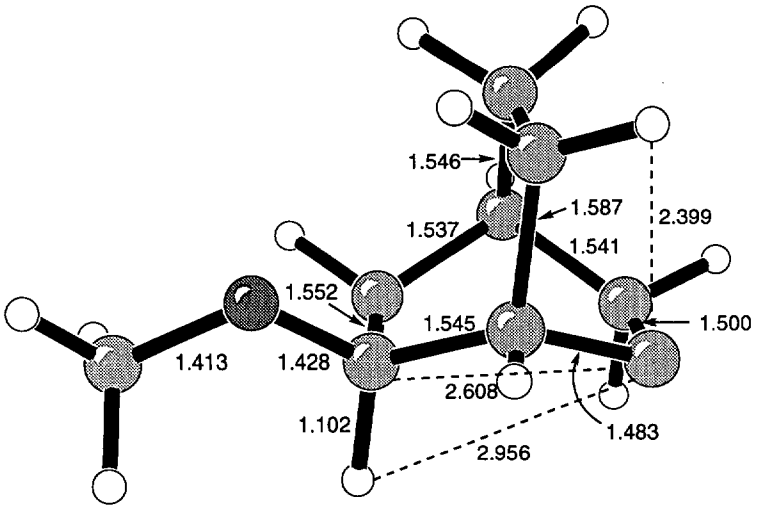


53 (R = CN)
E(RB+HF-LYP) = -404.176226 au
Zero Point Correction = 0.177223 au

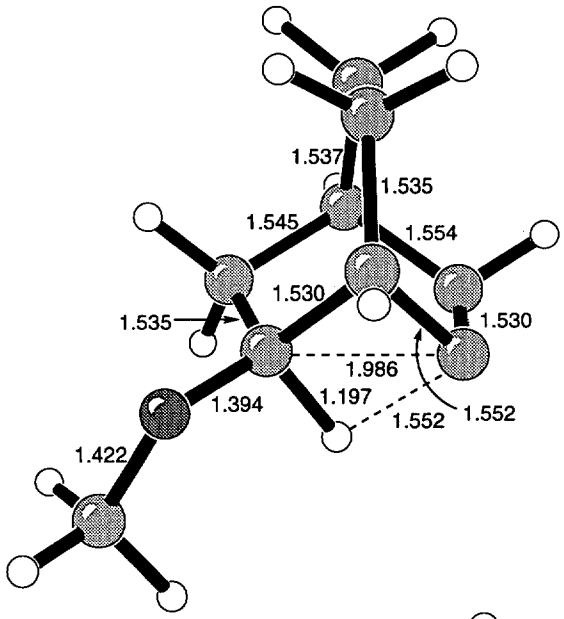


54 (R = CN)
E(RB+HF-LYP) = -404.178474 au
Zero Point Correction = 0.177628 au

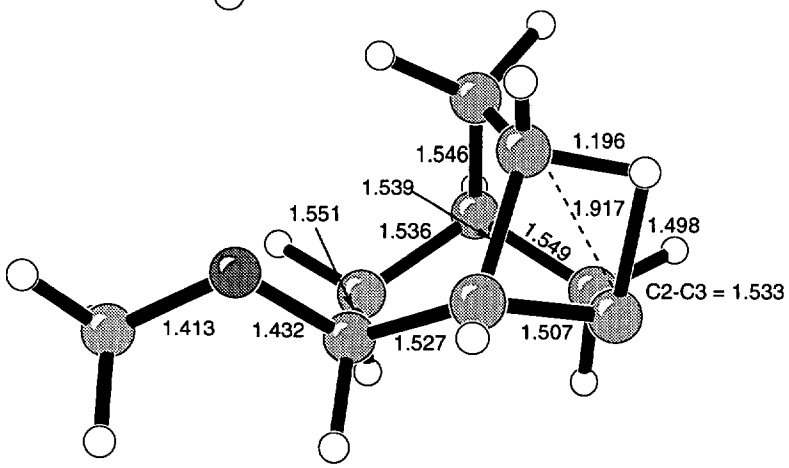
B3LYP/6-31G* Optimized Structures



10f (R = OCH_3)
E(RB+HF-LYP) = -426.465542 au
Zero Point Correction = 0.213127 au

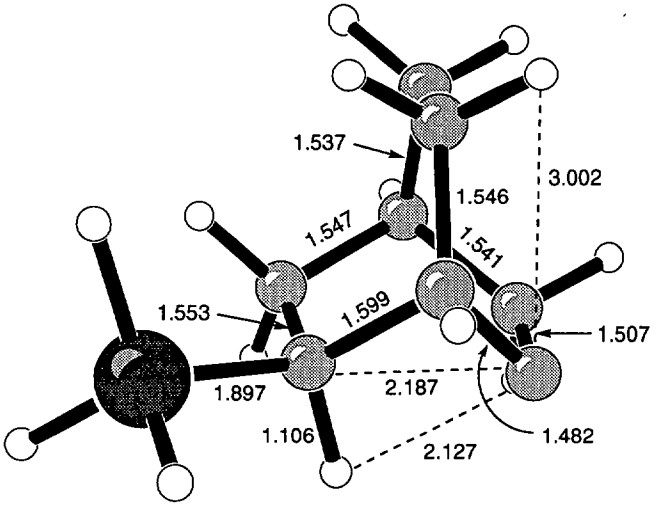


53 (R = OCH_3)
E(RB+HF-LYP) = -426.453788 au
Zero Point Correction = 0.211728 au

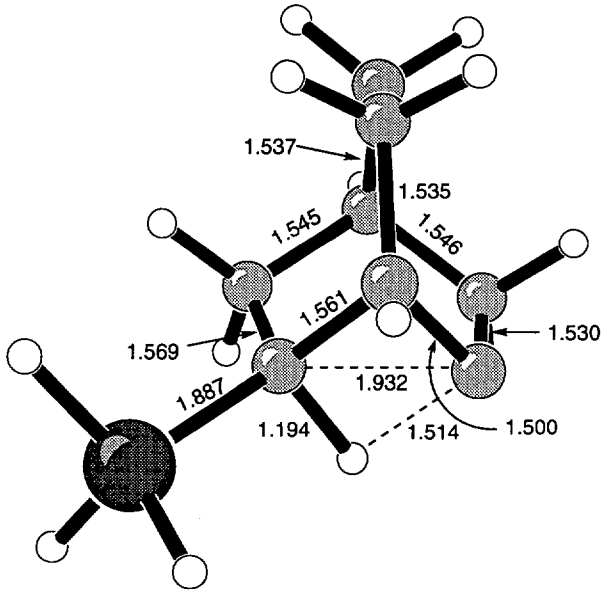


54 (R = OCH_3)
E(RB+HF-LYP) = -426.457571 au
Zero Point Correction = 0.211762 au

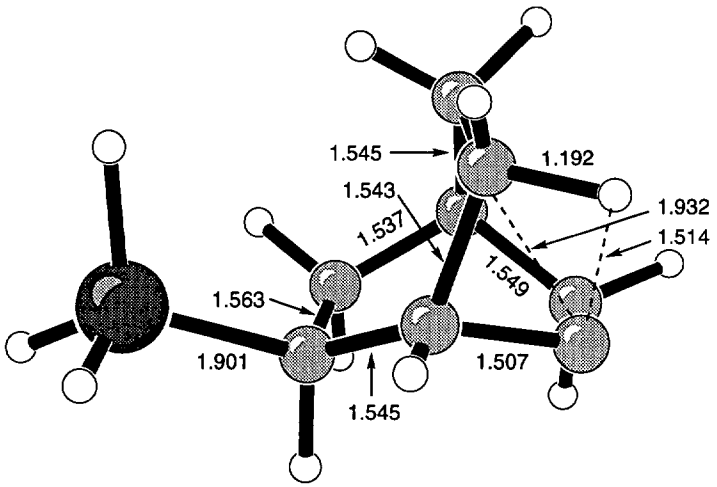
B3LYP/6-31G* Optimized Structures



10g (R = SiH_3)
E(RB+HF-LYP) = -602.639593 au
Zero Point Correction = 0.195443 au

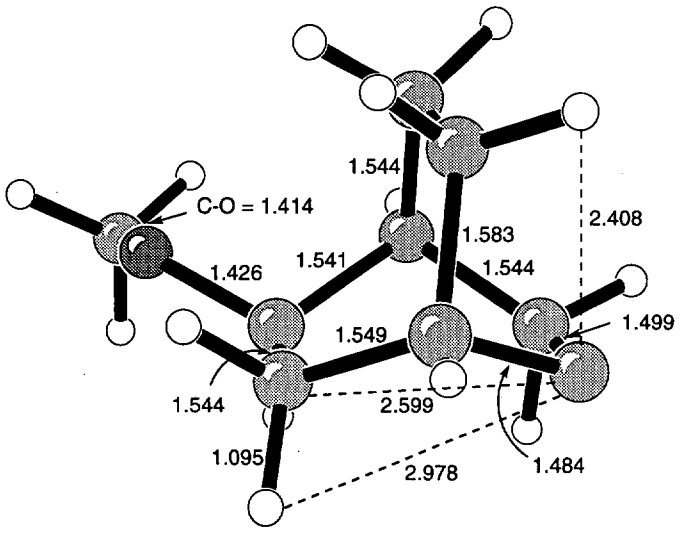


53 (R = SiH_3)
E(RB+HF-LYP) = -602.635467 au
Zero Point Correction = 0.193544 au



54 (R = SiH_3)
E(RB+HF-LYP) = -602.628025 au
Zero Point Correction = 0.193585 au

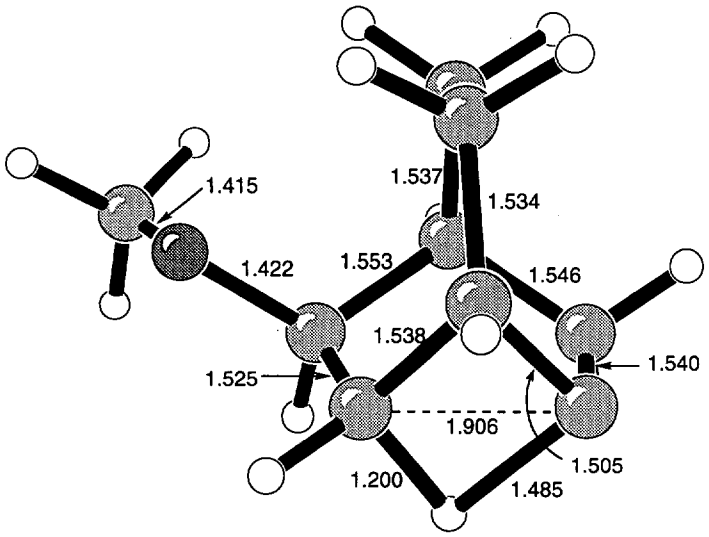
B3LYP/6-31G* Optimized Structures



11

E(RB+HF-LYP) = -426.466496 au

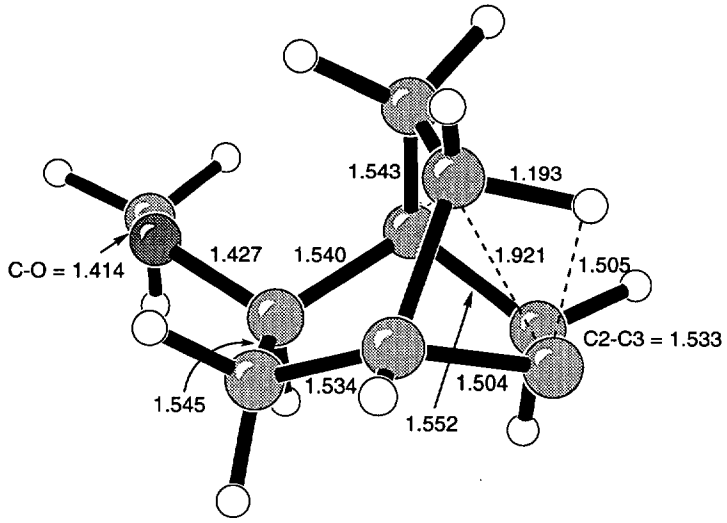
Zero Point Correction = 0.212936 au



55

E(RB+HF-LYP) = -426.454004 au

Zero Point Correction = 0.211741 au



54 (R = 5-OCH_3)

E(RB+HF-LYP) = -426.458645 au

Zero Point Correction = 0.211598 au

NMR Spectra of Compounds **37, 38** and **39c**

^{1}H NMR of **37**(R = $SiMe_3$) ($CDCl_3$) δ 1.92-1.30 (m, 9 H), 1.193 (d of d, *J* = 7.4, 3.3 Hz, 1 H), 0.637 (d of t, *J* = 7.4, 2.8 Hz, 1 H), -0.071 (s, 9 H).

^{13}C NMR of **37**(R = $SiMe_3$) ($CDCl_3$) δ 32.4 (CH_2), 32.1 (CH_2), 30.7 (CH), 27.9 (CH_2), 22.2 (CH), 16.9 (CH_2), 16.7 (CH), 14.0 (quat), -2.9 (CH_3).

^{13}C NMR of **37**(R = CH_3) ($CDCl_3$) δ 37.59 (CH_2), 32.2 (CH), 31.9 (CH_2), 27.5 (CH_2), 23.6 (CH), 23.3 (quat), 20.9 (CH_3), 20.6 (CH), 17.0 (CH_2).

^{1}H NMR of **38**(R = CH_3) ($CDCl_3$) δ 2.07 (m, 1 H), 1.84-1.74 (m, 2 H), 1.68-1.58 (m, 4 H), 1.25 (d, *J* = 7.2 Hz, 2 H), 1.01 (d, *J* = 7.2 Hz, 3 H), 0.92 (d of quintets, *J* = 2.6, 13.0 Hz, 1 H), 0.58 (d of d of d, *J* = 2.4, 7.8, 7.8 Hz, 1 H).

^{13}C NMR of **38**(R = CH_3) ($CDCl_3$) δ 37.3 (CH_2), 31.7 (CH_2), 30.4 (CH_2), 30.1 (CH), 25.7 (CH_3), 23.9 (CH), 19.8 (CH), 16.6 (CH), 16.2 (CH).

^{1}H NMR of **38**(R = SCH_3) ($CDCl_3$) δ 3.20 (d of d of d of d, *J* = 0.8, 2.7, 4.6, 10.8 Hz, 1 H), 2.13 (s, 3 H), 1.94-1.87 (m, 2 H), 1.75 (d, *J* = 11.7, 1 H), 1.70-1.63 (m, 2 H), 1.56 (d, *J* = 11.7, 1 H), 1.45-1.38 (m, 3 H), 1.01 (d of t, *J* = 2.6, 7.7 Hz, 1 H).

^{13}C NMR of **38**(R = SCH_3) ($CDCl_3$) δ 37.7 (d, *J* = 136 Hz), 36.6 (t, *J* = 132 Hz), 30.9 (t, *J* = 132 Hz), 30.5 (t, *J* = 130 Hz), 29.4 (d, *J* = 139 Hz), 17.9 (d, *J* = 162 Hz), 17.8 (d, *J* = 167 Hz), 17.1 (d, *J* = 171 Hz), 13.8 (q, *J* = 138 Hz).

^{13}C NMR of **37**(R = SCH_3) ($CDCl_3$) δ 36.5 (CH_2), 32.3 (CH), 31.8 (CH_2), 31.3 (quat), 26.9 (CH), 26.7 (CH_2), 24.4 (CH), 17.4 (CH_2), 14.3 (CH_3).

^{1}H NMR of **39** (R = SCH_3) ($CDCl_3$) δ 6.29 (m, 2 H), 2.66 (m, 1 H), 2.55 (m, 1 H), 2.49 (m, 1 H), 2.14 (m, 1 H), 2.07 (s, 3 H), 1.79 (m, 1 H), 1.55 (m, 1 H), 1.23 (m, 1 H), 1.16-1.04 (m, 2 H).

^{13}C NMR of **39** (R = SCH_3) ($CDCl_3$) δ 134.9 (d, *J* = 163 Hz), 134.2 (d, *J* = 162 Hz), 44.5 (d, *J* = 142 Hz), 33.8 (t, *J* = 131 Hz), 32.7 (d, *J* = 140 Hz), 30.1 (d, *J* = 137 Hz), 26.1 (t, *J* = 131 Hz), 18.9 (t, *J* = 131 Hz), 14.9 (q, *J* = 138 Hz).

^{1}H NMR of **37**(R = CO_2CH_3) ($CDCl_3$) δ 3.66 (s, 3 H), 2.05 (m, 1 H), 2.01 (m, 1 H), 1.94 (d of d, *J* = 3.6, 7.8 Hz, 1 H), 1.92-1.88 (m, 2 H), 1.77 (m, 1 H), 1.74 (d, *J* = 12.0 Hz, 1 H), 1.66 (d of t, *J* = 2.4, 8.4 Hz, 1 H), 1.58 (d, *J* = 12.0 Hz, 1 H), 1.42-1.37 (m, 2 H).

^{13}C NMR of **37**(R = CO_2CH_3) ($CDCl_3$) δ 175.5, 51.5, 31.2, 31.1, 30.8, 30.7, 30.4, 26.6, 24.6, 16.6.

^{1}H NMR of **38**(R = CO_2CH_3) ($CDCl_3$) δ 3.70 (s, 3 H), 2.92 (d of d of d, *J* = 2.4, 5.4, 12.0 Hz, 1 H), 1.89 (m, 1 H), 1.75 (d of quintets, *J* = 2.4, 13.2 Hz, 1 H), 1.70 (d, *J* = 12.0 Hz, 1 H), 1.69-1.58 (m, 3 H), 1.55 (d, *J* = 12.0 Hz, 1 H), 1.39-1.34 (m, *J* = 2 H), 0.99 (d of t, *J* = 2.4, 7.8 Hz, 1 H).

^{13}C NMR of **38**(R = CO_2CH_3) ($CDCl_3$) δ 177.6 (quat), 51.8 (q, *J* = 147 Hz), 34.8 (d, *J* = 128 Hz), 31.0 (t, *J* = 129 Hz), 30.8 (t, *J* = 130 Hz), 30.5 (t, *J* = 129 Hz), 28.9 (d, *J* = 139 Hz), 16.6 (d, *J* = 171 Hz), 16.3 (d, *J* = 170 Hz), 15.4 (d, *J* = 164 Hz).

^{13}C NMR of **38**(R = CN) ($CDCl_3$) δ 124.2, 32.7, 30.5, 30.3, 28.6, 19.9, 17.0, 16.2, 15.3.

^{1}H NMR of **38**(R = OCH_3) ($CDCl_3$) δ 3.73 (d of d of d, *J* = 3.1, 3.1, 9.2 Hz, 1 H), 3.31 (s, 3 H), 1.89 (m, 1 H), 1.72-1.58 (m, 4 H), 1.71 (d, *J* = 12.0 Hz, 1 H), 1.43 (d, *J* = 12.0 Hz, 1 H), 1.42-1.36 (m, 2 H), 1.09 (d of d of d, *J* = 3.3, 7.7, 7.7 Hz, 1 H).

^{13}C NMR of **38**(R = OCH_3) ($CDCl_3$) δ 74.2 (d, *J* = 145 Hz), 55.4 (q, *J* = 141 Hz), 36.2 (t, *J* = 127 Hz), 30.9 (t, *J* = 130 Hz), 30.7 (t, *J* = 128 Hz), 28.8 (d, *J* = 136 Hz), 17.2 (d, *J* = 160 Hz), 16.0 (d, *J* = 165 Hz), 15.8 (d, *J* = 169 Hz).