Dienamine Catalysis: Organocatalytic Asymmetric

γ -Amination of α,β -Unsaturated Aldehydes

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Experimental Section

General. The ^1H NMR and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz, respectively. The chemical shifts are reported in ppm relative to CHCl_3 ($\delta = 7.26$) for ^1H NMR and relative to the central CDCl_3 resonance ($\delta = 77.0$) for ^{13}C NMR. Purification of reaction products was carried out by flash chromatography (FC) using silica gel 60 (230-400 mesh from Merck). The enantiomeric excess (ee) was determined by HPLC using either a Chiralpak AD, a Chiralcel OD or a Chiralpak AS column. Optical rotation was measured on a Perkin-Elmer 241 polarimeter. Mass spectra were recorded on a micromass LCT spectrometer using electrospray (ES^+) ionisation techniques.

Materials. Commercially available starting materials and solvents were used without further purification. α,β -unsaturated aldehydes **1f**, **1g** and **1h** were prepared following a literature procedure.¹

General Procedure for the γ -Amination of α,β -Unsaturated Aldehydes.

The catalyst (15 mg, 25 μ mol, 0.1 eq) and benzoic acid (3 mg, 25 μ mol, 0.1 eq) were dissolved in 125 μ L of toluene [2M]. The α,β -unsaturated aldehyde (375 μ mol, 1.5 eq) and afterwards DEAD (39 μ L, 250 μ mol) were added. The reactions were monitored by NMR and upon full consumption of the DEAD, the raw reaction mixtures were purified by FC.

General Procedure for the Reduction and Esterification of γ -Aminated- α,β -Unsaturated Aldehydes.

The aldehyde was dissolved in 2 mL MeOH and NaBH₄ (10 mg) was added. After 30 min 1M HCl solution was added and the aq. phase extracted with CH₂Cl₂ (3 x 10 mL). The combined organic phases were washed with sat. NaCl solution and dried over Na₂SO₄. The solvent was evaporated after filtration to yield the crude alcohol. The alcohol was dissolved in 2 mL CH₂Cl₂ and Et₃N (1.3 eq) and 4-chlorobenzoylchloride (1.3 eq) were added. After 1-3 h the raw reaction mixtures were purified directly by FC.

Analytical and Spectroscopic Data.

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-pent-2-*E*-enal (6a).

The product was obtained following the standard procedure and purified by FC. ¹H NMR δ 9.56 (d, *J*=7.6, 1 H), 6.87 (dd, *J*=4.9, 15.4, 1 H), 6.34 (bs, 1 H), 6.14 (dd, *J*=7.5, 15.9, 1 H), 5.05-5.01 (m, 1 H), 4.24-4.17 (m, 4 H), 1.39 (d, *J*=7.0, 3 H), 1.27 (t, *J*=7.1, 6 H). ¹³C NMR δ 193.7, 156.9, 155.8, 155.4, 132.1, 62.9, 62.3, 54.3, 16.1, 14.4, 14.3. MS (TOF ES⁺): [M+Na]⁺ calcd for C₁₁H₁₈N₂NaO 281.1113; found 281.1000. [α]_D¹⁵ = +17.2 (*c* 1.1, CH₂Cl₂) from catalytic reaction (89% ee); [α]_D¹⁵ = +15.4 (*c* 1.3, CH₂Cl₂) from α -amination-Wittig sequence (81% ee).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-pent-2-*E*-enyl ester (Xa).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AS Column (hexane/*i*-PrOH (95/5)): flow rate 1.0 mL/min: τ_{major} = 26.9, τ_{minor} = 33.7. ¹H NMR δ 7.97 (d, *J*=8.6, 2 H), 7.40 (d, *J*=8.6, 2 H),

6.29 (bs, 1 H), 5.84 (m, 2 H), 4.85 (m, 1 H), 4.79 (d, $J=5.7$, 2 H), 4.17 (k, $J=7.2$, 4 H), 1.30 (d, $J=6.9$, 3 H), 1.25 (t, $J=7.1$, 6 H). ^{13}C NMR δ 165.3, 156.7, 155.6, 139.4, 134.1, 131.0, 128.6, 125.2, 65.0, 62.5, 62.0, 54.3, 16.7, 14.4, 14.3. MS (TOF ES $^{+}$): $[\text{M}+\text{Na}]^{+}$ calcd for $\text{C}_{18}\text{H}_{23}\text{ClN}_2\text{NaO}_6$ 421.1142; found 421.1136. $[\alpha]_{\text{D}}^{15} = +10.6$ (c 0.86, CH_2Cl_2).

4-(Hydrazine- N,N' -dicarboxylic acid ethyl ester)-hex-2- E -enal (6b).

The product was obtained following the standard procedure and purified by FC. ^1H NMR δ 9.54 (d, $J=7.6$, 1 H), 6.82 (dd, $J=6.5$, 16.0 Hz, 1 H), 6.36 (bs, 1 H), 6.16 (ddd, $J=1.2$, 7.6, 16.0, 1 H), 4.74 (m, 1 H), 4.20 (m, 4 H), 1.83 (m, 1 H), 1.68 (m, 1 H), 1.27 (dt, $J=1.7$, 7.1, 6 H), 0.97 (t, $J=7.4$, 3 H). ^{13}C NMR δ 193.7, 156.8, 155.7, 154.2, 132.9, 62.9, 62.4, 60.5, 23.9, 14.4, 14.4, 10.6. MS (TOF ES $^{+}$): $[\text{M}+\text{Na}]^{+}$ calcd for $\text{C}_{12}\text{H}_{20}\text{N}_2\text{NaO}_5$ 295.1270; found 295.1266. $[\alpha]_{\text{D}}^{15} = +8.7$ (c 1.1, CH_2Cl_2).

p -Chloro-benzoic acid 4-(hydrazine- N,N' -dicarboxylic acid ethyl ester)-hex-2- E -enyl ester (Xb). The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AS Column (hexane/ i -PrOH (90/10)): flow rate 1.0 mL/min: $\tau_{\text{major}} = 11.0$, $\tau_{\text{minor}} = 14.1$. ^1H NMR δ 7.98 (d, $J=8.5$, 2 H), 7.41 (d, $J=8.5$, 2 H), 6.16 (bs, 1 H), 5.85 (m, 2 H), 4.80 (d, $J=4.1$, 2 H), 4.55 (m, 1 H), 4.19 (p, $J=7.2$, 4 H), 1.75 (m, 1 H), 1.60 (m, 1 H), 1.26 (t, $J=7.2$, 6 H), 0.94 (t, $J=7.4$, 3 H). ^{13}C NMR δ 165.6, 157.0, 156.2, 139.7, 133.0, 131.3, 128.9, 128.8, 126.7, 65.3, 62.8, 62.3, 61.1, 24.7, 14.7, 14.6, 11.0. MS (TOF ES $^{+}$): $[\text{M}+\text{Na}]^{+}$ calcd for $\text{C}_{19}\text{H}_{25}\text{ClN}_2\text{NaO}_6$ 435.1299; found 435.1291. $[\alpha]_{\text{D}}^{15} = +7.8$ (c 1.4, CH_2Cl_2).

4-(Hydrazine- N,N' -dicarboxylic acid ethyl ester)-hept-2- E -enal (6c).

The product was obtained by following the standard procedure and purified by FC. ^1H NMR δ 9.53 (d, $J=7.6$, 1 H), 6.82 (dd, $J=6.6$, 15.8, 1 H), 6.3 (bs, 1H), 6.15 (ddd, $J=1.1$, 7.6, 15.8, 1 H), 4.83 (m, 4 H), 4.19 (m, 1 H), 1.79 (m, 1 H), 1.60 (m, 1 H), 1.38 (m, 2 H), 1.26 (dt, $J=2.60$, 7.1, 6 H), 0.95 (t, $J=7.3$, 3 H). ^{13}C NMR δ 193.9, 156.9, 155.7, 154.6,

132.7, 62.9, 62.4, 58.7, 32.6, 19.2, 14.4, 14.3, 13.7. MS (TOF ES⁺): [M+Na]⁺ calcd for C₁₃H₂₂N₂NaO₅ 309.1426; found 309.1435. [α]_D¹⁵ = +14.6 (c 1.0, CH₂Cl₂).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-hept-2-*E*-enyl ester (Xc).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AS Column (hexane/*i*-PrOH (90/10)): flow rate 1.0 mL/min: τ_{major} = 10.1, τ_{minor} = 12.1. ¹H NMR δ 7.98 (d, *J* = 8.6, 2 H), 7.41 (d, *J* = 8.6 Hz, 2 H), 6.13 (bs, 1 H), 5.85 (m, 2 H), 4.80 (m, 1 H), 4.65 (s, 1 H), 4.19 (p, *J* = 7.03, 7.03, 7.03 Hz, 1 H), 1.71 (s, 1 H), 1.54 (s, 1 H), 1.37 (s, 1 H), 1.26 (t, *J* = 7.10, 7.10 Hz, 1 H), 0.94 (t, *J* = 7.32, 7.32 Hz, 1 H). ¹³C NMR δ 165.4, 156.6, 155.9, 139.4, 133.0, 131.0, 128.7, 128.5, 126.2, 65.0, 62.5, 62.0, 58.9, 33.3, 19.2, 14.5, 14.4, 13.8. MS (TOF ES⁺): [M+Na]⁺ calcd for C₂₀H₂₇ClN₂NaO₆ 449.1455; found 449.1460. [α]_D¹⁵ = +6.1 (c 1.0, CH₂Cl₂).

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-dec-2-*E*-enal (6d). The product was obtained following the standard procedure and purified by FC. ¹H NMR δ 9.54 (d, *J* = 7.6, 1 H), 6.83 (dd, *J* = 6.5, 15.9, 1 H), 6.32 (bs, 1 H), 6.16 (ddd, *J* = 0.9, 7.6, 15.9, 1 H), 4.81 (m, 1 H), 4.20 (m, 4 H), 1.79 (m, 1 H), 1.61 (m, 1 H), 1.42-1.24 (m, 15 H), 0.88 (t, *J* = 6.9, 3 H). ¹³C NMR δ 193.9, 156.9, 155.7, 154.6, 132.7, 62.8, 62.3, 56.2, 31.6, 30.6, 28.9, 25.9, 22.5, 14.4, 14.3, 14.0. MS (TOF ES⁺): [M+Na]⁺ calcd for C₁₆H₂₈N₂NaO₅ 351.1896; found 351.1897. [α]_D¹⁵ = +14.1 (c 1.8, CH₂Cl₂).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-dec-2-*E*-enyl ester (Xd).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AS Column (hexane/*i*-PrOH (99/1)): flow rate 1.0 mL/min: $\tau_{\text{major}} = 39.3$, $\tau_{\text{minor}} = 52.5$. ^1H NMR δ 7.98 (d, $J=8.5$, 2 H), 7.41 (d, $J=8.5$, 2 H), 6.12 (m, 1 H), 5.85 (m, 2 H), 4.79 (d, $J=4.5$ Hz, 2 H), 4.63 (m, 1 H), 4.18 (p, $J=7.0$, 4 H), 1.71 (m, 1 H), 1.56 (m, 1 H), 1.35-1.22 (m, 14 H), 0.88 (t, $J=6.9$, 1 H). ^{13}C NMR δ 165.4, 156.6, 155.9, 139.4, 133.0, 131.0, 128.7, 128.5, 126.1, 65.0, 62.5, 62.0, 59.2, 31.7, 31.2, 29.0, 26.0, 22.5, 14.4, 14.3, 14.0. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{33}\text{ClN}_2\text{NaO}_6$ 491.1925; found 491.1931. $[\alpha]_{\text{D}}^{15} = +8.5$ (c 1.5, CH_2Cl_2).

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-non-2-*E*-6-*Z*-dienal (6e). The product was obtained following the standard procedure and purified by FC. ^1H NMR δ 9.53 (d, $J=7.6$, 1 H), 6.85 (dd, $J=6.1$, 15.9, 1 H), 6.34 (bs, 1 H), 6.18 (dd, $J=7.6$, 15.9, 1 H), 5.56-5.49 (m, 1 H), 5.31-5.25 (m, 1 H), 4.84 (m, 1 H), 4.22-4.16 (m, 4 H), 2.62-2.54 (m, 1 H), 2.45-2.38 (m, 1 H), 2.06 (p, $J=7.4$, 2 H), 1.28-1.24 (m, 6 H), 0.97 (t, $J=7.5$, 3 H). ^{13}C NMR δ 193.8, 154.2, 135.3, 132.7, 123.2, 62.9, 62.3, 28.7, 20.7, 14.3, 14.0. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{24}\text{N}_2\text{NaO}_5$ 335.1577; found 335.1567. $[\alpha]_{\text{D}}^{15} = +16.5$ (c 1.12, CH_2Cl_2).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-non-2-*E*-6-*Z*-dienyl ester (Xe).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AS Column (hexane/*i*-PrOH (95/5)): flow rate 1.0

mL/min: $\tau_{\text{major}} = 17.4$, $\tau_{\text{minor}} = 20.9$. ^1H NMR δ 7.98 (d, $J=8.7$, 2 H), 7.41 (d, $J=8.6$, 2 H), 6.14 (bs, 1 H), 5.94-5.83 (m, 2 H), 5.51-5.45 (m, 1 H), 5.34-5.27 (m, 1 H), 4.80 (d, $J=4.3$, 2 H), 4.71-4.65 (m, 1 H), 4.22-4.15 (m, 4 H), 2.55-2.46 (m, 1 H), 2.39-2.31 (m, 1 H), 2.11-2.03 (m, 2 H), 1.26 (t, $J=7.1$, 6 H), 0.98 (t, $J=7.5$, 3 H). ^{13}C NMR δ 165.4, 156.7, 155.8, 139.4, 134.4, 132.5, 131.0, 128.7, 126.2, 124.1, 65.0, 62.6, 62.1, 59.4, 53.4, 29.4, 20.7, 14.4, 14.1. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{22}\text{H}_{29}\text{ClN}_2\text{NaO}_6$ 475.1606; found 475.1605. $[\alpha]_{\text{D}}^{15} = +7.6$ (c 0.91, CH_2Cl_2).

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-phenyl-pent-2-*E*-enal (6f). The product was obtained following the standard procedure and purified by FC. ^1H NMR δ 9.54 (d, $J=7.5$, 1 H), 7.34-7.20 (m, 5 H), 6.93 (dd, $J=6.2$, 15.9, 1 H), 6.30 (bs, 1 H), 6.16, (dd, $J=7.5$, 15.9, 1 H), 5.16-5.15 (m, 1 H), 4.25-4.12 (m, 4 H), 3.18 (dd, $J=8.5$, 13.9, 1 H), 3.02 (dd, $J=7.2$, 14.0, 1 H), 1.29 (t, $J=7.1$, 3 H), 1.22 (t, $J=7.1$, 3 H). ^{13}C NMR δ 193.1, 156.8, 155.4, 153.0, 136.7, 133.1, 128.9, 128.7, 127.0, 62.8, 62.3, 60.8, 37.4, 14.3. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{NaO}_5$ 357.1421; found 357.1419. $[\alpha]_{\text{D}}^{15} = +15.9$ (c 0.97, CH_2Cl_2).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-phenyl-pent-2-*E*-enyl ester (Xf).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralcel OD Column (hexane/*i*-PrOH (90/10)): flow rate 1.0 mL/min: $\tau_{\text{major}} = 15.3$, $\tau_{\text{minor}} = 24.2$. ^1H NMR δ 7.97 (d, $J=8.7$, 2 H), 7.42 (d, $J=8.7$, 2 H), 7.29-7.19 (m, 5 H), 6.14 (bs, 1 H), 5.98 (dd, $J=7.0$, 15.7, 1 H), 5.79 (dt, $J=5.8$, 15.7, 1 H), 4.96 (q, $J=6.9$, 1 H), 4.77 (d, $J=5.8$, 2 H), 4.22-4.10 (m, 4 H), 3.10 (dd, $J=7.7$, 13.8, 1 H), 2.93 (dd, $J=7.5$, 13.9, 1 H), 1.27 (t, $J=7.1$, 3 H), 1.21 (t, $J=7.1$, 3 H). ^{13}C NMR δ 165.3, 156.8, 155.5, 139.4, 137.5, 132.1, 131.0, 129.1, 128.6, 128.5, 126.5, 64.9, 62.5, 62.2, 60.8, 38.1, 38.0, 14.4. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{27}\text{ClN}_2\text{NaO}_6$ 497.1450; found 497.1436. $[\alpha]_{\text{D}}^{15} = +2.0$ (c 0.96, CH_2Cl_2).

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-methyl-hex-2-*E*-enal (6g). The product was obtained following the standard procedure and purified by FC. ^1H NMR δ 9.55 (d, $J=7.6$, 1 H), 6.75 (dd, $J=8.5$, 15.8, 1 H), 6.38 (bs, 1 H), 6.19 (ddd, $J=0.7$, 7.6, 15.8, 1 H), 4.38 (t, $J=9.1$ Hz, 1 H), 4.23-4.14 (m, 4 H), 2.11-2.00 (m, 1 H), 1.29-1.23 (m, 6 H), 1.01 (d, $J=6.6$, 3 H), 0.91 (d, $J=6.8$, 3 H). ^{13}C NMR δ 193.9, 156.9, 155.8, 152.5, 134.1, 66.2/65.5, 62.8, 62.3, 29.1, 19.8/19.5, 14.4. MS (TOF ES $^+$): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{13}\text{H}_{22}\text{N}_2\text{NaO}_5$ 309.1426; found: 309.1425. $[\alpha]_{\text{D}}^{15} = -15.7$ (c 0.73, CHCl_3).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-methyl-hex-2-*E*-enyl ester (Xg).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AD Column (hexane/*i*-PrOH (90/10)): flow rate 1.0 mL/min: $\tau_{\text{minor}}=14.3$, $\tau_{\text{major}}=15.8$. ^1H NMR δ 7.98 (d, $J=8.7$, 2 H), 7.41 (d, $J=8.7$, 2 H), 6.15 (bs, 1 H), 5.92-5.79 (m, 2 H), 4.81 (d, $J=4.6$, 2 H), 4.25-4.13 (m, 5 H), 1.99-1.87 (m, 1 H), 1.26 (t, $J=7.1$, 6 H), 1.00 (d, $J=6.6$, 3 H), 0.89 (d, $J=6.8$, 3 H). ^{13}C NMR δ 165.4, 156.7, 156.0, 139.4, 131.6, 131.0, 128.7, 127.6, 125.5, 66.4, 65.0, 62.5, 62.0, 29.5, 19.9, 19.7, 14.5, 14.4. MS (TOF ES $^+$): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{20}\text{H}_{27}\text{ClN}_2\text{NaO}_6$ 449.1455; found: 449.1460. $[\alpha]_{\text{D}}^{15} = -3.2$ (c 0.69, CHCl_3).

4-(Hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-methylsulfanyl-pent-2-*E*-enal (6h). The product was obtained following the standard procedure and purified by FC. ^1H NMR δ 9.55 (d, $J=7.5$, 1 H), 6.89 (dd, $J=6.2$, 16.0, 1 H), 6.47 (bs, 1 H), 6.24 (ddd, $J=1.1$, 7.5, 16.0, 1 H), 4.99 (bs, 1 H), 4.26-4.15 (m, 4 H), 2.92 (dd, $J=8.8$, 13.6, 1 H), 2.77 (dd, $J=6.5$, 13.6, 1 H), 2.13 (s, 3 H), 1.27 (t, $J=7.1$, 6 H). ^{13}C NMR δ 193.5, 156.6, 155.6, 152.7, 133.2, 63.0, 62.4, 58.0/56.9, 35.4/34.8, 15.3, 14.4. MS (TOF ES $^+$): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{12}\text{H}_{20}\text{N}_2\text{NaO}_5\text{S}$ 327.0991; found 327.0988. $[\alpha]_{\text{D}}^{15} = +15.5$ (c 1.0, CHCl_3).

***p*-Chloro-benzoic acid 4-(hydrazine-*N,N'*-dicarboxylic acid ethyl ester)-5-methylsulfanyl-pent-2-*E*-enyl ester (Xh).** The product was obtained following the standard procedure and purified by FC. The enantiomeric excess was determined by HPLC using a Daicel Chiralpak AD Column (hexane/*i*-PrOH (90/10)): flow rate 1.0 mL/min: $\tau_{\text{minor}}=21.2$, $\tau_{\text{major}}=26.8$. ^1H NMR δ 7.97 (d, $J=8.6$, 2 H), 7.40 (d, $J=8.6$, 2 H), 6.35 (bs, 1 H), 5.98-5.87 (m, 2 H), 4.87-4.78 (m, 3 H), 4.23-4.13 (m, 4 H), 2.85 (dd, $J=8.7$, 13.6, 1 H), 2.71 (dd, $J=6.5$, 13.6, 1 H), 2.11 (s, 3 H), 1.26 (dt, $J=3.9$, 7.1, 6 H). ^{13}C NMR δ 165.3, 156.9, 155.8, 139.4, 131.3, 131.0, 128.6, 128.4, 127.0, 64.8, 62.7/62.1, 58.2/57.2, 35.8, 15.4, 14.4. MS (TOF ES⁺): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{19}\text{H}_{25}\text{ClN}_2\text{NaO}_6\text{S}$ 467.1020; found 467.1040. $[\alpha]_{\text{D}}^{15} = +8.4$ (*c* 1.8, CHCl_3).

Dienamine *in situ* NMR.

^1H NMR in C_6D_6 : 2-pentenal **1a** [0.5 M] and catalyst **2a** (10 mol%) after 30 min

Determination of the Absolute Configuration of **6a**.

The crude α -aminated propionaldehyde (see left) was synthesized, following a literature procedure.²

The desired compound **6a** was then obtained by subjecting the α -aminated aldehyde to a Wittig reaction in accordance with literature procedure¹ and the product was purified by FC. The enantiomeric excess was determined after reduction and esterification in accordance with the general procedure. The product obtained by *S*-proline and *S*-**2a** have the same absolute configuration.

Diels-Alder Reaction with *N*-Methylmaleimide.

The catalyst **2a** (149 mg, 0.25 mmol), benzoic acid (31 mg, 0.25 mmol) and 2-*E*-pentenal **1a** (37 μ L, 0.375 mmol) were suspended in 125 μ L toluene. After 10 min stirring *N*-methylmaleimide (28 mg, 0.25 mmol) was added. The raw reaction mixture was purified directly by FC, yielding 67 mg of **8** (35% yield) as a yellow oil and as a mixture of two diastereomers in a ratio of 2:1.

4-{2-[Bis-(3,5-bis-trifluoromethyl-phenyl)-trimethylsilylanyloxy-methyl]pyrrolidin-1-yl}-2,7-dimethyl-3a,4,7,7a-tetrahydro-isoindole-1,3-dione (8).

^1H NMR δ 8.00-7.86 (m, 6H), 5.91-5.82 (m, 1H), 5.74-5.64 (m, 1H), 4.74/4.61 (dd, $J=1.6$, 8.2 / $J=2.1$, 9.1, 1H), 4.06/3.82 (bs, 1H), 3.53/3.43 (t, $J=8.3/8.9$, 1H), 2.97-2.93/2.83-2.78 (m, 1H), 2.93/2.87 (s, 3H), 2.61-2.52 (m, 1H), 2.50-2.37 (m, 1H), 2.32-2.10 (m, 1H), 2.07-1.95 (m, 1H), 1.70-1.57 (m, 1H), 1.51/0.96 (d, $J=7.4/6.9$, 3H), 1.48-1.20 (m, 2H), -0.14/-0.17 (s, 9H). ^{13}C NMR δ 178.9, 178.0, 177.6, 145.9, 145.7, 143.9, 143.6, 134.4, 133.4, 131.8, 131.6, 131.5, 131.4, 131.3, 131.2, 131.1, 130.9, 130.8, 130.7, 130.6, 130.5, 130.4, 129.3, 129.1, 128.8, 128.2, 127.9, 127.3, 126.2, 126.1, 124.6, 124.5, 121.7, 120.6, 119.2, 119.1, 83.8, 83.5, 68.8, 67.9, 57.2, 52.9, 49.7, 48.5, 47.0, 45.5, 40.7, 40.4, 29.9, 28.7, 28.6, 28.4, 24.9, 24.7, 22.6, 22.5, 19.3, 17.1, 1.7, 1.6. MS (TOF ES^+): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{34}\text{H}_{35}\text{F}_{12}\text{N}_2\text{O}_3\text{Si}$ 775.2225; found 775.2214.

Computational Details. All molecules were optimized at the B3LYP/6-31G(d) level of theory using the Gaussian 03 program.³ All optimized structures were verified as either a minimum or a transition state by a frequency calculation, i.e. having zero or one imaginary frequencies, respectively. The imaginary frequency of the optimized transition states were confirmed to correspond to the correct motion on the potential energy surface by visualization with the GaussView program.

The continuum solvation effects were modelled by using the implementation of the conductor-like screening solvation model (CPCM) in Gaussian 03. The solvation effects were estimated from a single-point calculation of the gas-phase optimized structures at the B3LYP/6-31G(d) level of theory, i.e. B3LYP/6-31G(d) (CPCM)//B3LYP/6-31G(d).

TS1_{ROT}

Charge Multiplicity: 0 1

scf done: -2740.171033

C	-0.338372	-1.015302	1.769757
N	-1.721896	-1.463832	1.868714
C	-1.842315	-2.850075	2.327353
C	-0.404495	-3.385362	2.347710
C	0.449335	-2.118144	2.517255
H	-0.236599	-0.052139	2.281985
H	-2.296470	-2.859286	3.330966
H	-2.500773	-3.432106	1.669553
H	-0.251354	-4.105460	3.157261
H	-0.162353	-3.876657	1.403102
H	0.508834	-1.841252	3.576370
H	1.469418	-2.244378	2.150209
C	-2.752988	-0.567922	2.119810
C	-4.021329	-0.873707	2.454078
H	-2.468944	0.475422	2.001523
H	-4.324538	-1.917370	2.532332
C	-5.078348	0.158602	2.621186
C	-5.513334	0.661983	3.783778
H	-5.557022	0.509781	1.704018
H	-6.316590	1.399498	3.751233
C	-5.005726	0.307406	5.151817
H	-4.647544	1.199657	5.683572
H	-4.184088	-0.412424	5.098246
H	-5.805052	-0.123522	5.770603
C	0.202875	-0.778358	0.284067
O	0.215129	-2.047641	-0.347398
Si	0.275267	-2.664288	-1.927757
C	-1.417723	-3.342517	-2.404420
H	-1.328817	-3.950502	-3.313924
H	-1.817172	-3.992470	-1.616499
H	-2.158029	-2.562199	-2.603670
C	1.483323	-4.112216	-1.835878
H	2.514620	-3.808146	-1.622682
H	1.182967	-4.826814	-1.060333
H	1.494897	-4.651435	-2.791514
C	0.866446	-1.400358	-3.198340
H	0.931581	-1.886258	-4.180567
H	0.180987	-0.552784	-3.297736
H	1.861071	-1.004100	-2.965022
C	-0.710170	0.186989	-0.507983

C	-2.001928	-0.243843	-0.846096
C	-2.868512	0.573241	-1.573368
C	-2.468844	1.840596	-1.992237
C	-1.182903	2.272092	-1.676181
C	-0.314124	1.456458	-0.946429
H	-2.334249	-1.221937	-0.526720
H	-3.144631	2.477524	-2.549698
H	0.679256	1.830179	-0.736968
C	1.639201	-0.238169	0.445437
C	1.906080	0.938571	1.164017
C	3.214045	1.391581	1.343854
C	4.292983	0.682699	0.814907
C	4.037889	-0.493827	0.116484
C	2.729653	-0.950347	-0.055846
H	1.096640	1.526818	1.582277
H	5.307258	1.039180	0.949588
H	2.564356	-1.888503	-0.563846
C	-4.235627	0.045926	-1.924361
C	-0.693659	3.602926	-2.186968
C	3.468404	2.626231	2.171080
C	5.165939	-1.264696	-0.519113
F	4.935369	-2.597961	-0.488429
F	6.343789	-1.039097	0.097475
F	5.322912	-0.925849	-1.819182
F	4.582634	3.273510	1.770543
F	2.438847	3.497368	2.100122
F	3.636391	2.317829	3.477245
F	0.209378	4.159371	-1.350439
F	-1.705887	4.482736	-2.341152
F	-0.089732	3.477979	-3.391190
F	-5.030122	0.998882	-2.451944
F	-4.154744	-0.956112	-2.836767
F	-4.868148	-0.464555	-0.846183

TS2_{ROT}

Charge Multiplicity: 0 1

scf done: -2740.171442

C	-0.264026	-0.644369	1.984413
N	-1.632230	-1.107229	2.177373
C	-1.711187	-2.362201	2.929182
C	-0.256877	-2.832426	3.066540
C	0.554542	-1.531445	2.952978
H	-0.197104	0.409633	2.275839
H	-2.171164	-2.166326	3.910679
H	-2.345835	-3.095617	2.414990
H	-0.086706	-3.351458	4.014728
H	0.007563	-3.511523	2.253391
H	0.600182	-1.028209	3.925863
H	1.579758	-1.701847	2.619535
C	-2.694511	-0.213193	2.228146
C	-3.952231	-0.479976	2.627657
H	-2.445244	0.787876	1.883292
H	-4.221949	-1.489059	2.936809
C	-5.038317	0.533324	2.583864
C	-5.483432	1.227469	3.636873
H	-5.521844	0.694063	1.615533
H	-5.009721	1.067286	4.606873

C	-6.604912	2.226231	3.599928
H	-7.017019	2.329805	2.590241
H	-6.268669	3.217429	3.933871
H	-7.423169	1.931944	4.271618
C	0.278898	-0.718773	0.482069
O	0.342386	-2.094338	0.145957
Si	0.407811	-3.050884	-1.253814
C	-1.243421	-3.928791	-1.492070
H	-1.134533	-4.718794	-2.246309
H	-1.570131	-4.410493	-0.562471
H	-2.045761	-3.265175	-1.827599
C	1.714978	-4.363036	-0.885649
H	2.730444	-3.959515	-0.801750
H	1.490073	-4.888011	0.050358
H	1.729118	-5.113122	-1.686506
C	0.875794	-2.077548	-2.801148
H	1.033130	-2.779509	-3.630228
H	0.093066	-1.376885	-3.108458
H	1.804436	-1.510035	-2.674084
C	-0.664914	0.014164	-0.500077
C	-1.934665	-0.533778	-0.737084
C	-2.828663	0.069754	-1.622470
C	-2.478543	1.232734	-2.304889
C	-1.214457	1.776532	-2.089787
C	-0.318753	1.175603	-1.201316
H	-2.229104	-1.434058	-0.215646
H	-3.174979	1.705129	-2.986583
H	0.655410	1.629237	-1.075638
C	1.692858	-0.102231	0.515987
C	1.909652	1.209397	0.967594
C	3.197892	1.742858	1.039706
C	4.305219	0.982722	0.665212
C	4.100139	-0.323290	0.227835
C	2.812564	-0.858721	0.163876
H	1.075543	1.839269	1.257041
H	5.303773	1.400089	0.717795
H	2.685955	-1.887271	-0.138242
C	-4.175538	-0.571133	-1.835303
C	-0.776115	2.986589	-2.873980
C	3.394988	3.133796	1.587227
C	5.265965	-1.154005	-0.243272
F	5.063502	-2.472897	-0.018734
F	6.414266	-0.806171	0.373375
F	5.468062	-1.009488	-1.572514
F	4.513903	3.709124	1.100027
F	2.354056	3.940348	1.286645
F	3.508193	3.121073	2.934999
F	0.077251	3.758624	-2.166338
F	-1.824191	3.757821	-3.233262
F	-0.135606	2.633076	-4.012058
F	-4.975660	0.170814	-2.627253
F	-4.052764	-1.789678	-2.420618
F	-4.825002	-0.768726	-0.667943

TS3_{ROT}

Charge Multiplicity: 0 1

scf done: -2740.171442

C	-0.264026	-0.644369	1.984413
N	-1.632230	-1.107229	2.177373
C	-1.711187	-2.362201	2.929182
C	-0.256877	-2.832426	3.066540
C	0.554542	-1.531445	2.952978
H	-0.197104	0.409633	2.275839
H	-2.171164	-2.166326	3.910679
H	-2.345835	-3.095617	2.414990
H	-0.086706	-3.351458	4.014728
H	0.007563	-3.511523	2.253391
H	0.600182	-1.028209	3.925863
H	1.579758	-1.701847	2.619535
C	-2.694511	-0.213193	2.228146
C	-3.952231	-0.479976	2.627657
H	-2.445244	0.787876	1.883292
H	-4.221949	-1.489059	2.936809
C	-5.038317	0.533324	2.583864
C	-5.483432	1.227469	3.636873
H	-5.521844	0.694063	1.615533
H	-5.009721	1.067286	4.606873
C	-6.604912	2.226231	3.599928
H	-7.017019	2.329805	2.590241
H	-6.268669	3.217429	3.933871
H	-7.423169	1.931944	4.271618
C	0.278898	-0.718773	0.482069
O	0.342386	-2.094338	0.145957
Si	0.407811	-3.050884	-1.253814
C	-1.243421	-3.928791	-1.492070
H	-1.134533	-4.718794	-2.246309
H	-1.570131	-4.410493	-0.562471
H	-2.045761	-3.265175	-1.827599
C	1.714978	-4.363036	-0.885649
H	2.730444	-3.959515	-0.801750
H	1.490073	-4.888011	0.050358
H	1.729118	-5.113122	-1.686506
C	0.875794	-2.077548	-2.801148
H	1.033130	-2.779509	-3.630228
H	0.093066	-1.376885	-3.108458
H	1.804436	-1.510035	-2.674084
C	-0.664914	0.014164	-0.500077
C	-1.934665	-0.533778	-0.737084
C	-2.828663	0.069754	-1.622470
C	-2.478543	1.232734	-2.304889
C	-1.214457	1.776532	-2.089787
C	-0.318753	1.175603	-1.201316
H	-2.229104	-1.434058	-0.215646
H	-3.174979	1.705129	-2.986583
H	0.655410	1.629237	-1.075638
C	1.692858	-0.102231	0.515987
C	1.909652	1.209397	0.967594
C	3.197892	1.742858	1.039706
C	4.305219	0.982722	0.665212
C	4.100139	-0.323290	0.227835
C	2.812564	-0.858721	0.163876
H	1.075543	1.839269	1.257041
H	5.303773	1.400089	0.717795
H	2.685955	-1.887271	-0.138242

C	-4.175538	-0.571133	-1.835303
C	-0.776115	2.986589	-2.873980
C	3.394988	3.133796	1.587227
C	5.265965	-1.154005	-0.243272
F	5.063502	-2.472897	-0.018734
F	6.414266	-0.806171	0.373375
F	5.468062	-1.009488	-1.572514
F	4.513903	3.709124	1.100027
F	2.354056	3.940348	1.286645
F	3.508193	3.121073	2.934999
F	0.077251	3.758624	-2.166338
F	-1.824191	3.757821	-3.233262
F	-0.135606	2.633076	-4.012058
F	-4.975660	0.170814	-2.627253
F	-4.052764	-1.789678	-2.420618
F	-4.825002	-0.768726	-0.667943

(E,s-cis,Z)-4a

Charge Multiplicity: 0 1

scf done: -2740.176034

C	-0.215871	-0.437084	2.082115
N	-1.587845	-0.794613	2.416478
C	-1.682497	-2.003880	3.239785
C	-0.239515	-2.519549	3.353887
C	0.620276	-1.274016	3.078560
H	-0.079017	0.634486	2.262594
H	-2.105340	-1.734372	4.219365
H	-2.356304	-2.744405	2.789266
H	-0.042814	-2.953520	4.338823
H	-0.043180	-3.283119	2.598981
H	0.746358	-0.689698	3.997421
H	1.614672	-1.523473	2.703744
C	-2.589571	0.159004	2.460361
C	-3.857914	-0.036111	2.895155
H	-2.294220	1.124913	2.061407
H	-4.162499	-1.042680	3.176146
C	-4.907956	0.978823	2.945257
C	-4.815839	2.302701	3.181862
H	-5.913224	0.584599	2.789078
H	-5.742743	2.874461	3.148014
C	-3.582256	3.089546	3.523864
H	-3.162211	3.610435	2.650262
H	-2.794701	2.445865	3.931761
H	-3.811115	3.865070	4.265519
C	0.216553	-0.682342	0.563394
O	0.235617	-2.087759	0.370982
Si	0.217539	-3.174467	-0.934756
C	-1.466628	-4.016339	-1.033745
H	-1.400096	-4.890822	-1.693836
H	-1.785846	-4.377915	-0.048643
H	-2.255916	-3.369638	-1.428072
C	1.498473	-4.487314	-0.486706
H	2.525925	-4.106708	-0.461291
H	1.284104	-4.925392	0.495356
H	1.472281	-5.301888	-1.221487
C	0.653597	-2.365984	-2.582893
H	0.706495	-3.142459	-3.357050

H	-0.096601	-1.635647	-2.902364
H	1.626446	-1.862436	-2.560243
C	-0.786157	-0.041718	-0.423270
C	-2.072224	-0.596542	-0.510882
C	-3.017974	-0.091834	-1.402149
C	-2.708304	0.982140	-2.234988
C	-1.432903	1.535804	-2.162175
C	-0.481968	1.029230	-1.270945
H	-2.336267	-1.426569	0.129270
H	-3.445748	1.379810	-2.921424
H	0.500682	1.482192	-1.262150
C	1.638759	-0.097415	0.437988
C	1.905652	1.251825	0.719274
C	3.204854	1.758844	0.652701
C	4.274295	0.933916	0.305676
C	4.019995	-0.408736	0.038207
C	2.721789	-0.916336	0.112914
H	1.102053	1.931421	0.981162
H	5.281252	1.329988	0.249833
H	2.559284	-1.969676	-0.058302
C	-4.364859	-0.762234	-1.484758
C	-1.038261	2.646886	-3.100810
C	3.457395	3.198642	1.022523
C	5.137710	-1.321560	-0.396237
F	4.937438	-2.591264	0.027308
F	6.333166	-0.916390	0.078828
F	5.238593	-1.370005	-1.744050
F	4.557864	3.686378	0.413462
F	2.415950	3.989974	0.685305
F	3.644183	3.338920	2.354689
F	-0.185694	3.515904	-2.514149
F	-2.108447	3.348870	-3.528044
F	-0.413005	2.165507	-4.199933
F	-5.267247	-0.011689	-2.148111
F	-4.277998	-1.949753	-2.140762
F	-4.868045	-1.031577	-0.263825

(E,s-trans,Z)-4a

Charge Multiplicity: 0 1

scf done: -2740.181842

C	-0.277882	-1.167414	1.725463
N	-1.696096	-1.492598	1.822330
C	-1.940509	-2.914299	2.086374
C	-0.557943	-3.576155	1.995894
C	0.417263	-2.425370	2.296317
H	-0.074116	-0.293664	2.353294
H	-2.380218	-3.022011	3.089813
H	-2.657831	-3.335381	1.370065
H	-0.459450	-4.403610	2.704980
H	-0.380650	-3.965048	0.991273
H	0.528468	-2.296790	3.379258
H	1.410655	-2.594978	1.876878
C	-2.619770	-0.546397	2.229141
C	-3.913597	-0.767274	2.564665
H	-2.229132	0.469034	2.255769
H	-4.319718	-1.772823	2.505806
C	-4.788750	0.309119	2.990066

C	-6.087069	0.228815	3.343344
H	-4.324906	1.296508	3.023403
C	0.250466	-0.788749	0.265913
O	0.201267	-1.978613	-0.504425
Si	0.205302	-2.413399	-2.146585
C	-1.515471	-2.996066	-2.652319
H	-1.452236	-3.540637	-3.603195
H	-1.933893	-3.686881	-1.910364
H	-2.228528	-2.178209	-2.792889
C	1.375605	-3.891934	-2.243375
H	2.421748	-3.635827	-2.040236
H	1.082044	-4.670137	-1.528880
H	1.339136	-4.336481	-3.245914
C	0.795948	-1.033723	-3.290682
H	0.873304	-1.431539	-4.310949
H	0.103354	-0.186635	-3.321855
H	1.784869	-0.651118	-3.015201
C	-0.635777	0.288833	-0.397873
C	-1.936313	-0.074850	-0.780061
C	-2.783085	0.831775	-1.414997
C	-2.358170	2.131453	-1.686591
C	-1.067533	2.501326	-1.317992
C	-0.214650	1.591627	-0.685078
H	-2.289498	-1.075375	-0.574173
H	-3.019455	2.839817	-2.170880
H	0.784601	1.921159	-0.432402
C	1.709671	-0.327514	0.459986
C	2.032527	0.749347	1.301291
C	3.359185	1.132416	1.504718
C	4.401359	0.450479	0.877124
C	4.090932	-0.628233	0.053569
C	2.764034	-1.015538	-0.143076
H	1.252975	1.314772	1.799873
H	5.430463	0.752514	1.031434
H	2.554652	-1.881081	-0.753171
C	-4.143705	0.365337	-1.863517
C	-0.550383	3.872678	-1.668737
C	3.670021	2.256683	2.460025
C	5.183130	-1.353346	-0.689505
F	4.889205	-2.663779	-0.855664
F	6.366073	-1.278138	-0.046191
F	5.366166	-0.833891	-1.924638
F	4.807366	2.898745	2.121679
F	2.676313	3.170835	2.494814
F	3.831678	1.800195	3.722826
F	0.332227	4.323926	-0.750536
F	-1.547930	4.777440	-1.757609
F	0.090112	3.868795	-2.860369
F	-4.983522	1.395073	-2.092351
F	-4.055693	-0.339021	-3.023316
F	-4.721255	-0.448433	-0.959000
C	-6.947402	-1.001859	3.380492
H	-6.407107	-1.906603	3.087086
H	-7.354502	-1.170144	4.387565
H	-7.811718	-0.899956	2.709143
H	-6.584483	1.153061	3.635470

(E,s-trans,E)-4a

Charge Multiplicity: 0 1

scf done: -2740.183693

C	-0.228031	-0.838053	1.931756
N	-1.618800	-1.246842	2.097201
C	-1.754001	-2.583869	2.684739
C	-0.325363	-3.142385	2.726468
C	0.553533	-1.881267	2.764748
H	-0.102351	0.165474	2.352465
H	-2.184192	-2.491772	3.694124
H	-2.436803	-3.210126	2.096385
H	-0.168760	-3.788647	3.595358
H	-0.110229	-3.721440	1.826244
H	0.636660	-1.509663	3.792721
H	1.563871	-2.059910	2.392556
C	-2.617597	-0.307940	2.293273
C	-3.887873	-0.547969	2.695797
H	-2.312130	0.713422	2.075828
H	-4.218938	-1.566997	2.884316
C	-4.862432	0.509997	2.880613
C	-6.135811	0.335957	3.277860
H	-4.516427	1.526274	2.677286
H	-6.486242	-0.677208	3.482693
C	-7.137124	1.437195	3.465768
H	-6.703404	2.417199	3.237000
H	-7.514548	1.469772	4.498006
H	-8.015583	1.299696	2.819098
C	0.294451	-0.745597	0.424481
O	0.334410	-2.072900	-0.074210
Si	0.433571	-2.836264	-1.588815
C	-1.240553	-3.574313	-2.044601
H	-1.114350	-4.279980	-2.875876
H	-1.665043	-4.136662	-1.204023
H	-1.978211	-2.829572	-2.357697
C	1.644813	-4.259773	-1.320255
H	2.668269	-3.928486	-1.109850
H	1.324496	-4.892909	-0.484274
H	1.686176	-4.894136	-2.214666
C	1.051822	-1.696494	-2.959563
H	1.139837	-2.275022	-3.888309
H	0.367469	-0.864894	-3.155780
H	2.040159	-1.276127	-2.743190
C	-0.651080	0.102032	-0.457183
C	-1.923057	-0.416487	-0.746092
C	-2.816487	0.275733	-1.562035
C	-2.467790	1.507438	-2.113954
C	-1.205227	2.027295	-1.841437
C	-0.305401	1.332265	-1.027425
H	-2.216127	-1.367027	-0.323245
H	-3.166058	2.050378	-2.739444
H	0.670861	1.766751	-0.858220
C	1.717962	-0.156896	0.518430
C	1.958496	1.101234	1.094058
C	3.255928	1.601923	1.215123
C	4.350229	0.860874	0.768450
C	4.121689	-0.395124	0.213988
C	2.824508	-0.898931	0.102507

H	1.136097	1.715270	1.444402
H	5.356040	1.254075	0.856253
H	2.681019	-1.893975	-0.290622
C	-4.142819	-0.358678	-1.892484
C	-0.770628	3.317640	-2.487512
C	3.481666	2.930312	1.891856
C	5.265622	-1.207513	-0.335416
F	5.067764	-2.533432	-0.150452
F	6.440124	-0.884377	0.242603
F	5.408134	-1.016876	-1.667050
F	4.586326	3.547284	1.423224
F	2.436368	3.766646	1.713048
F	3.645492	2.781622	3.226088
F	0.087160	4.005833	-1.702622
F	-1.820266	4.123971	-2.752318
F	-0.136130	3.093531	-3.661236
F	-5.038223	0.543231	-2.343628
F	-4.002121	-1.297239	-2.865936
F	-4.682615	-0.982041	-0.827789

(E,s-cis,E)-4a

Charge Multiplicity: 0 1

scf done: -2740.177072

C	-0.157403	-0.617228	2.023981
N	-1.486871	-1.141406	2.320448
C	-1.403710	-2.357954	3.136583
C	-0.108987	-2.156317	3.934771
C	0.806627	-1.429236	2.936762
H	-0.137903	0.448343	2.284542
H	-2.291760	-2.434742	3.769096
H	-1.350475	-3.254236	2.504920
H	-0.316337	-1.520939	4.803881
H	0.323238	-3.094360	4.297826
H	1.535215	-0.777984	3.426555
H	1.357361	-2.156961	2.336495
C	-2.577955	-0.290296	2.393522
C	-3.862532	-0.628570	2.650566
H	-2.337834	0.751473	2.184302
H	-4.134878	-1.679975	2.720561
C	-4.945495	0.342063	2.789322
C	-4.845013	1.607963	3.232373
H	-5.934608	-0.017090	2.497202
H	-3.880387	1.965736	3.595450
C	-5.977893	2.591801	3.277617
H	-6.916285	2.137782	2.940190
H	-5.781510	3.464689	2.638365
H	-6.134856	2.980922	4.293529
C	0.284491	-0.715662	0.495492
O	0.323943	-2.098465	0.186817
Si	0.321521	-3.086861	-1.192649
C	-1.350991	-3.941576	-1.359430
H	-1.261081	-4.789425	-2.050743
H	-1.686987	-4.343218	-0.395759
H	-2.138586	-3.288365	-1.746918
C	1.620179	-4.409722	-0.834995
H	2.642609	-4.017427	-0.790458
H	1.415876	-4.909606	0.119208

H	1.600930	-5.177708	-1.618503
C	0.749088	-2.158205	-2.778811
H	0.823190	-2.879748	-3.602805
H	-0.016520	-1.425751	-3.053700
H	1.709807	-1.635070	-2.716692
C	-0.721490	-0.005965	-0.439717
C	-1.988175	-0.584850	-0.608508
C	-2.928624	-0.025981	-1.472164
C	-2.636513	1.134887	-2.186529
C	-1.382234	1.717835	-2.027060
C	-0.433124	1.151941	-1.170326
H	-2.238154	-1.482280	-0.060874
H	-3.366819	1.569654	-2.858387
H	0.540192	1.620303	-1.108838
C	1.697607	-0.100492	0.433369
C	1.940980	1.218447	0.847485
C	3.232605	1.748597	0.839330
C	4.316279	0.977523	0.420688
C	4.084687	-0.336051	0.020567
C	2.794305	-0.867665	0.035983
H	1.125355	1.854805	1.173496
H	5.317246	1.392264	0.411960
H	2.648484	-1.900999	-0.239486
C	-4.240674	-0.736701	-1.679748
C	-1.057653	3.000576	-2.748394
C	3.458686	3.149317	1.348769
C	5.222251	-1.180881	-0.492403
F	5.020594	-2.495659	-0.244134
F	6.398749	-0.834970	0.069797
F	5.367140	-1.052261	-1.830655
F	4.569593	3.702193	0.819984
F	2.417452	3.959040	1.056580
F	3.605622	3.166514	2.693388
F	-1.395299	4.081964	-2.009471
F	-1.723020	3.098910	-3.919241
F	0.262228	3.104135	-3.017849
F	-5.182953	0.077662	-2.197034
F	-4.097649	-1.775834	-2.545083
F	-4.724143	-1.253035	-0.532902

TS4a

Charge Multiplicity: 0 1

scf done: -3385.172553

C	3.468526	-0.700015	-0.742129
C	2.103385	-0.648343	-0.460317
C	1.507639	-1.781385	0.117216
C	2.272900	-2.907737	0.427668
C	3.640947	-2.941693	0.161887
C	4.230587	-1.827917	-0.431061
C	1.257704	0.588586	-0.839057
C	0.154438	0.029760	-1.831263
N	-0.917371	0.980945	-2.209007
C	-0.852654	1.288945	-3.651648
C	-0.219856	0.031943	-4.255515
C	0.773211	-0.430200	-3.176769
C	-2.064499	0.927477	-1.493345
C	-3.277540	1.602214	-1.809598

C	-4.439977	1.467815	-1.072585
C	-4.584283	0.805630	0.164709
C	1.589770	-4.073837	1.095290
F	1.265457	-3.784766	2.377008
C	5.713294	-1.799250	-0.694545
F	6.380774	-1.185247	0.309905
C	0.641392	1.285603	0.398301
C	0.667056	0.756472	1.692259
C	0.127432	1.464045	2.770630
C	-0.443725	2.719546	2.586799
C	-0.480805	3.253832	1.298360
C	0.051663	2.547155	0.220816
C	-1.183988	4.563800	1.058864
F	-1.099565	5.383208	2.127801
C	0.103562	0.828723	4.135983
F	-1.036243	0.114007	4.323924
O	2.022453	1.537481	-1.565543
Si	3.162157	2.758999	-1.279586
C	2.390425	4.420700	-1.723340
C	4.572469	2.447111	-2.496343
C	3.807282	2.773747	0.493911
F	-0.673907	5.226430	-0.004791
F	-2.500677	4.374274	0.807624
F	0.149363	1.750396	5.120776
F	1.133931	-0.021291	4.318829
F	0.435054	-4.398527	0.468489
F	2.365350	-5.177220	1.115736
F	6.005843	-1.118575	-1.827886
F	6.230762	-3.038443	-0.817909
N	-3.809025	-1.171200	-0.535555
C	-2.993288	-1.519820	0.569620
O	-1.774772	-1.456141	0.648404
N	-3.067164	-1.011561	-1.623081
C	-3.760035	-1.149356	-2.847821
O	-4.798531	-2.016886	-2.938947
C	-4.980265	-3.204665	-2.136647
C	-6.266851	-3.117645	-1.334707
O	-3.419940	-0.557641	-3.855831
O	-3.780363	-1.975965	1.559988
C	-3.109326	-2.418993	2.769081
C	-2.578458	-3.837743	2.630506
H	-0.342764	-0.801781	-1.331179
H	-1.847922	1.475514	-4.050346
H	-0.224283	2.175773	-3.801093
H	-1.008930	-0.708076	-4.411416
H	0.265609	0.230395	-5.216320
H	0.924309	-1.512781	-3.185088
H	1.744450	0.047628	-3.321633
H	-1.909374	0.578096	-0.485838
H	-3.359756	2.071050	-2.783619
H	-5.358246	1.709887	-1.608307
H	1.618331	4.746098	-1.020047
H	3.166421	5.196536	-1.743241
H	1.940434	4.385730	-2.722988
H	5.152248	1.541175	-2.287720
H	4.189455	2.364878	-3.520535
H	5.272832	3.291846	-2.476167

H	3.025178	3.017640	1.220066
H	4.252501	1.816592	0.787070
H	4.589464	3.538645	0.583323
H	0.014827	2.981674	-0.768720
H	-0.846512	3.272985	3.427058
H	1.119522	-0.205438	1.889606
H	0.443167	-1.801220	0.332039
H	4.228152	-3.820693	0.397517
H	3.945006	0.132370	-1.236833
H	-2.311553	-1.713558	3.012761
H	-3.888008	-2.359848	3.533314
H	-5.030685	-4.024981	-2.862313
H	-1.773025	-3.889205	1.893994
H	-2.179041	-4.173614	3.594422
H	-3.379462	-4.523159	2.334322
H	-6.185164	-2.336753	-0.575417
H	-7.113738	-2.895532	-1.992547
H	-6.460916	-4.076042	-0.838203
H	-4.116873	-3.369092	-1.490933
C	-3.792204	1.170694	1.398159
H	-3.798208	0.374008	2.145381
H	-2.763772	1.464083	1.189639
H	-4.280966	2.040400	1.861589
H	-5.599597	0.489285	0.395755

TS4b

Charge Multiplicity: 0 1

scf done: -3385.186234

C	3.553422	-0.552634	-0.719536
C	2.189794	-0.553844	-0.423293
C	1.644160	-1.704656	0.167861
C	2.457492	-2.794021	0.487834
C	3.823368	-2.774645	0.210304
C	4.362182	-1.646466	-0.404430
C	1.291844	0.643336	-0.805755
C	0.234919	0.036500	-1.823515
N	-0.876320	0.935333	-2.208101
C	-0.822021	1.249149	-3.649026
C	-0.119246	0.027549	-4.248631
C	0.894817	-0.374248	-3.164991
C	-2.023361	0.842551	-1.492866
C	-3.233756	1.538391	-1.767099
C	-4.355721	1.420073	-0.964957
C	-4.419086	0.663617	0.214426
C	-5.721079	0.403661	0.913448
C	1.833522	-3.973027	1.189731
F	0.661603	-4.330489	0.615123
C	5.816942	-1.621978	-0.794699
F	6.327859	-0.368635	-0.739479
C	0.613751	1.298494	0.422302
C	0.677402	0.787760	1.722294
C	0.065249	1.453667	2.788655
C	-0.623612	2.645931	2.585739
C	-0.688056	3.167693	1.293402
C	-0.075698	2.506208	0.230254
C	-1.483407	4.419669	1.030993
F	-1.505692	5.235849	2.105862

C	0.110584	0.844797	4.165656
F	-0.938164	0.005901	4.370939
O	2.025529	1.634365	-1.508480
Si	3.059916	2.933103	-1.161611
C	2.202224	4.528895	-1.682376
C	4.577222	2.701422	-2.261744
C	3.581300	3.006876	0.650471
F	-0.981476	5.127534	-0.007953
F	-2.768370	4.131477	0.724072
F	0.048887	1.783917	5.132822
F	1.232420	0.123404	4.363169
F	2.637619	-5.056109	1.181005
F	1.558733	-3.686100	2.483372
F	6.001207	-2.063307	-2.059232
F	6.567145	-2.401789	0.011561
N	-3.716615	-1.275456	-0.583552
C	-2.890238	-1.607011	0.520644
O	-1.670596	-1.544283	0.585364
N	-2.980145	-1.060127	-1.665433
C	-3.661319	-1.198035	-2.898016
O	-4.611761	-2.155713	-3.024223
C	-4.688302	-3.377145	-2.256131
C	-5.990944	-3.436433	-1.478071
O	-3.377003	-0.540081	-3.881055
O	-3.667750	-2.030673	1.533560
C	-2.989417	-2.396905	2.763795
C	-2.423541	-3.807385	2.700530
H	-0.222499	-0.826029	-1.337225
H	-1.825336	1.380946	-4.049796
H	-0.239587	2.167320	-3.797187
H	-0.864861	-0.756917	-4.406047
H	0.357030	0.248347	-5.209150
H	1.121666	-1.443467	-3.178617
H	1.831011	0.172000	-3.299502
H	-1.850423	0.506439	-0.481541
H	-3.332453	2.060625	-2.711932
H	-5.293748	1.792317	-1.375453
H	-3.541099	0.664483	0.854771
H	-6.553174	0.356950	0.204038
H	-5.936629	1.201471	1.639703
H	-5.678093	-0.539411	1.464490
H	2.913336	5.364060	-1.648560
H	1.834898	4.455446	-2.713215
H	1.354742	4.792437	-1.042564
H	5.240410	1.896082	-1.927025
H	4.285727	2.487408	-3.296713
H	5.171190	3.624150	-2.272715
H	4.361292	3.770373	0.766847
H	2.754866	3.275298	1.316214
H	4.001018	2.056741	0.999447
H	-0.130573	2.934180	-0.760912
H	-1.084469	3.167339	3.416547
H	1.218863	-0.124077	1.933475
H	0.582702	-1.765238	0.388823
H	4.450768	-3.620887	0.462520
H	3.990117	0.299248	-1.218513
H	-2.210336	-1.660785	2.973224

H	-3.771591	-2.317450	3.522606
H	-4.645492	-4.178807	-3.002682
H	-1.608958	-3.876063	1.975446
H	-2.027632	-4.085035	3.684239
H	-3.204939	-4.525848	2.431353
H	-6.002880	-2.666563	-0.703391
H	-6.844058	-3.286224	-2.147989
H	-6.096454	-4.419544	-1.003743
H	-3.823249	-3.473641	-1.599025

TS5a

Charge Multiplicity: 0 1

scf done: -3385.170561

C	0.219511	-1.234307	-0.539077
N	-1.065222	-0.591444	-0.873272
C	-1.534952	-0.974029	-2.218681
C	-0.980646	-2.392436	-2.382430
C	0.299257	-2.440841	-1.515946
H	0.171285	-1.548605	0.508214
H	-2.625333	-0.968592	-2.234944
H	-1.134167	-0.271591	-2.956772
H	-1.730701	-3.089688	-2.004146
H	-0.776975	-2.631611	-3.429960
H	0.356544	-3.383332	-0.964480
H	1.198072	-2.362381	-2.130106
C	-1.785348	0.105215	-0.000377
C	-2.989923	0.752859	-0.274178
H	-1.391703	0.128708	1.013122
H	-3.322941	0.823090	-1.301050
C	-3.831054	1.203937	0.736053
C	-5.177893	1.534064	0.467708
H	-3.521552	1.079288	1.772878
C	1.433266	-0.232535	-0.690468
O	1.460580	0.125492	-2.057817
Si	2.475123	0.618003	-3.324239
C	1.271142	0.734658	-4.765772
H	1.790148	1.038755	-5.682868
H	0.788010	-0.229383	-4.961830
H	0.482297	1.471192	-4.573805
C	3.816173	-0.652798	-3.705294
H	4.656282	-0.617516	-3.005160
H	3.420019	-1.675001	-3.709892
H	4.218434	-0.455681	-4.707461
C	3.253041	2.314895	-3.022554
H	3.652908	2.683793	-3.976431
H	2.529296	3.057387	-2.668248
H	4.091627	2.300760	-2.317474
C	1.178135	1.022057	0.171474
C	0.691608	2.191965	-0.410224
C	0.452369	3.330136	0.364278
C	0.666683	3.311171	1.738621
C	1.129175	2.133703	2.331709
C	1.387812	1.002814	1.557341
H	0.497084	2.215140	-1.474588
H	0.474962	4.192026	2.339161
H	1.762072	0.107380	2.042860
C	2.763058	-0.876453	-0.234358

C	2.885826	-2.177161	0.261060
C	4.132303	-2.681701	0.651500
C	5.280609	-1.903911	0.546579
C	5.164110	-0.599281	0.064456
C	3.921674	-0.090734	-0.300495
H	2.023381	-2.822282	0.364994
H	6.243834	-2.297343	0.848911
H	3.853282	0.939294	-0.628732
C	-0.035276	4.572311	-0.336295
C	1.421997	2.103938	3.811172
C	4.226160	-4.109196	1.130635
C	6.394761	0.244339	-0.144992
F	6.881364	0.076412	-1.399112
F	7.381586	-0.078351	0.712548
F	6.130633	1.560596	-0.000607
F	4.288506	-4.970442	0.091061
F	5.322232	-4.313096	1.887819
F	3.146069	-4.455304	1.864971
F	1.234998	0.869549	4.327773
F	0.632731	2.958893	4.492647
F	2.702578	2.450741	4.066944
F	-0.198777	5.607030	0.508916
F	0.843101	4.960418	-1.293284
F	-1.214273	4.355945	-0.957545
N	-5.919776	-0.277359	0.374536
N	-5.330948	-1.031427	-0.554579
C	-7.286208	-0.024637	0.244907
C	-4.473543	-1.980310	-0.024353
O	-7.877408	0.945205	0.697107
O	-3.753502	-2.692710	-0.722491
O	-4.539667	-2.140964	1.337487
O	-7.920540	-1.083245	-0.316970
C	-9.358093	-0.998517	-0.316476
H	-9.666680	-0.102239	-0.865451
H	-9.712428	-0.888626	0.714158
C	-9.881266	-2.268031	-0.963821
H	-9.565138	-3.151685	-0.400206
H	-10.976609	-2.248492	-0.993194
H	-9.508032	-2.364515	-1.988392
C	-3.846481	-3.273464	1.877563
H	-4.396443	-3.528175	2.788814
H	-3.910608	-4.107770	1.173811
C	-2.390758	-2.958975	2.199730
H	-1.915384	-3.815551	2.692722
H	-1.844806	-2.745104	1.275814
H	-2.318589	-2.095235	2.870470
C	-5.563935	2.123661	-0.875499
H	-5.000281	3.044175	-1.075292
H	-5.368194	1.418164	-1.691312
H	-6.628176	2.364156	-0.879152
H	-5.767103	1.880487	1.308890

TS5b

Charge Multiplicity: 0 1

scf done: -3385.181540

C	0.031743	-1.189191	-0.447779
N	-1.214345	-0.545067	-0.923956

C	-1.818042	-1.277234	-2.052610
C	-1.335630	-2.709699	-1.820092
C	0.062764	-2.544971	-1.200747
H	-0.065339	-1.336439	0.632113
H	-2.905362	-1.203658	-1.980367
H	-1.467410	-0.853368	-3.000560
H	-2.013597	-3.179431	-1.103188
H	-1.318289	-3.298732	-2.741820
H	0.295290	-3.372454	-0.526902
H	0.833700	-2.518452	-1.974781
C	-1.883960	0.348391	-0.199672
C	-3.125151	0.904596	-0.503384
H	-1.429764	0.604723	0.752728
H	-3.575305	0.717101	-1.471214
C	-3.892985	1.510621	0.488114
C	-5.298731	1.512302	0.368023
H	-3.445952	1.672998	1.468448
H	-5.692042	1.717106	-0.624232
C	-6.161207	2.005657	1.501591
H	-5.858471	1.545250	2.446780
H	-7.207875	1.760627	1.311216
H	-6.081159	3.096892	1.601590
C	1.296086	-0.285454	-0.721477
O	1.352149	-0.093254	-2.117705
Si	2.341296	-0.109315	-3.488876
C	1.095774	-0.188532	-4.898058
H	1.604802	-0.162773	-5.869356
H	0.502618	-1.109479	-4.859184
H	0.400355	0.658148	-4.866928
C	3.493785	-1.601743	-3.560018
H	4.362905	-1.504882	-2.902034
H	2.979337	-2.536188	-3.307326
H	3.870910	-1.706512	-4.585709
C	3.341425	1.489157	-3.628830
H	3.722373	1.583172	-4.654126
H	2.733536	2.379014	-3.427402
H	4.212021	1.521495	-2.964450
C	1.110449	1.084343	-0.032173
C	0.857895	2.231182	-0.782325
C	0.677283	3.468145	-0.156463
C	0.710460	3.573532	1.230002
C	0.944116	2.422666	1.987737
C	1.159767	1.194537	1.364496
H	0.803986	2.157766	-1.860369
H	0.567881	4.531947	1.714016
H	1.373826	0.324444	1.977074
C	2.593417	-0.913486	-0.164407
C	2.646227	-2.079402	0.602179
C	3.869679	-2.570234	1.077135
C	5.060436	-1.913204	0.790479
C	5.012646	-0.736397	0.039287
C	3.795931	-0.236153	-0.410153
H	1.746742	-2.625129	0.855453
H	6.005233	-2.297614	1.155856
H	3.782012	0.701152	-0.952704
C	0.424607	4.675823	-1.022775
C	0.895607	2.493663	3.492721

C	3.877312	-3.859892	1.859442
C	6.290711	-0.049548	-0.365332
F	6.771975	-0.575753	-1.517930
F	7.254132	-0.184834	0.566553
F	6.106115	1.270408	-0.584169
F	3.727975	-4.926754	1.042956
F	5.027927	-4.030654	2.539880
F	2.861387	-3.900860	2.749039
F	-0.356150	2.246389	3.949351
F	1.250889	3.710761	3.950658
F	1.710525	1.582526	4.064870
F	0.474742	5.825217	-0.321344
F	1.341730	4.760295	-2.015774
F	-0.786324	4.612005	-1.616442
N	-5.732355	-0.372828	0.220777
N	-4.751436	-1.238328	-0.049754
C	-6.813604	-0.436478	-0.680564
C	-3.991497	-1.597591	1.048189
O	-7.512740	0.508518	-1.012512
O	-3.075807	-2.416975	0.981090
O	-4.326615	-0.980991	2.224491
O	-7.086836	-1.713738	-1.026762
C	-8.285472	-1.891848	-1.807193
H	-8.200637	-1.314005	-2.733810
H	-9.139574	-1.492786	-1.249671
C	-8.427556	-3.378927	-2.075827
H	-8.511492	-3.938018	-1.138488
H	-9.327025	-3.565862	-2.673138
H	-7.560692	-3.760090	-2.625006
C	-3.655139	-1.455817	3.405485
H	-4.336569	-1.208778	4.224769
H	-3.549640	-2.542128	3.341025
C	-2.295607	-0.801310	3.615607
H	-1.866451	-1.130205	4.569606
H	-1.609601	-1.094013	2.815364
H	-2.373239	0.290927	3.640193

TS6a

Charge Multiplicity: 0 1

scf done: -3385.16615731

C	0.003375	-1.999900	-1.880282
C	-0.035853	-0.963664	-0.739196
N	-1.384032	-0.397127	-0.890217
C	-1.852936	-0.440858	-2.293262
C	-0.889148	-1.417917	-2.998928
C	1.152537	0.090899	-0.788513
O	1.196728	0.585463	-2.113879
Si	1.947574	1.876041	-2.943603
C	2.612342	1.103543	-4.531148
C	-2.129035	-0.073431	0.148920
C	-3.506593	0.311884	0.114080
N	-4.370725	-1.297607	-0.029428
N	-4.886016	-1.765106	1.124890
C	-4.012227	-2.509661	1.864655
O	-4.324645	-3.125506	2.872652
C	2.422371	-0.721087	-0.450269
C	3.468552	-0.819864	-1.366822

C	4.616777	-1.561002	-1.081684
C	4.737746	-2.250777	0.120729
C	3.681878	-2.191543	1.030445
C	2.540484	-1.439444	0.749818
C	3.779315	-2.896548	2.360698
F	4.158153	-2.043706	3.337948
C	5.737540	-1.545728	-2.089022
F	6.643709	-2.514578	-1.861781
C	0.903257	1.260507	0.195514
C	-0.082912	2.201582	-0.139330
C	-0.365858	3.283512	0.691562
C	0.331326	3.461678	1.885959
C	1.323164	2.544513	2.220903
C	1.610503	1.459447	1.385902
C	-1.395380	4.290597	0.245805
F	-0.874074	5.142598	-0.673417
C	2.078320	2.679245	3.520184
F	1.594777	1.832616	4.455417
F	-2.456216	3.692356	-0.338355
F	-1.850806	5.037320	1.268240
F	1.994885	3.926777	4.023911
F	3.387241	2.385110	3.360989
F	2.587226	-3.415368	2.730006
F	4.675874	-3.901652	2.332031
F	6.391919	-0.361351	-2.064529
F	5.269315	-1.703567	-3.349252
C	-3.993663	0.982512	1.337314
C	-4.890502	1.978808	1.384379
C	3.336392	2.684891	-1.956762
C	0.645244	3.154380	-3.417248
C	-5.248403	-1.161050	-1.099067
O	-5.069351	-0.419837	-2.068842
O	-6.257592	-2.048916	-1.038593
C	-7.121306	-2.085319	-2.193119
C	-8.185534	-3.131735	-1.918530
O	-2.675885	-2.478459	1.430995
C	-1.775399	-3.266739	2.228478
C	-1.791797	-4.732238	1.815071
H	0.000819	-1.445663	0.238290
H	-2.898898	-0.750951	-2.314358
H	-1.801198	0.568164	-2.718880
H	-1.441365	-2.206595	-3.516505
H	-0.281975	-0.890693	-3.736359
H	-0.425640	-2.932693	-1.500787
H	1.018803	-2.208930	-2.220647
H	-1.639514	-0.163252	1.112158
H	-3.836774	0.735546	-0.827422
H	-3.595050	0.602582	2.276585
H	1.066110	3.833930	-4.169385
H	-0.235082	2.681562	-3.869690
H	0.304947	3.770244	-2.579062
H	3.414366	0.374927	-4.367410
H	1.813155	0.596017	-5.084346
H	3.015352	1.886756	-5.185461
H	3.746442	3.514634	-2.547068
H	2.988780	3.103576	-1.006733
H	4.163305	1.999500	-1.742118

H	-0.629561	2.099435	-1.066693
H	0.112260	4.300487	2.535215
H	2.412573	0.792611	1.674350
H	1.743581	-1.428126	1.485875
H	5.623288	-2.834965	0.339060
H	3.385871	-0.338709	-2.329392
H	-7.553612	-1.091557	-2.349155
H	-6.526100	-2.328746	-3.080075
H	-0.782872	-2.827360	2.064625
H	-2.040586	-3.161885	3.283612
H	-8.873698	-3.194316	-2.769007
H	-7.733689	-4.116533	-1.763580
H	-8.760305	-2.875052	-1.023366
H	-1.048097	-5.297194	2.389980
H	-2.778485	-5.160715	2.007943
H	-1.561114	-4.841337	0.749133
C	-5.587497	2.644165	0.233102
H	-6.668452	2.681721	0.417804
H	-5.248465	3.683450	0.123099
H	-5.433035	2.129563	-0.718763
H	-5.151265	2.361970	2.370698

TS6b

Charge Multiplicity: 0 1

scf done: -3385.168048

C	0.148435	-1.737171	-2.324892
C	-0.006987	-0.840776	-1.079487
N	-1.335105	-0.242354	-1.293155
C	-1.742740	-0.237060	-2.717522
C	-0.629851	-1.014552	-3.443215
C	1.196206	0.184406	-0.877445
O	1.453142	0.773194	-2.139246
Si	2.345884	2.107152	-2.721778
C	3.244474	1.452069	-4.245152
C	-2.137736	0.037749	-0.284230
C	-3.514267	0.399778	-0.360512
N	-4.232935	-1.329382	-0.274226
N	-4.753097	-1.643510	0.922450
C	-3.881906	-2.305858	1.751121
O	-4.209952	-2.780213	2.827331
C	2.376834	-0.701891	-0.421980
C	3.523360	-0.827586	-1.209181
C	4.571680	-1.667496	-0.830920
C	4.492837	-2.422740	0.337680
C	3.343155	-2.324438	1.118337
C	2.298509	-1.477889	0.742765
C	3.206272	-3.105801	2.401335
F	3.321120	-2.297426	3.477636
C	5.818730	-1.709568	-1.677709
F	6.463906	-2.887042	-1.563967
C	0.836480	1.293218	0.141580
C	-0.088182	2.272612	-0.256281
C	-0.453005	3.314319	0.593134
C	0.098485	3.413340	1.870619
C	1.029465	2.459376	2.269958
C	1.398580	1.413628	1.416395
C	-1.393316	4.377483	0.085225

F	-0.716190	5.336015	-0.596338
C	1.626204	2.514302	3.654942
F	0.988917	1.672981	4.497285
F	-2.310632	3.871524	-0.766024
F	-2.052237	4.992002	1.087132
F	1.547331	3.751359	4.185663
F	2.927763	2.152322	3.643810
F	1.992992	-3.699012	2.484050
F	4.141797	-4.067682	2.511690
F	6.687463	-0.738550	-1.317320
F	5.537757	-1.518932	-2.987597
C	-4.057527	1.138870	0.795000
C	-4.765821	2.269071	0.681926
C	-5.320458	3.054385	1.832188
C	3.565590	2.786860	-1.455284
C	1.152607	3.456050	-3.280471
C	-5.048836	-1.428080	-1.393010
O	-4.861074	-0.849774	-2.464397
O	-6.007629	-2.360055	-1.225752
C	-6.801251	-2.648331	-2.394611
C	-7.803160	-3.716958	-1.997970
O	-2.552581	-2.370251	1.314329
C	-1.676881	-3.114429	2.180597
C	-1.779385	-4.614361	1.939723
H	-0.075008	-1.436747	-0.168967
H	-2.730579	-0.700033	-2.798384
H	-1.833274	0.798086	-3.067398
H	-1.050320	-1.720127	-4.164703
H	0.030984	-0.332257	-3.980343
H	-0.312891	-2.705738	-2.105467
H	1.192906	-1.912433	-2.587512
H	-1.707054	-0.102683	0.700580
H	-3.876093	0.716021	-1.333426
H	-3.864217	0.715541	1.779796
H	-4.947957	2.677748	-0.312921
H	-5.129196	2.558519	2.789136
H	-6.404705	3.193367	1.730660
H	-4.873345	4.057614	1.867619
H	1.690061	4.177795	-3.908856
H	0.340118	3.041441	-3.889559
H	0.704436	4.016824	-2.454538
H	4.004284	0.695486	-4.018697
H	2.536932	1.007642	-4.955182
H	3.752187	2.275819	-4.762409
H	4.149471	3.589860	-1.923501
H	3.063940	3.215930	-0.582081
H	4.276164	2.032503	-1.100847
H	-0.519792	2.231997	-1.246887
H	-0.184393	4.220976	2.534946
H	2.151601	0.716864	1.760907
H	1.418415	-1.437700	1.376029
H	5.299090	-3.086627	0.625050
H	3.591205	-0.292578	-2.144324
H	-7.293297	-1.729429	-2.730115
H	-6.142658	-2.983651	-3.203280
H	-0.666941	-2.757308	1.945515
H	-1.907061	-2.873776	3.221785

H	-8.437906	-3.968945	-2.855011
H	-7.292455	-4.625848	-1.664563
H	-8.442747	-3.365940	-1.182275
H	-1.041712	-5.145045	2.553601
H	-2.777285	-4.968916	2.209396
H	-1.590065	-4.854083	0.887427

DEAD 5

Charge Multiplicity: 0 1

scf done: -645.014926

N	0.271528	0.314098	-0.464572
N	-0.271503	-0.314031	0.464362
C	1.582122	0.821743	-0.109408
C	-1.582087	-0.821686	0.109192
O	-2.482175	0.157700	0.115376
O	2.482153	-0.157701	-0.115289
C	-3.860602	-0.252803	-0.110173
H	-3.923659	-0.706763	-1.103559
H	-4.116601	-1.017838	0.628924
C	3.860583	0.252767	0.110295
H	4.116709	1.017589	-0.628979
H	3.923572	0.706986	1.103566
O	-1.771680	-1.999699	-0.060397
O	1.771777	1.999782	0.059930
C	4.724976	-0.985771	-0.012842
H	4.435148	-1.739604	0.725509
H	4.638169	-1.426297	-1.010850
H	5.773624	-0.719354	0.157715
C	-4.725069	0.985643	0.013377
H	-5.773713	0.719198	-0.157153
H	-4.638198	1.425907	1.011494
H	-4.435364	1.739694	-0.724800

9a

Charge Multiplicity: 0 1

scf done: -3385.234563

C	3.475262	-0.654978	-0.506016
C	2.096532	-0.561990	-0.308002
C	1.432454	-1.679894	0.221734
C	2.141427	-2.826975	0.584701
C	3.522631	-2.899168	0.411515
C	4.181239	-1.804873	-0.146053
C	1.307631	0.688469	-0.745789
C	0.320276	0.166390	-1.898298
N	-0.827321	1.028970	-2.206140
C	-0.770047	1.493072	-3.604814
C	0.090877	0.448827	-4.328939
C	1.069494	-0.035092	-3.242800
C	-2.038887	0.694812	-1.525715
C	-3.187308	1.667242	-1.667032
C	-4.429448	1.272509	-1.378320
C	-4.807886	-0.126012	-0.910192
C	1.385328	-3.968445	1.214761
F	0.230589	-4.227400	0.557153
C	5.659121	-1.878979	-0.426408
F	6.245986	-0.661045	-0.343004

C	0.530811	1.362781	0.406412
C	0.393712	0.841600	1.695710
C	-0.322415	1.534349	2.679117
C	-0.913812	2.763087	2.401426
C	-0.773296	3.295388	1.119197
C	-0.057540	2.610111	0.139296
C	-1.349495	4.644879	0.784674
F	-2.286315	5.035855	1.672327
C	-0.400188	0.953776	4.065830
F	-0.604885	-0.386925	4.034931
O	2.168938	1.662800	-1.319071
Si	3.254280	2.852403	-0.789737
C	2.542986	4.552714	-1.190337
C	4.815866	2.616775	-1.825330
C	3.672875	2.716674	1.045353
F	-0.390334	5.604251	0.771095
F	-1.920607	4.656990	-0.442900
F	-1.402471	1.496864	4.789212
F	0.744721	1.150997	4.755948
F	2.106801	-5.109622	1.230783
F	1.046677	-3.690897	2.495128
F	5.909420	-2.348642	-1.669563
F	6.295228	-2.695579	0.440250
N	-3.564841	-0.937865	-0.697314
C	-3.013803	-1.445672	0.469674
O	-1.819875	-1.666117	0.605265
N	-2.615187	-0.702625	-1.711541
C	-2.982783	-1.186624	-2.973333
O	-3.568049	-2.408585	-2.991484
C	-3.067823	-3.508443	-2.188970
C	-4.237273	-4.247176	-1.562504
O	-2.821374	-0.567026	-4.002041
O	-3.935355	-1.718769	1.407837
C	-3.421224	-2.200325	2.682995
C	-3.065935	-3.678009	2.637329
H	-0.068296	-0.788571	-1.536567
H	-1.772361	1.571701	-4.024661
H	-0.292284	2.483326	-3.639222
H	-0.549622	-0.365810	-4.674761
H	0.611340	0.865179	-5.198182
H	1.361900	-1.080677	-3.377594
H	1.978424	0.568473	-3.251298
H	-1.770006	0.642970	-0.466894
H	-2.969053	2.694628	-1.941100
H	-5.262796	1.965513	-1.473075
H	3.326222	5.314754	-1.088024
H	2.184044	4.591998	-2.225982
H	1.716075	4.844290	-0.535809
H	5.390648	1.727263	-1.544273
H	4.574878	2.537595	-2.891912
H	5.478956	3.482336	-1.701629
H	4.440077	3.461395	1.293972
H	2.809124	2.906157	1.690416
H	4.078147	1.731897	1.303097
H	0.033320	3.033643	-0.850900
H	-1.474232	3.291989	3.162406
H	0.835053	-0.110680	1.958866

H	0.355545	-1.673045	0.356361
H	4.070273	-3.788815	0.697991
H	4.004990	0.166730	-0.964185
H	-2.561230	-1.590950	2.967668
H	-4.245384	-2.007672	3.373757
H	-2.525262	-4.162331	-2.881812
H	-2.201380	-3.852747	1.992740
H	-2.815111	-4.020524	3.647967
H	-3.913596	-4.270931	2.277407
H	-4.755230	-3.618756	-0.831963
H	-4.953793	-4.554054	-2.331158
H	-3.875689	-5.146733	-1.051467
H	-2.362463	-3.144482	-1.439402
C	-5.782286	-0.044198	0.270741
H	-6.130639	-1.029510	0.581561
H	-5.340659	0.461034	1.133155
H	-6.647947	0.540051	-0.060599
H	-5.340486	-0.631320	-1.729580

9b

Charge Multiplicity: 0 1

scf done: -3385.197199

C	0.101058	-0.982115	-0.783056
N	-1.046193	-0.170463	-1.237680
C	-1.330635	-0.403315	-2.668976
C	-0.954325	-1.877257	-2.850737
C	0.152246	-2.153016	-1.804950
H	-0.120753	-1.330797	0.230515
H	-2.389139	-0.237727	-2.867409
H	-0.716674	0.273139	-3.271022
H	-1.847357	-2.474515	-2.649445
H	-0.619596	-2.087218	-3.870582
H	-0.023478	-3.108313	-1.301728
H	1.136895	-2.205142	-2.271000
C	-1.855947	0.475692	-0.408582
C	-2.975608	1.227961	-0.778869
H	-1.628243	0.363021	0.648875
H	-3.164487	1.405271	-1.829322
C	-3.934933	1.586794	0.144135
C	-5.337622	1.840404	-0.280311
H	-3.769471	1.405058	1.204038
C	1.427427	-0.124448	-0.721506
O	1.709506	0.281043	-2.046456
Si	2.954844	0.278302	-3.201522
C	2.049801	0.789256	-4.769549
H	2.746321	0.851203	-5.614615
H	1.266879	0.071059	-5.038521
H	1.578447	1.772742	-4.658912
C	3.732718	-1.425166	-3.423557
H	4.238543	-1.786528	-2.522563
H	2.997762	-2.179879	-3.726375
H	4.486025	-1.370448	-4.220249
C	4.286648	1.557092	-2.804485
H	4.820883	1.812374	-3.728862
H	3.856713	2.487810	-2.415050
H	5.036105	1.201313	-2.090702
C	1.168664	1.128997	0.141654

C	1.035886	2.387106	-0.444173
C	0.782106	3.515410	0.342128
C	0.635082	3.402927	1.720919
C	0.754582	2.142293	2.310653
C	1.027782	1.018789	1.531798
H	1.131941	2.485414	-1.518256
H	0.438419	4.277907	2.328196
H	1.147840	0.057310	2.021426
C	2.602444	-0.908326	-0.094784
C	2.554775	-2.262834	0.247906
C	3.673511	-2.904603	0.789740
C	4.863023	-2.211246	0.995750
C	4.913167	-0.855279	0.672662
C	3.793506	-0.211267	0.150700
H	1.652598	-2.844092	0.110671
H	5.727091	-2.709953	1.417415
H	3.845803	0.851500	-0.058081
C	0.693748	4.855636	-0.343172
C	0.527419	1.975812	3.792092
C	3.592496	-4.379808	1.095381
C	6.183554	-0.063111	0.851776
F	6.757616	0.207000	-0.347337
F	7.094066	-0.721511	1.592852
F	5.944842	1.124964	1.445229
F	3.798037	-5.121600	-0.015416
F	4.512567	-4.755238	2.005418
F	2.374939	-4.716565	1.574760
F	-0.757929	1.642488	4.050321
F	0.792338	3.108187	4.472633
F	1.299910	0.994051	4.305762
F	0.364670	5.845120	0.509174
F	1.874218	5.185043	-0.916489
F	-0.227478	4.839510	-1.330997
N	-5.786278	0.414985	-0.402194
N	-5.381492	-0.286524	-1.521831
C	-6.597457	-0.066951	0.617913
C	-4.644449	-1.395952	-1.275428
O	-6.815665	0.536657	1.659721
O	-4.186740	-2.132368	-2.154202
O	-4.391638	-1.680677	0.070251
O	-7.168311	-1.240354	0.287179
C	-8.033595	-1.799841	1.292746
H	-8.819636	-1.076774	1.533779
H	-7.454915	-1.973180	2.206948
C	-8.602529	-3.088454	0.727882
H	-7.802903	-3.796271	0.487123
H	-9.270357	-3.554154	1.461297
H	-9.172227	-2.894121	-0.186290
C	-3.752139	-2.928943	0.325549
H	-4.226114	-3.717183	-0.267949
H	-2.699046	-2.885360	0.008052
C	-3.853521	-3.207698	1.817281
H	-3.358042	-4.154177	2.063911
H	-3.382904	-2.409151	2.401748
H	-4.901589	-3.275942	2.126451
C	-5.575697	2.619928	-1.569276
H	-5.183494	2.084545	-2.436164

H	-6.651345	2.752731	-1.722228
H	-5.109473	3.609351	-1.502438
H	-5.913591	2.262718	0.541905

9c

Charge Multiplicity: 0 1

scf done: -3385.186693

C	0.012818	-1.169815	-2.627957
C	-0.205380	-0.459678	-1.276917
N	-1.445731	0.306405	-1.544786
C	-1.613372	0.613793	-2.988958
C	-0.496634	-0.179976	-3.693095
C	1.039683	0.388166	-0.784597
O	1.440302	1.205577	-1.870425
Si	2.491150	2.528841	-2.117327
C	3.408570	2.117351	-3.714102
C	-2.389253	0.406493	-0.634199
C	-3.839850	0.643005	-0.855570
N	-4.259401	-0.735648	-0.464517
N	-4.670464	-0.951169	0.838183
C	-3.914416	-1.823676	1.546995
O	-4.184505	-2.217913	2.672453
C	2.122226	-0.664505	-0.452000
C	3.331811	-0.680639	-1.146398
C	4.317264	-1.628050	-0.867507
C	4.107363	-2.609710	0.097212
C	2.886489	-2.629630	0.769241
C	1.905470	-1.673293	0.498019
C	2.596099	-3.670982	1.821330
F	2.439426	-3.102433	3.036138
C	5.630784	-1.519093	-1.597288
F	6.379641	-2.630571	-1.472761
C	0.676813	1.283872	0.426713
C	-0.091462	2.433480	0.184704
C	-0.418292	3.315349	1.212756
C	-0.004024	3.065888	2.520875
C	0.757319	1.929010	2.773320
C	1.101890	1.052343	1.739426
C	-1.142757	4.594511	0.882857
F	-0.266907	5.561310	0.505978
C	1.192567	1.606229	4.182332
F	0.340414	0.744675	4.773697
F	-2.004712	4.433904	-0.145247
F	-1.833035	5.073236	1.933564
F	1.248684	2.712270	4.952693
F	2.415433	1.031398	4.199230
F	1.448977	-4.334159	1.546935
F	3.581123	-4.584002	1.919038
F	6.360153	-0.480214	-1.126126
F	5.443856	-1.291640	-2.918601
C	-4.457974	1.705383	0.013082
C	-4.827535	2.922327	-0.400708
C	3.705465	2.793633	-0.699109
C	1.474582	4.089017	-2.417572
C	-4.257066	-1.684604	-1.471058
O	-3.791441	-1.489989	-2.593890
O	-4.846552	-2.823910	-1.087164

C	-4.888998	-3.868900	-2.080768
C	-5.684373	-5.016977	-1.488449
O	-2.713613	-2.245763	0.917601
C	-1.992673	-3.252864	1.641958
C	-2.563472	-4.645750	1.408771
H	-0.449944	-1.170598	-0.487109
H	-2.600783	0.266758	-3.292202
H	-1.531259	1.694724	-3.141742
H	-0.885211	-0.701155	-4.571730
H	0.308477	0.482881	-4.011761
H	-0.604573	-2.073434	-2.634673
H	1.052512	-1.461220	-2.786541
H	-2.119127	0.118200	0.375106
H	-4.071217	0.789606	-1.908391
H	-4.599527	1.407052	1.046704
H	2.115800	4.851380	-2.878353
H	0.648238	3.901402	-3.114126
H	1.057243	4.525826	-1.505447
H	4.075202	1.251707	-3.628557
H	2.706191	1.914204	-4.531288
H	4.025644	2.971976	-4.018841
H	4.283747	3.704821	-0.900018
H	3.204333	2.933540	0.264085
H	4.421161	1.971286	-0.593703
H	-0.418853	2.657596	-0.821280
H	-0.259914	3.748969	3.321961
H	1.730033	0.205781	1.981973
H	0.970152	-1.728836	1.045663
H	4.868775	-3.348551	0.313293
H	3.506435	0.035733	-1.934343
H	-5.350223	-3.476708	-2.992556
H	-3.863207	-4.165080	-2.327372
H	-0.962136	-3.197598	1.271917
H	-2.005796	-3.009892	2.707722
H	-5.743431	-5.838607	-2.211009
H	-5.211178	-5.389453	-0.574975
H	-6.701373	-4.697224	-1.241502
H	-1.952937	-5.397004	1.924496
H	-3.583147	-4.697712	1.799160
H	-2.577453	-4.887069	0.339786
C	-4.736131	3.515177	-1.778273
H	-5.713424	3.897797	-2.098970
H	-4.045871	4.368783	-1.782641
H	-4.392005	2.803352	-2.535130
H	-5.250575	3.586570	0.352995

9d

Charge Multiplicity: 0 1

scf done: -3385.18975883

C	0.206721	-1.175216	-2.733189
C	-0.082985	-0.513575	-1.371737
N	-1.358927	0.187517	-1.642520
C	-1.545901	0.488159	-3.085556
C	-0.357207	-0.197741	-3.783530
C	1.110051	0.385757	-0.829270
O	1.583272	1.153234	-1.922761
Si	2.638886	2.477408	-2.144382

C	3.685525	2.008059	-3.642377
C	-2.296956	0.260466	-0.725141
C	-3.750130	0.485152	-0.932722
N	-4.164129	-0.896481	-0.552552
N	-4.549781	-1.119865	0.757841
C	-3.776306	-1.993173	1.446127
O	-4.021345	-2.396109	2.574434
C	2.173362	-0.633738	-0.362306
C	3.419371	-0.698581	-0.986443
C	4.380553	-1.629918	-0.591249
C	4.110583	-2.544074	0.423629
C	2.856546	-2.512182	1.031401
C	1.899312	-1.572533	0.643312
C	2.489065	-3.514739	2.097311
F	1.908545	-2.910930	3.155469
C	5.736199	-1.580641	-1.247536
F	6.425978	-2.724495	-1.077847
C	0.643397	1.342594	0.295361
C	-0.139740	2.447590	-0.076900
C	-0.562800	3.385422	0.860404
C	-0.228557	3.242289	2.208001
C	0.550331	2.154944	2.588195
C	0.989395	1.219091	1.643987
C	-1.304792	4.610745	0.393395
F	-0.440385	5.609441	0.082066
C	0.913861	1.943861	4.037974
F	0.150817	0.984322	4.599082
F	-2.033141	4.368744	-0.718633
F	-2.139398	5.089365	1.337051
F	0.753749	3.068249	4.764915
F	2.201489	1.551553	4.165453
F	1.602588	-4.422952	1.626637
F	3.562897	-4.193240	2.545173
F	6.485451	-0.574692	-0.739711
F	5.632739	-1.353538	-2.578023
C	-4.357638	1.546177	-0.056922
C	-4.767056	2.725829	-0.530227
C	-5.330767	3.833678	0.310594
C	3.723561	2.823617	-0.641657
C	1.632696	4.008431	-2.592953
C	-4.176826	-1.837397	-1.565266
O	-3.729421	-1.634935	-2.693967
O	-4.761242	-2.979525	-1.180775
C	-4.821457	-4.016023	-2.182161
C	-5.606726	-5.168819	-1.585417
O	-2.585047	-2.404015	0.790436
C	-1.848660	-3.418973	1.487954
C	-2.425926	-4.809015	1.253769
H	-0.303309	-1.256569	-0.605022
H	-2.499292	0.056522	-3.391679
H	-1.562424	1.573102	-3.233605
H	-0.684707	-0.720510	-4.685889
H	0.401651	0.533270	-4.064798
H	-0.340316	-2.122578	-2.771475
H	1.267821	-1.383587	-2.880394
H	-2.013918	-0.029941	0.279985
H	-3.991719	0.654775	-1.981584

H	-4.436669	1.293286	0.996171
H	-4.690362	2.929062	-1.600581
H	-5.442009	3.525997	1.355093
H	-6.313899	4.150330	-0.060563
H	-4.677023	4.714929	0.281560
H	2.299793	4.763379	-3.028370
H	0.870255	3.779726	-3.347585
H	1.133829	4.472160	-1.736690
H	4.358212	1.161435	-3.463925
H	3.050798	1.750744	-4.498694
H	4.309525	2.859329	-3.942235
H	4.360998	3.689789	-0.862067
H	3.137175	3.070665	0.249387
H	4.386029	1.988566	-0.390499
H	-0.403946	2.591048	-1.115460
H	-0.559262	3.967797	2.941476
H	1.626403	0.413818	1.985656
H	0.936726	-1.584416	1.144407
H	4.854104	-3.269831	0.728961
H	3.642668	-0.035497	-1.808251
H	-5.298833	-3.616210	-3.082275
H	-3.800413	-4.310396	-2.449572
H	-0.826938	-3.360316	1.095002
H	-1.836905	-3.187228	2.556371
H	-5.679533	-5.984223	-2.313774
H	-5.117269	-5.549354	-0.683900
H	-6.618843	-4.850630	-1.317242
H	-1.803513	-5.565827	1.746666
H	-3.436022	-4.864862	1.667771
H	-2.465697	-5.038433	0.182834

9e

Charge Multiplicity: 0 1

scf done: -3385.191452

C	0.177664	-1.260277	-0.217893
N	-1.143291	-0.658654	-0.519918
C	-1.766128	-1.278501	-1.714648
C	-1.221467	-2.706929	-1.662529
C	0.179842	-2.585153	-1.027943
H	0.217998	-1.434503	0.861398
H	-2.854946	-1.257241	-1.605423
H	-1.447812	-0.725203	-2.603495
H	-1.895423	-3.285059	-1.025723
H	-1.186652	-3.165555	-2.654771
H	0.392608	-3.440308	-0.381558
H	0.959056	-2.543285	-1.792074
C	-1.781130	0.133064	0.314892
C	-3.073382	0.653688	0.093560
H	-1.286935	0.324177	1.264840
H	-3.504334	0.569936	-0.893894
C	-3.880352	1.001001	1.141018
C	-5.351567	1.008674	0.951943
H	-3.479288	1.069343	2.150793
H	-5.615691	1.861539	0.309908
C	-6.143391	1.138199	2.255376
H	-5.985043	0.259429	2.882956
H	-7.206871	1.232926	2.027223

H	-5.827044	2.038051	2.798740
C	1.354319	-0.284267	-0.610896
O	1.225974	-0.074233	-1.999319
Si	2.052695	0.177805	-3.458555
C	0.658541	0.154566	-4.721880
H	1.051547	0.324132	-5.731786
H	0.135949	-0.808735	-4.728385
H	-0.082859	0.936731	-4.521900
C	3.284971	-1.199511	-3.833883
H	4.225033	-1.102315	-3.282663
H	2.866751	-2.190377	-3.621358
H	3.530758	-1.173907	-4.903453
C	2.909909	1.862541	-3.515937
H	3.177202	2.077792	-4.559012
H	2.259831	2.676892	-3.176293
H	3.840087	1.912309	-2.939082
C	1.189290	1.060278	0.132344
C	0.699947	2.183015	-0.534026
C	0.561342	3.404830	0.130712
C	0.879178	3.517498	1.480171
C	1.345059	2.389095	2.160125
C	1.507248	1.175380	1.493196
H	0.438257	2.108020	-1.581168
H	0.781603	4.467164	1.992301
H	1.907530	0.326169	2.037303
C	2.730924	-0.876503	-0.231821
C	2.917197	-2.063057	0.482331
C	4.204953	-2.517104	0.792701
C	5.329261	-1.806856	0.384126
C	5.149515	-0.614730	-0.318785
C	3.869334	-0.148057	-0.598798
H	2.076093	-2.654120	0.820557
H	6.324360	-2.163938	0.621372
H	3.756656	0.804851	-1.100564
C	0.041698	4.587310	-0.647505
C	1.633438	2.477786	3.638198
C	4.362313	-3.826019	1.526917
C	6.336891	0.136658	-0.862411
F	6.618290	-0.268363	-2.125512
F	7.445093	-0.059021	-0.123737
F	6.103839	1.466028	-0.921245
F	4.290637	-4.875344	0.678918
F	5.547802	-3.903071	2.163122
F	3.387515	-3.994164	2.447037
F	0.520171	2.234711	4.366425
F	2.076963	3.702678	3.985806
F	2.563068	1.577389	4.021486
F	0.197920	5.744950	0.022393
F	0.685143	4.708140	-1.833568
F	-1.271471	4.450787	-0.928663
N	-5.803079	-0.200712	0.147126
N	-4.946859	-1.223761	-0.297070
C	-6.932381	0.047382	-0.603123
C	-4.440216	-2.008882	0.665734
O	-7.560945	1.102731	-0.568738
O	-3.609561	-2.909751	0.471229
O	-4.857916	-1.722363	1.966845

O	-7.308502	-1.019150	-1.341383
C	-8.522247	-0.836569	-2.091242
H	-8.411036	0.023872	-2.760192
H	-9.343912	-0.610233	-1.402767
C	-8.768445	-2.122337	-2.860096
H	-8.874803	-2.970328	-2.176064
H	-9.687064	-2.035020	-3.451375
H	-7.936394	-2.334679	-3.539121
C	-4.397765	-2.624100	2.981356
H	-5.148410	-2.564519	3.776534
H	-4.381193	-3.639606	2.577755
C	-3.019001	-2.244878	3.510152
H	-2.724939	-2.913402	4.328685
H	-2.280831	-2.334948	2.707950
H	-3.014298	-1.217196	3.892786

9f

Charge Multiplicity: 0 1

scf done: -3385.23456259

C	3.421315	-0.801127	-0.493552
C	2.050683	-0.623782	-0.294758
C	1.324728	-1.688301	0.260859
C	1.963154	-2.872102	0.636666
C	3.336266	-3.029850	0.461316
C	4.058158	-1.983994	-0.112527
C	1.328201	0.654012	-0.766334
C	0.315291	0.146205	-1.908289
N	-0.828441	1.017871	-2.205250
C	-0.814179	1.433883	-3.621245
C	0.026686	0.366588	-4.334642
C	1.039759	-0.071441	-3.262303
C	-2.025764	0.729595	-1.477959
C	-3.166340	1.706252	-1.650051
C	-4.396517	1.364451	-1.259531
C	-4.758187	0.028999	-0.640686
C	-5.921023	-0.659250	-1.373769
C	1.118336	-3.977182	1.217303
F	0.195891	-4.413109	0.326315
C	5.529227	-2.150280	-0.389335
F	6.186408	-0.967240	-0.335342
C	0.587013	1.399646	0.364434
C	0.450210	0.935359	1.675402
C	-0.225026	1.693733	2.639225
C	-0.778674	2.929493	2.317904
C	-0.637955	3.404513	1.013401
C	0.042202	2.656727	0.054165
C	-1.177425	4.755881	0.628834
F	-2.081176	5.217762	1.516757
C	-0.297272	1.178019	4.051677
F	-0.538424	-0.156321	4.084920
O	2.239718	1.566271	-1.362845
Si	3.377496	2.717054	-0.858171
C	2.744326	4.439111	-1.295225
C	4.924549	2.385072	-1.888540
C	3.790526	2.601658	0.979415
F	-0.188373	5.681262	0.550635
F	-1.775120	4.729447	-0.585348

F	-1.273171	1.780663	4.764042
F	0.863165	1.374881	4.715647
F	1.856394	-5.045617	1.585949
F	0.434698	-3.561161	2.307687
F	5.751267	-2.664500	-1.620322
F	6.116588	-2.981430	0.497756
N	-3.552413	-0.848927	-0.550936
C	-3.037686	-1.296602	0.655196
O	-1.874827	-1.624344	0.829208
N	-2.605712	-0.674507	-1.574300
C	-2.957733	-1.246060	-2.807040
O	-3.425384	-2.513411	-2.762440
C	-2.857903	-3.519249	-1.883100
C	-3.978362	-4.317562	-1.240555
O	-2.864773	-0.662778	-3.865619
O	-3.993189	-1.356755	1.602254
C	-3.548946	-1.752954	2.931520
C	-3.347871	-3.255266	3.049626
H	-0.078073	-0.804510	-1.540764
H	-1.828491	1.496414	-4.014310
H	-0.340722	2.423519	-3.704863
H	-0.621112	-0.462338	-4.629414
H	0.517745	0.752560	-5.234433
H	1.354003	-1.112961	-3.378492
H	1.934083	0.552148	-3.303816
H	-1.736016	0.734276	-0.421919
H	-2.949253	2.698183	-2.033495
H	-5.223740	2.062842	-1.366817
H	-5.070717	0.206210	0.392599
H	-5.666842	-0.888018	-2.412030
H	-6.796297	0.000277	-1.375485
H	-6.192424	-1.589303	-0.865871
H	3.555962	5.170243	-1.188463
H	2.406327	4.478116	-2.337942
H	1.917766	4.773215	-0.660960
H	5.454563	1.473493	-1.590057
H	4.678369	2.296352	-2.953168
H	5.630237	3.218725	-1.782748
H	4.608807	3.297070	1.207033
H	2.944112	2.868449	1.620143
H	4.126576	1.598295	1.263578
H	0.139184	3.038914	-0.952191
H	-1.310191	3.508151	3.063240
H	0.860443	-0.021897	1.969508
H	0.251782	-1.612615	0.407390
H	3.831042	-3.945417	0.761509
H	3.997740	-0.021233	-0.968457
H	-2.632851	-1.209107	3.170467
H	-4.356401	-1.403663	3.579022
H	-2.246162	-4.163683	-2.525123
H	-2.489248	-3.580870	2.457625
H	-3.157989	-3.511746	4.098358
H	-4.242924	-3.795872	2.723803
H	-4.569645	-3.695463	-0.561866
H	-4.645570	-4.729860	-2.004290
H	-3.554883	-5.150080	-0.667420
H	-2.206453	-3.057407	-1.139814

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