Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


# Effect of Configuration of 2-Vinyldiazocarbonyl Compounds on Their Reactivity: Experimental and Computational Study

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## Supporting Information

## Characterization data for isolated compounds

**Dimethyl ester of 1*H*-pyrazole-5-dicarboxylic acid (3a)**. Yield 0.63 g (86%), colorless solid, mp 150-152 °C (from benzene).[14b] $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.4 (br s, 1 H, N-H), 7.35 (s, 1 H, C-H), 3.96 (s, 6 H, $OCH_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 160.7 (2***C***OOMe), 139.8 ($C^{3,5}$), 111.4 ($C^4$), 52.4 (OMe) ppm.

**Dimethyl ester of 4-methyl-1*H*-pyrazole-3,5-dicarboxylic acid (3c)**. Yield 0.76 g (96%), colorless solid, mp 128-129 °C ($Et_2O$).[14a] $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.8 (br. s, 1 H, N-H), 3.85 (m, 6 H, $OCH_3$), 2.50 (m, 3 H, $CH_3$) ppm.

**Diethyl ester of 4-methyl-1*H*-pyrazole-3,5-dicarboxylic acid (3d)**. Yield 0.77 g (86%), colorless solid, mp 108-109 °C (from $Et_2O$).[14b] $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.3 (br. s, 1 H, N-H), 4.45-4.38 (m, 4 H, OC***H***$_2$$CH_3$), 2.58-2.57 (m, 3 H, $CH_3$), 1.45-1.39 (m, 6 H, $OCH_2C$***H***$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 161.1 (2COOEt), 137.6 ($C^{3,5}$), 124.8 ($C^4$), 61.3 (2***C***$H_2CH_3$), 14.2 ($2CH_2$***C***$H_3$), 9.5 ($CH_3$) ppm.

**Dimethyl ester of 3-(*tert*-buthyldimethylsiloxy)-1*H*-pyrazole-3,5-dicarboxylic acid (3e)**. Yield 110 mg (87%), colorless solid, mp 111-112 °C (from $Et_2O$), *Rf* 0.30 (hexane/EtOAc 1:1). IR (KBr): ν 1720 cm$^{-1}$ (CO), 1561 cm$^{-1}$,1463 cm$^{-1}$ (cycle, γ). $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 3.90 (s, 6 H, OMe), 1.02 (s, 9 H, *t*-Bu), 0.17 (s, 6 H, $CH_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 160.4 (2COOMe), 143.2 ($C^{3,5}$), 51.7 (2OMe), 25.4 (C-(***C***$H_3$)$_3$), 18.4 (***C***-$(CH_3)_3$), -4.7 (Si-Me) ppm. HRMS (ESI-BrukerICR): Calc. for $C_{13}H_{23}N_2O_5Si$ ($M+H^+$) 315.1376, found 315.1371.

**Methyl ester of 3-acetyl-4-methyl-1*H*-pyrazole-5-carboxylic acid (3f)**. Yield 0.62 mg (85%), colorless solid, mp 146-148 °C (from $Et_2O$) [14b], *Rf* 0.38 (petroleum ether/EtOAc 2:1). $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 11.8 (br. s, 1 H, N-H), 3.94 (s, 3 H, $OCH_3$), 2.62 (s, 3 H, $CH_3$), 2.55 (s, 3 H, $CH_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 194.9 (***C***$OCH_3$), 161.0 (***C***$OOCH_3$), 148.6 ($C^5$), 133.6 ($C^3$), 124.0 ($C^4$), 52.5 (COO***C***$H_3$), 28.0 (CO***C***$H_3$), 9.9 ($CH_3$) ppm. EI-MS: 182 $[M+H]^+$.

**Dimethyl ester of 4-hydroxy-1*H*-pyrazole-3,5-dicarboxylic acid (5)**. Yield 0.67 g (87%), colorless solid, mp 240-241 °C (from acetone). [14c] $^{1}$H NMR (400 MHz, *d*-DMSO, 25ºC) δ = 12.3 (br. s, 1 H, N-H), 12.3 (br. s, 1 H, O-H), 4.39 (s, 6 H, OMe) ppm.

**Ethyl ester of 5-ethoxyfurane-2-carboxylic acid (6b)**. Yield 32-33%, colorless solid, mp 35-36 °C (from hexane), [11c] *Rf* 0.52 (hexane/EtOAc 1:1). IR (KBr): ν 2985 cm$^{-1}$ (CH δ), 1719 cm$^{-1}$ (CO), 1595 cm$^{-1}$,1534 cm$^{-1}$ (cycle, γ). $^{1}$H NMR (400 MHz, $CDCl_3$, 25ºC) δ = 7.10 (d, 1 H, $C^4$-H, $^{3}J_{H,H}$ 3.6 Hz), 5.30 (d, $^{3}J_{H,H}$ 3.6 Hz, 1 H, $C^5$-H), 4.30 (q, $^{3}J_{H,H}$ 7.1 Hz, 2 H, $CH_2$), 4.19 (q, $^{3}J_{H,H}$ 7.0 Hz, 2 H, $CH_2$), 1.41 (t, $^{3}J_{H,H}$ 7.0 Hz, 3 H, $CH_3$), 1.33 (t, $^{3}J_{H,H}$ 7.1 Hz, 3 H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$, 25ºC) δ = 162.8 (COOEt), 158.5 ($C^5$), 134.7 ($C^2$), 121.2 ($C^3$), 105.0 ($C^4$), 67.1, 60.4 (2***C***$H_2CH_3$), 14.5, 14.4 ($2CH_2$***C***$H_3$) ppm. HRMS (ESI-GCT): Calc. for $C_9H_{12}O_4$ ($M^+$) 184.0736, found 184.0728.

**Diethyl ester of 1*H*-pyrazole-3,5-dicarboxylic acid (3b)**. Yield 59-68%, colorless solid, mp 51-55 °C (from $Et_2O$). [11a] $^{1}$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 12.3 (br. s 1 H, N-H), 7.31 (s, 1 H, C-H), 4.39 (q, $^{3}J_{H,H}$ 7.0 Hz, 4-H, $CH_2$), 1.37 (t, $^{3}J_{H,H}$ 7.1 Hz, 6 H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$, 25ºC) δ = 160.3 (COOEt), 140.1 ($C^{3,5}$), 111.2 ($C^4$), 61.6 ($CH_2$), 14.1 ($CH_3$) ppm. EI-MS: 212.1 $[M]^+$.

**Diethyl ester of 4-phenyl-1*H*-pyrazole-3,5-dicarboxylic acid (3i)**. Yield 0.27 g (87%)**,** colorless oil. [11b] $^1$H NMR (400 MHz, $CDCl_3$, 25ºC) δ = 11.18 (br. s, 1 H, N-H), 7.37-7.31 (m, 5 H, H-arom.), 4.24 (q, $^3J_{H,H}$ 7.0 Hz, 4 H, OC***H***$_2$CH$_3$), 1.17 (t, $^3J_{H,H}$ 7.0 Hz, 3 H, OCH$_2$C*H*$_3$) ppm.

**Ethyl ester of 5-ethoxy-3,4-propanofurane-2-carboxylic acid (6j)**. Yield 0.15 g (42%), colorless oil, *Rf* 0.47 (hexane/EtOAc 1:1). IR (KBr): ν 1707 cm$^{-1}$ (CO), 1645 cm$^{-1}$,1445 cm$^{-1}$ (cycle, γ). $^1$H NMR (400 MHz, $CDCl_3$, 25ºC) δ = 4.27 (q, $^3J_{H,H}$ 7.1 Hz, 2 H, C***H***$_2$CH$_3$), 4.26 (q, $^3J_{H,H}$ 7.1 Hz, 2 H, C***H***$_2$CH$_3$), 2.80-2.77 (m, 2 H), 2.62-2.58 (m, 2 H), 2.39-2.31 (m, 2 H), 1.37 (t, $^3J_{H,H}$ 7.1 Hz, 3 H, CH$_3$), 1.31 (t, $^3J_{H,H}$ 7.1 Hz, 3 H, CH$_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$, 25ºC) δ = 158.4 (COOEt), 153.3 (C$^5$), 147.4 (C$^2$), 125.5 (C$^3$), 105.8 (C$^4$), 66.6, 59.6 (***C***H$_2$CH$_3$), 31.1, 25.5, 23.2 (CH$_2$CH$_2$CH$_2$), 14.6, 14.2 (CH$_2$***C***H$_3$) ppm. HRMS (ESI-GCT): Calc. for $C_{12}H_{16}O_4$ (M$^+$) 224.1049, found 224.1052.

**Methyl 2-acethyl-3-(trifluoromethyl)cycloprop-2-ene-1-carboxylate (9)**. *(Not isolated in the pure state)* $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ: 2.57 (s, 3 H, COCH$_3$), 2.99 (s, 1 H, CH), 3.75 (s, 3H, OCH$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 182.5 (***C***OCH$_3$), 170.3 (***C***O$_2$CH$_3$), 119.0 (q, $^1J_{C,F}$ 268.7 Hz, CF$_3$), 114.7 (q, $^2J_{C,F}$ 5.5 Hz, C$^2$), 108.1 (q, $^2J_{C,F}$ 51.5 Hz, ***C***-CF$_3$), 52.6 (CO$_2$***C***H$_3$), 30.8 (CO***C***H$_3$), 26.4 (C$^1$H) ppm.

**Methyl 2-acetyl-1,5-dimethyl-4-trifluoromethyl-8-oxatricyclo-[3.2.1.0$^{2,4}$]oct-6-en-3-oate (10)**. Yield 140 mg (28%), colorless oil, *Rf* 0.4 (petroleum ether/*t*-BuOMe 1:1). [12d] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 1.62 (s, 3 H, CH$_3$), 2.29 (s, 3 H, COCH$_3$), 3.21 (s, 1H, CH), 3.73 (s, 3 H, COOCH$_3$), 4.91 (d, $^3J_{H,H}$ 2 Hz, 1H, CH), 6.50 (C H, $^3J_{H,H}$ 6 Hz), 6.72 (dd, $^3J_{H,H}$ 6 Hz, $^3J_{HH}$ 2 Hz, 1 H, CH=) ppm.

**Dimethyl ester of 1*H*-pyrazole-5-dicarboxylic acid (3a)**. Yield 0.63 g (86%), colorless solid, mp 150-152 °C (from benzene).[14b] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.4 (br s, 1 H, N-H), 7.35 (s, 1 H, C-H), 3.96 (s, 6 H, OCH$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 160.7 (2***C***OOMe), 139.8 (C$^{3,5}$), 111.4 (C$^4$), 52.4 (OMe) ppm.

**Dimethyl ester of 4-methyl-1*H*-pyrazole-3,5-dicarboxylic acid (3c)**. Yield 0.76 g (96%), colorless solid, mp 128-129 °C ($Et_2O$).[14a] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.8 (br. s, 1 H, N-H), 3.85 (m, 6 H, OCH$_3$), 2.50 (m, 3 H, CH$_3$) ppm.

**Diethyl ester of 4-methyl-1*H*-pyrazole-3,5-dicarboxylic acid (3d)**. Yield 0.77 g (86%), colorless solid, mp 108-109 °C (from $Et_2O$).[14b] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 10.3 (br. s, 1 H, N-H), 4.45-4.38 (m, 4 H, OC***H***$_2$CH$_3$), 2.58-2.57 (m, 3 H, CH$_3$), 1.45-1.39 (m, 6 H, OCH$_2$C***H***$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 161.1 (2COOEt), 137.6 (C$^{3,5}$), 124.8 (C$^4$), 61.3 (2***C***H$_2$CH$_3$), 14.2 (2CH$_2$***C***H$_3$), 9.5 (CH$_3$) ppm.

**Dimethyl ester of 3-(*tert*-buthyldimethylsiloxy)-1*H*-pyrazole-3,5-dicarboxylic acid (3e)**. Yield 110 mg (87%), colorless solid, mp 111-112 °C (from $Et_2O$), *Rf* 0.30 (hexane/EtOAc 1:1). IR (KBr): ν 1720 cm$^{-1}$ (CO), 1561 cm$^{-1}$,1463 cm$^{-1}$ (cycle, γ). $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 3.90 (s, 6 H, OMe), 1.02 (s, 9 H, *t*-Bu), 0.17 (s, 6 H, CH$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 160.4 (2COOMe), 143.2 (C$^{3,5}$), 51.7 (2OMe), 25.4 (C-(***C***H$_3$)$_3$), 18.4 (***C***-(CH$_3$)$_3$), -4.7 (Si-Me) ppm. HRMS (ESI-BrukerICR): Calc. for $C_{13}H_{23}N_2O_5Si$ (M+H$^+$) 315.1376, found 315.1371.

**Methyl ester of 3-acetyl-4-methyl-1*H*-pyrazole-5-carboxylic acid (3f)**. Yield 0.62 mg (85%), colorless solid, mp 146-148 °C (from $Et_2O$) [14b], *Rf* 0.38 (petroleum ether/EtOAc 2:1). $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 11.8 (br. s, 1 H, N-H), 3.94 (s, 3 H, OCH$_3$), 2.62 (s, 3 H, CH$_3$), 2.55 (s, 3 H, CH$_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 194.9 (***C***OCH$_3$), 161.0 (***C***OOCH$_3$), 148.6 (C$^5$), 133.6 (C$^3$), 124.0 (C$^4$), 52.5 (COO***C***H$_3$), 28.0 (CO***C***H$_3$), 9.9 (CH$_3$) ppm. EI-MS: 182 [M+H]$^+$.

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**Diethyl ester of 1*H*-pyrazole-3,5-dicarboxylic acid (3b)**. Yield 59-68%, colorless solid, mp 51-55 °C (from $Et_2O$). [11a] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 12.3 (br. s 1 H, N-H), 7.31 (s, 1 H, C-H), 4.39 (q, $^3J_{H,H}$ 7.0 Hz, 4-H, $CH_2$), 1.37 (t, $^3J_{H,H}$ 7.1 Hz, 6 H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$, 25ºC) δ = 160.3 (COOEt), 140.1 (C$^{3,5}$), 111.2 (C$^4$), 61.6 ($CH_2$), 14.1 ($CH_3$) ppm. EI-MS: 212.1 [*M*]$^+$.

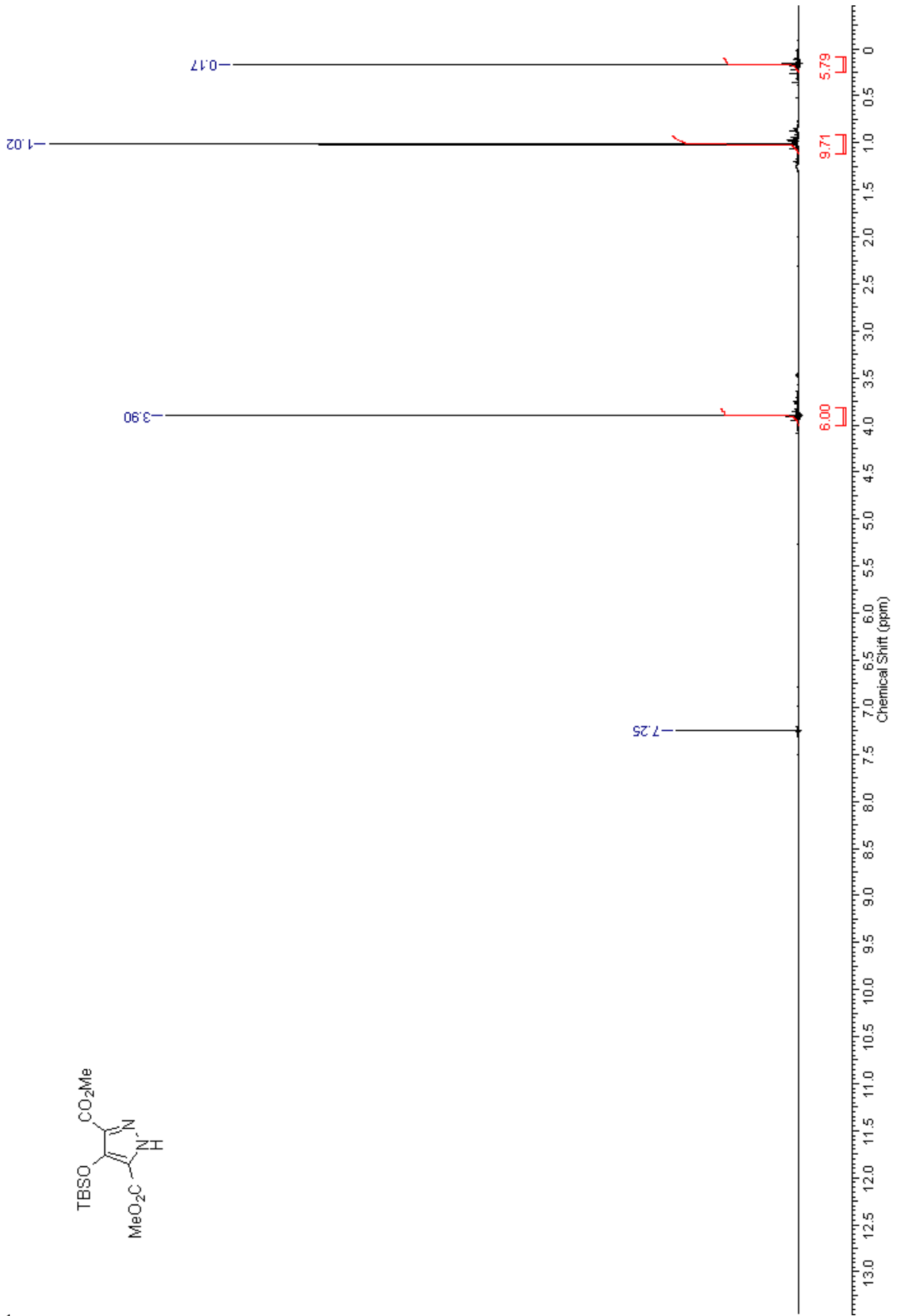
**Cyclization of Vinyldiazoacetate *H*-2i to Produce Pyrazole (3i)**. Heating of the neat diazo compound **2i** (1 mmol) at 120 °C for 2 h (until decoloration of reaction mixture) followed by cooling and washing with petroleum ether produced pyrazole **3i**.

**Diethyl ester of 4-phenyl-1*H*-pyrazole-3,5-dicarboxylic acid (3i)**. Yield 0.27 g (87%)**,** colorless oil. [11b] $^1$H NMR (400 MHz, $CDCl_3$, 25ºC) δ = 11.18 (br. s, 1 H, N-H), 7.37-7.31 (m, 5 H, H-arom.), 4.24 (q, $^3J_{H,H}$ 7.0 Hz, 4 H, OC***H***$_2$CH$_3$), 1.17 (t, $^3J_{H,H}$ 7.0 Hz, 3 H, OCH$_2$C***H***$_3$) ppm.

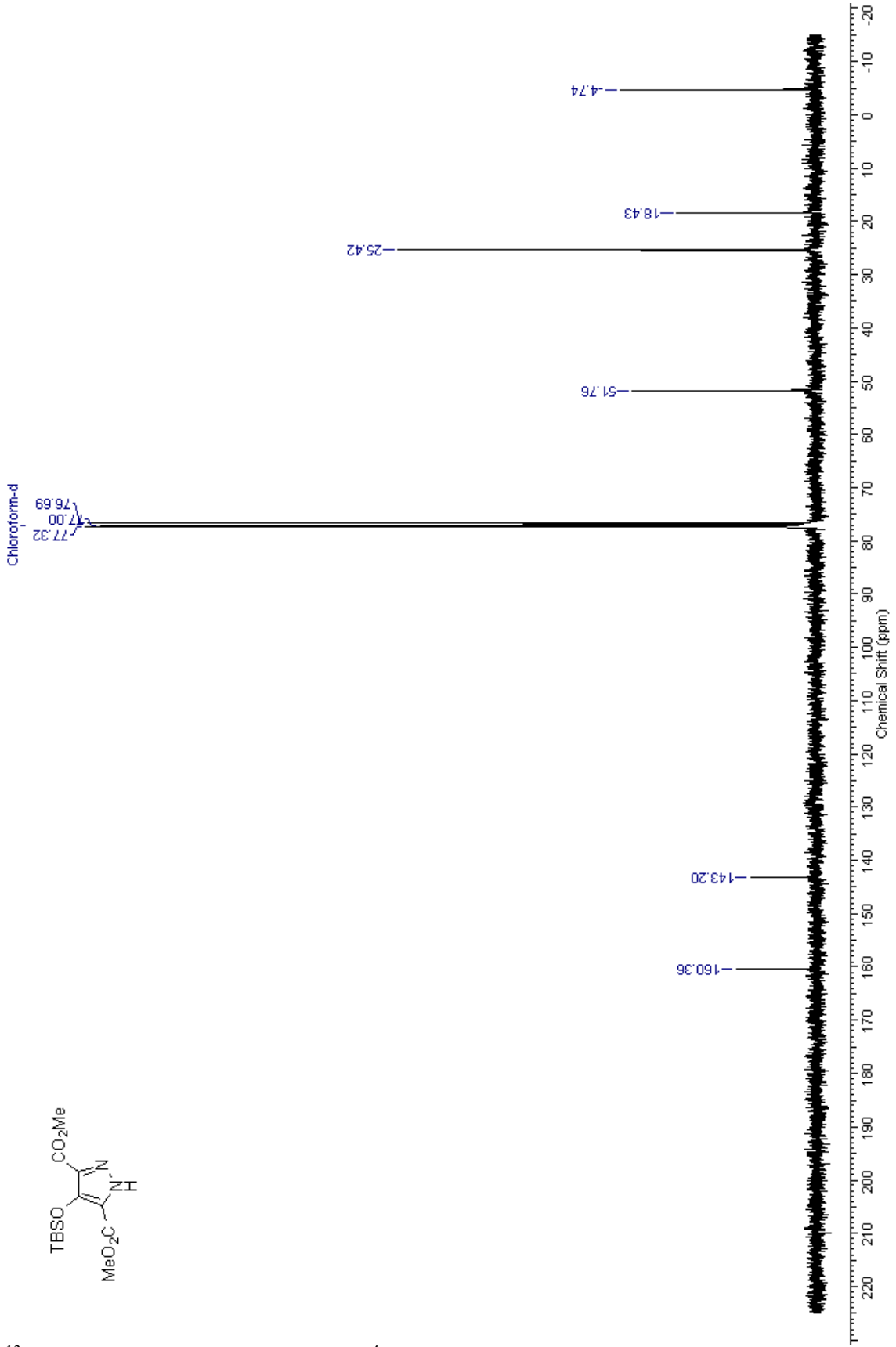
**Ethyl ester of 5-ethoxy-3,4-propanofurane-2-carboxylic acid (6j)**. Yield 0.15 g (42%), colorless oil, *Rf* 0.47 (hexane/EtOAc 1:1). IR (KBr): ν 1707 cm$^{-1}$ (CO), 1645 cm$^{-1}$,1445 cm$^{-1}$ (cycle, γ). $^1$H NMR (400 MHz, $CDCl_3$, 25ºC) δ = 4.27 (q, $^3J_{H,H}$ 7.1 Hz, 2 H, C***H***$_2$CH$_3$), 4.26 (q, $^3J_{H,H}$ 7.1 Hz, 2 H, C***H***$_2$CH$_3$), 2.80-2.77 (m, 2 H), 2.62-2.58 (m, 2 H), 2.39-2.31 (m, 2 H), 1.37 (t, $^3J_{H,H}$ 7.1 Hz, 3 H, $CH_3$), 1.31 (t, $^3J_{H,H}$ 7.1 Hz, 3 H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$, 25ºC) δ = 158.4 (COOEt), 153.3 (C$^5$), 147.4 (C$^2$), 125.5 (C$^3$), 105.8 (C$^4$), 66.6, 59.6 (***C***$H_2$CH$_3$), 31.1, 25.5, 23.2 ($CH_2CH_2CH_2$), 14.6, 14.2 (CH$_2$***C***H$_3$) ppm. HRMS (ESI-GCT): Calc. for $C_{12}H_{16}O_4$ ($M^+$) 224.1049, found 224.1052.

**Methyl 2-acethyl-3-(trifluoromethyl)cycloprop-2-ene-1-carboxylate (9)**. *(Not isolated in the pure state)* $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ: 2.57 (s, 3 H, $COCH_3$), 2.99 (s, 1 H, CH), 3.75 (s, 3H, $OCH_3$) ppm. $^{13}$C NMR (75 MHz, $CDCl_3$, 25ºC) δ = 182.5 (***C***O$CH_3$), 170.3 (***C***$O_2CH_3$), 119.0 (q, $^1J_{C,F}$ 268.7 Hz, $CF_3$), 114.7 (q, $^2J_{C,F}$ 5.5 Hz, C$^2$), 108.1 (q, $^2J_{C,F}$ 51.5 Hz, ***C***-$CF_3$), 52.6 ($CO_2$***C***$H_3$), 30.8 (CO***C***$H_3$), 26.4 (C$^1$H) ppm.

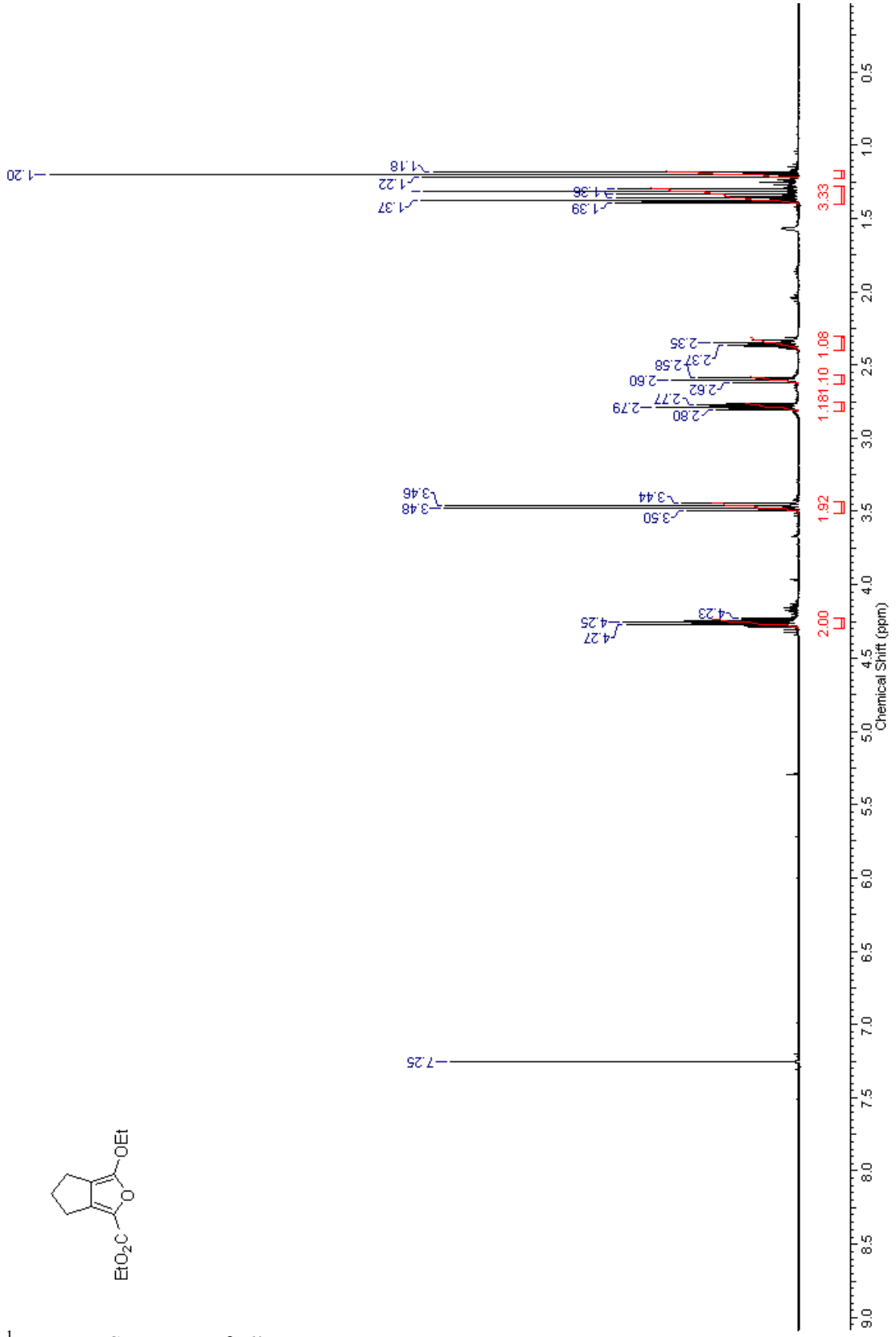
**Methyl 2-acetyl-1,5-dimethyl-4-trifluoromethyl-8-oxatricyclo-[3.2.1.0$^{2,4}$]oct-6-en-3-oate (10)**. Yield 140 mg (28%), colorless oil, *Rf* 0.4 (petroleum ether/*t*-BuOMe 1:1). [12d] $^1$H NMR (300 MHz, $CDCl_3$, 25ºC) δ = 1.62 (s, 3 H, $CH_3$), 2.29 (s, 3 H, $COCH_3$), 3.21 (s, 1H, CH), 3.73 (s, 3 H, $COOCH_3$), 4.91 (d, $^3J_{H,H}$ 2 Hz, 1H, CH), 6.50 (C H, $^3J_{H,H}$ 6 Hz), 6.72 (dd, $^3J_{H,H}$ 6 Hz, $^3J_{HH}$ 2 Hz, 1 H, CH=) ppm.



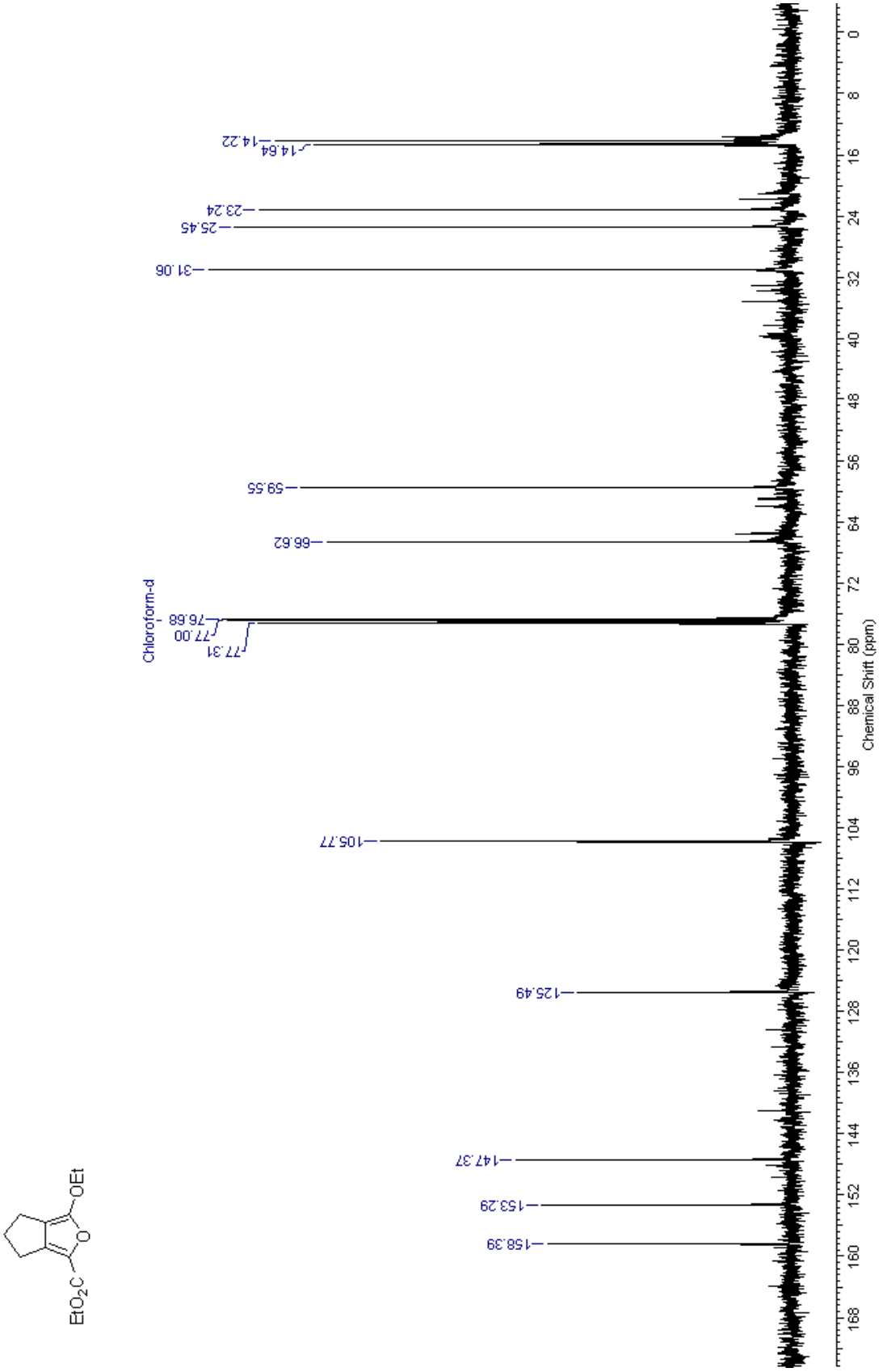

$^{1}$H NMR Spectrum of **3e**




$^{13}C$ NMR Spectrum of **3e** (missed $C^4$ around 124-128 ppm)



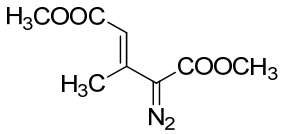

$^{1}$H NMR Spectrum of **6j**




$^{13}$C NMR Spectrum of **6j**

# Cartesian coordinates and energies for all calculated structures

## *s-trans*-1c

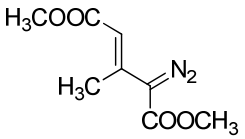



Sum of electronic and zero-point Energies= -720.965454
Sum of electronic and thermal Energies= -720.950526
Sum of electronic and thermal Enthalpies= -720.949582
Sum of electronic and thermal Free Energies= -721.008627

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.230253 | 0.816388 | -0.000038 |
| 2 | 6 | 0 | 1.201185 | 0.511268 | 0.000092 |
| 3 | 6 | 0 | -1.137375 | -0.182206 | -0.000147 |
| 4 | 7 | 0 | 2.032771 | 1.543007 | 0.000152 |
| 5 | 6 | 0 | 1.868802 | -0.795896 | 0.000024 |
| 6 | 8 | 0 | -3.239212 | 1.022853 | -0.000123 |
| 7 | 8 | 0 | -3.196404 | -1.210783 | 0.000107 |
| 8 | 6 | 0 | -4.623574 | -1.196040 | 0.000132 |
| 9 | 6 | 0 | -2.599798 | -0.004226 | -0.000067 |
| 10 | 8 | 0 | 1.305952 | -1.860377 | 0.000004 |
| 11 | 8 | 0 | 3.204767 | -0.659677 | -0.000018 |
| 12 | 6 | 0 | 3.952190 | -1.880916 | -0.000102 |
| 13 | 7 | 0 | 2.731228 | 2.413299 | 0.000198 |
| 14 | 1 | 0 | -0.808411 | -1.210600 | -0.000138 |
| 15 | 1 | 0 | -5.002535 | -0.689922 | -0.888945 |
| 16 | 1 | 0 | -5.002485 | -0.690975 | 0.889845 |
| 17 | 1 | 0 | -4.930092 | -2.239628 | -0.000419 |
| 18 | 1 | 0 | 4.997759 | -1.582736 | -0.000186 |
| 19 | 1 | 0 | 3.724033 | -2.466631 | 0.890780 |
| 20 | 1 | 0 | 3.723880 | -2.466605 | -0.890961 |
| 21 | 6 | 0 | -0.558559 | 2.286202 | -0.000157 |
| 22 | 1 | 0 | -1.629442 | 2.450543 | -0.000412 |
| 23 | 1 | 0 | -0.128822 | 2.769494 | 0.882687 |
| 24 | 1 | 0 | -0.128401 | 2.769334 | -0.882897 |

***s-cis*-1c**

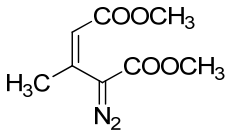



Sum of electronic and zero-point Energies= -720.964629
Sum of electronic and thermal Energies= -720.949438
Sum of electronic and thermal Enthalpies= -720.948494
Sum of electronic and thermal Free Energies= -721.009088

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.219701 | -0.456878 | -0.030504 |
| 2 | 6 | 0 | -1.087906 | 0.205011 | -0.023381 |
| 3 | 6 | 0 | 1.346778 | 0.289446 | 0.004632 |
| 4 | 7 | 0 | -1.102998 | 1.529711 | -0.041979 |
| 5 | 6 | 0 | -2.420880 | -0.410072 | 0.019248 |
| 6 | 8 | 0 | 3.122136 | -1.354696 | -0.033722 |
| 7 | 8 | 0 | 3.580939 | 0.831919 | 0.046551 |
| 8 | 6 | 0 | 4.968514 | 0.497535 | 0.056659 |
| 9 | 6 | 0 | 2.729370 | -0.212493 | 0.000580 |
| 10 | 8 | 0 | -2.644797 | -1.590828 | 0.083461 |
| 11 | 8 | 0 | -3.382085 | 0.529047 | -0.018075 |
| 12 | 6 | 0 | -4.726752 | 0.042584 | 0.050976 |
| 13 | 7 | 0 | -1.080023 | 2.644000 | -0.058922 |
| 14 | 1 | 0 | 1.293286 | 1.370758 | 0.045819 |
| 15 | 1 | 0 | 5.239892 | -0.047528 | -0.848505 |
| 16 | 1 | 0 | 5.211347 | -0.111595 | 0.928580 |
| 17 | 1 | 0 | 5.500716 | 1.445254 | 0.099871 |
| 18 | 1 | 0 | -5.358782 | 0.926207 | 0.008548 |
| 19 | 1 | 0 | -4.937668 | -0.616341 | -0.791624 |
| 20 | 1 | 0 | -4.888319 | -0.494476 | 0.986102 |
| 21 | 6 | 0 | 0.190670 | -1.957416 | -0.086618 |
| 22 | 1 | 0 | 1.197018 | -2.355160 | -0.150278 |
| 23 | 1 | 0 | -0.308037 | -2.355363 | 0.799029 |
| 24 | 1 | 0 | -0.394817 | -2.287573 | -0.946504 |

***s-trans*-2c**

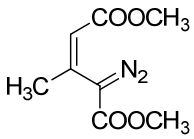



Sum of electronic and zero-point Energies= -720.961799
Sum of electronic and thermal Energies= -720.946937
Sum of electronic and thermal Enthalpies= -720.945993
Sum of electronic and thermal Free Energies= -721.004265

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.215562 | 1.650726 | 0.264274 |
| 2 | 6 | 0 | -1.109546 | 0.517364 | 0.001304 |
| 3 | 6 | 0 | 1.119072 | 1.533909 | 0.212328 |
| 4 | 7 | 0 | -2.291584 | 0.777621 | -0.518008 |
| 5 | 6 | 0 | -0.882313 | -0.879884 | 0.391543 |
| 6 | 8 | 0 | 1.462955 | -0.351394 | -1.226368 |
| 7 | 8 | 0 | 3.048669 | 0.239437 | 0.239226 |
| 8 | 6 | 0 | 3.842784 | -0.849733 | -0.235472 |
| 9 | 6 | 0 | 1.845444 | 0.366630 | -0.336729 |
| 10 | 8 | 0 | 0.029850 | -1.257239 | 1.079553 |
| 11 | 8 | 0 | -1.847237 | -1.682241 | -0.083492 |
| 12 | 6 | 0 | -1.732777 | -3.061850 | 0.278377 |
| 13 | 7 | 0 | -3.292439 | 1.004336 | -0.963960 |
| 14 | 1 | 0 | 1.738953 | 2.350811 | 0.563239 |
| 15 | 1 | 0 | 4.059105 | -0.730390 | -1.298160 |
| 16 | 1 | 0 | 3.323368 | -1.795187 | -0.075120 |
| 17 | 1 | 0 | 4.763296 | -0.820954 | 0.342985 |
| 18 | 1 | 0 | -2.568745 | -3.562199 | -0.204478 |
| 19 | 1 | 0 | -0.787533 | -3.468805 | -0.081093 |
| 20 | 1 | 0 | -1.793998 | -3.179100 | 1.360854 |
| 21 | 6 | 0 | -0.875112 | 2.942661 | 0.661626 |
| 22 | 1 | 0 | -1.517519 | 3.311749 | -0.144768 |
| 23 | 1 | 0 | -1.503894 | 2.802898 | 1.544950 |
| 24 | 1 | 0 | -0.130715 | 3.710032 | 0.870503 |

***s-cis*-2c**

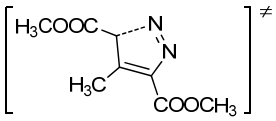



Sum of electronic and zero-point Energies= -720.966296
Sum of electronic and thermal Energies= -720.951234
Sum of electronic and thermal Enthalpies= -720.950290
Sum of electronic and thermal Free Energies= -721.009581

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.118516 | 1.277089 | -0.251562 |
| 2 | 6 | 0 | 0.791217 | 0.138632 | -0.206240 |
| 3 | 6 | 0 | -1.467473 | 1.195740 | -0.197699 |
| 4 | 7 | 0 | 0.392706 | -1.027583 | -0.697533 |
| 5 | 6 | 0 | 2.196307 | 0.177756 | 0.205100 |
| 6 | 8 | 0 | -1.851204 | -1.023982 | 0.629994 |
| 7 | 8 | 0 | -3.575040 | 0.270051 | 0.023193 |
| 8 | 6 | 0 | -4.454117 | -0.781406 | 0.426293 |
| 9 | 6 | 0 | -2.263149 | 0.023282 | 0.183073 |
| 10 | 8 | 0 | 2.748890 | 1.138727 | 0.678488 |
| 11 | 8 | 0 | 2.800799 | -1.003907 | 0.000862 |
| 12 | 6 | 0 | 4.173711 | -1.074230 | 0.397669 |
| 13 | 7 | 0 | 0.064905 | -1.995697 | -1.135202 |
| 14 | 1 | 0 | -2.041121 | 2.097959 | -0.368693 |
| 15 | 1 | 0 | -4.325589 | -1.002602 | 1.486759 |
| 16 | 1 | 0 | -4.263709 | -1.684170 | -0.155801 |
| 17 | 1 | 0 | -5.460113 | -0.414340 | 0.236418 |
| 18 | 1 | 0 | 4.487558 | -2.092793 | 0.182719 |
| 19 | 1 | 0 | 4.772222 | -0.364784 | -0.174596 |
| 20 | 1 | 0 | 4.274684 | -0.862738 | 1.462425 |
| 21 | 6 | 0 | 0.524328 | 2.630297 | -0.415417 |
| 22 | 1 | 0 | 1.011534 | 2.931551 | 0.513231 |
| 23 | 1 | 0 | 1.293430 | 2.614792 | -1.189740 |
| 24 | 1 | 0 | -0.233581 | 3.370019 | -0.671172 |

**$TS_{s\text{-}cis\text{-}1c \rightarrow 3c}$**



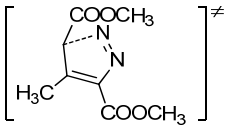

Imaginary Freq. = -474.1075 $cm^{-1}$

Sum of electronic and zero-point Energies= -720.919870
Sum of electronic and thermal Energies= -720.905915
Sum of electronic and thermal Enthalpies= -720.904970
Sum of electronic and thermal Free Energies= -720.961047

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.030074 | -0.266283 | -0.280555 |
| 2 | 6 | 0 | -1.123303 | 0.594566 | -0.108757 |
| 3 | 6 | 0 | 1.229952 | 0.354609 | -0.345091 |
| 4 | 7 | 0 | -0.696573 | 1.889893 | 0.078855 |
| 5 | 6 | 0 | -2.573043 | 0.378836 | 0.012742 |
| 6 | 8 | 0 | 2.536881 | -1.293834 | 0.785215 |
| 7 | 8 | 0 | 3.545646 | 0.339712 | -0.376910 |
| 8 | 6 | 0 | 4.807349 | -0.180532 | 0.045678 |
| 9 | 6 | 0 | 2.464878 | -0.313158 | 0.081309 |
| 10 | 8 | 0 | -3.369409 | 1.267755 | 0.172408 |
| 11 | 8 | 0 | -2.896909 | -0.914683 | -0.054427 |
| 12 | 6 | 0 | -4.294043 | -1.204604 | 0.083501 |
| 13 | 7 | 0 | 0.380953 | 2.279145 | 0.222888 |
| 14 | 1 | 0 | 1.379573 | 1.145702 | -1.078776 |
| 15 | 1 | 0 | 4.945959 | -1.197086 | -0.324901 |
| 16 | 1 | 0 | 4.876695 | -0.179818 | 1.134229 |
| 17 | 1 | 0 | 5.556913 | 0.482174 | -0.380613 |
| 18 | 1 | 0 | -4.378187 | -2.285391 | 0.002050 |
| 19 | 1 | 0 | -4.657785 | -0.866983 | 1.054218 |
| 20 | 1 | 0 | -4.861205 | -0.716137 | -0.709222 |
| 21 | 6 | 0 | -0.210349 | -1.757935 | -0.324430 |
| 22 | 1 | 0 | -0.637004 | -2.121288 | 0.612123 |
| 23 | 1 | 0 | -0.912230 | -2.013563 | -1.119688 |
| 24 | 1 | 0 | 0.738731 | -2.255472 | -0.498285 |

**$TS_{s\text{-}cis\text{-}2c\rightarrow 3c}$**



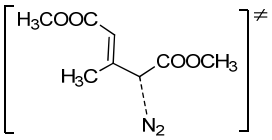

Imaginary Freq. = -448.8673 $cm^{-1}$

Sum of electronic and zero-point Energies= -720.916368
Sum of electronic and thermal Energies= -720.902233
Sum of electronic and thermal Enthalpies= -720.901289
Sum of electronic and thermal Free Energies= -720.957979

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.126312 | 0.857010 | -0.436471 |
| 2 | 6 | 0 | -0.867971 | -0.306823 | -0.280402 |
| 3 | 6 | 0 | 1.250242 | 0.735592 | -0.741165 |
| 4 | 7 | 0 | -0.116537 | -1.426914 | -0.610181 |
| 5 | 6 | 0 | -2.281946 | -0.566463 | 0.035058 |
| 6 | 8 | 0 | 1.950434 | -0.435266 | 1.236243 |
| 7 | 8 | 0 | 3.470205 | 0.389740 | -0.192505 |
| 8 | 6 | 0 | 4.496083 | -0.128307 | 0.657105 |
| 9 | 6 | 0 | 2.210713 | 0.160125 | 0.217337 |
| 10 | 8 | 0 | -2.784793 | -1.658791 | -0.008997 |
| 11 | 8 | 0 | -2.933971 | 0.549892 | 0.366375 |
| 12 | 6 | 0 | -4.324005 | 0.382334 | 0.675412 |
| 13 | 7 | 0 | 0.932770 | -1.478654 | -1.071434 |
| 14 | 1 | 0 | 1.686227 | 1.506809 | -1.366905 |
| 15 | 1 | 0 | 4.416487 | -1.213277 | 0.736038 |
| 16 | 1 | 0 | 4.429725 | 0.312685 | 1.652577 |
| 17 | 1 | 0 | 5.435895 | 0.147659 | 0.184139 |
| 18 | 1 | 0 | -4.680129 | 1.368326 | 0.963255 |
| 19 | 1 | 0 | -4.865356 | 0.021446 | -0.199560 |
| 20 | 1 | 0 | -4.446729 | -0.322584 | 1.497747 |
| 21 | 6 | 0 | -0.774709 | 2.213151 | -0.415565 |
| 22 | 1 | 0 | -1.718963 | 2.225821 | -0.957448 |
| 23 | 1 | 0 | -0.985749 | 2.496465 | 0.619402 |
| 24 | 1 | 0 | -0.092606 | 2.951311 | -0.834722 |

**TS*s-trans*-1c→carbene**

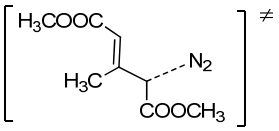



Imaginary Freq. = -247.0739 $cm^{-1}$
Sum of electronic and zero-point Energies= -720.912712
Sum of electronic and thermal Energies= -720.896919
Sum of electronic and thermal Enthalpies= -720.895975
Sum of electronic and thermal Free Energies= -720.957430

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.177451 | 0.759679 | 0.279886 |
| 2 | 6 | 0 | -1.110983 | 0.335613 | 0.754139 |
| 3 | 6 | 0 | 1.127423 | -0.197243 | 0.127755 |
| 4 | 7 | 0 | -2.347166 | 1.716095 | -0.195010 |
| 5 | 6 | 0 | -1.758884 | -0.902427 | 0.355177 |
| 6 | 8 | 0 | 3.103668 | 1.138105 | -0.232081 |
| 7 | 8 | 0 | 3.245465 | -1.089018 | -0.067411 |
| 8 | 6 | 0 | 4.650797 | -0.981771 | -0.300528 |
| 9 | 6 | 0 | 2.565265 | 0.069131 | -0.065253 |
| 10 | 8 | 0 | -1.284613 | -1.947102 | 0.748524 |
| 11 | 8 | 0 | -2.896570 | -0.804584 | -0.331461 |
| 12 | 6 | 0 | -3.576017 | -2.047629 | -0.564284 |
| 13 | 7 | 0 | -3.134931 | 2.463887 | -0.294591 |
| 14 | 1 | 0 | 0.864013 | -1.243537 | 0.211126 |
| 15 | 1 | 0 | 5.125641 | -0.390883 | 0.483753 |
| 16 | 1 | 0 | 4.842716 | -0.517697 | -1.269041 |
| 17 | 1 | 0 | 5.030146 | -2.000729 | -0.287539 |
| 18 | 1 | 0 | -4.485584 | -1.783794 | -1.097846 |
| 19 | 1 | 0 | -2.958483 | -2.708970 | -1.172034 |
| 20 | 1 | 0 | -3.815441 | -2.532344 | 0.382241 |
| 21 | 6 | 0 | 0.423583 | 2.245706 | 0.201378 |
| 22 | 1 | 0 | 1.454745 | 2.487342 | 0.441967 |
| 23 | 1 | 0 | 0.229569 | 2.595490 | -0.817263 |
| 24 | 1 | 0 | -0.248046 | 2.769681 | 0.881648 |

**TS*s-cis*-1c→carbene**



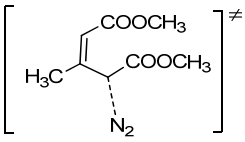

Imaginary Freq. = -215.6733 $cm^{-1}$

Sum of electronic and zero-point Energies= -720.913668
Sum of electronic and thermal Energies= -720.897869
Sum of electronic and thermal Enthalpies= -720.896925
Sum of electronic and thermal Free Energies= -720.958065

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.196085 | -0.507402 | -0.469391 |
| 2 | 6 | 0 | 1.135537 | -0.180873 | -0.798434 |
| 3 | 6 | 0 | -1.197194 | 0.302239 | -0.058274 |
| 4 | 7 | 0 | 1.194889 | 1.904236 | -0.595435 |
| 5 | 6 | 0 | 2.307149 | -0.584831 | -0.022923 |
| 6 | 8 | 0 | -3.003442 | -1.275349 | -0.067710 |
| 7 | 8 | 0 | -3.365995 | 0.862848 | 0.498683 |
| 8 | 6 | 0 | -4.744254 | 0.537722 | 0.675230 |
| 9 | 6 | 0 | -2.574545 | -0.156887 | 0.107193 |
| 10 | 8 | 0 | 2.637118 | -1.747933 | 0.003836 |
| 11 | 8 | 0 | 2.992999 | 0.411577 | 0.533107 |
| 12 | 6 | 0 | 4.224307 | 0.028032 | 1.167166 |
| 13 | 7 | 0 | 1.415075 | 2.925662 | -0.906818 |
| 14 | 1 | 0 | -1.012627 | 1.343581 | 0.165227 |
| 15 | 1 | 0 | -4.864861 | -0.230287 | 1.440564 |
| 16 | 1 | 0 | -5.178605 | 0.182749 | -0.260653 |
| 17 | 1 | 0 | -5.228855 | 1.459739 | 0.989070 |
| 18 | 1 | 0 | 4.647831 | 0.951708 | 1.553063 |
| 19 | 1 | 0 | 4.030893 | -0.671064 | 1.980415 |
| 20 | 1 | 0 | 4.897829 | -0.426216 | 0.440329 |
| 21 | 6 | 0 | -0.356302 | -1.998020 | -0.770662 |
| 22 | 1 | 0 | -0.680058 | -2.503557 | 0.139192 |
| 23 | 1 | 0 | -1.128268 | -2.117316 | -1.530007 |
| 24 | 1 | 0 | 0.569863 | -2.447646 | -1.124193 |

**TS$_{s\text{-}trans\text{-}2c \rightarrow carbene}$**



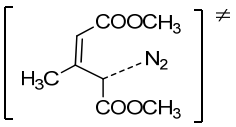

Imaginary Freq. = -278.3554 $cm^{-1}$

Sum of electronic and zero-point Energies= -720.909389
Sum of electronic and thermal Energies= -720.893849
Sum of electronic and thermal Enthalpies= -720.892904
Sum of electronic and thermal Free Energies= -720.953349

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.104124 | 1.260403 | 0.458119 |
| 2 | 6 | 0 | -0.622965 | 0.345469 | -0.371031 |
| 3 | 6 | 0 | 1.434111 | 1.085242 | 0.643215 |
| 4 | 7 | 0 | -2.356661 | 1.335060 | -0.762700 |
| 5 | 6 | 0 | -1.174485 | -0.889116 | 0.202723 |
| 6 | 8 | 0 | 1.709365 | -0.697299 | -0.902099 |
| 7 | 8 | 0 | 3.499145 | 0.133316 | 0.169729 |
| 8 | 6 | 0 | 4.312898 | -0.803199 | -0.537079 |
| 9 | 6 | 0 | 2.183586 | 0.075986 | -0.102376 |
| 10 | 8 | 0 | -0.442822 | -1.674318 | 0.752965 |
| 11 | 8 | 0 | -2.474474 | -1.106929 | -0.032665 |
| 12 | 6 | 0 | -2.964811 | -2.380907 | 0.402419 |
| 13 | 7 | 0 | -3.106449 | 1.732352 | -1.449181 |
| 14 | 1 | 0 | 1.978225 | 1.737816 | 1.312817 |
| 15 | 1 | 0 | 4.289753 | -0.598834 | -1.608703 |
| 16 | 1 | 0 | 3.968053 | -1.822332 | -0.357285 |
| 17 | 1 | 0 | 5.321136 | -0.671229 | -0.150653 |
| 18 | 1 | 0 | -4.024117 | -2.383272 | 0.156732 |
| 19 | 1 | 0 | -2.449975 | -3.184929 | -0.123823 |
| 20 | 1 | 0 | -2.824329 | -2.499216 | 1.477353 |
| 21 | 6 | 0 | -0.605509 | 2.407837 | 1.133863 |
| 22 | 1 | 0 | -0.976042 | 3.115247 | 0.387607 |
| 23 | 1 | 0 | -1.458264 | 2.052070 | 1.716408 |
| 24 | 1 | 0 | 0.085923 | 2.934347 | 1.790161 |

**$TS_{s\text{-}cis\text{-}2c \rightarrow carbene}$**



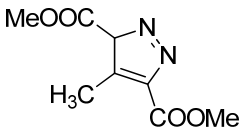

Imaginary Freq. = -264.3041 $cm^{-1}$

Sum of electronic and zero-point Energies= -720.908614
Sum of electronic and thermal Energies= -720.893105
Sum of electronic and thermal Enthalpies= -720.892161
Sum of electronic and thermal Free Energies= -720.952308

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.058481 | 1.302982 | -0.152013 |
| 2 | 6 | 0 | 0.770714 | 0.336338 | 0.490656 |
| 3 | 6 | 0 | -1.391758 | 1.180815 | -0.370904 |
| 4 | 7 | 0 | 0.281513 | -1.507977 | -0.447281 |
| 5 | 6 | 0 | 2.197967 | 0.226319 | 0.324546 |
| 6 | 8 | 0 | -1.931972 | -0.855510 | 0.779685 |
| 7 | 8 | 0 | -3.537172 | 0.348308 | -0.219013 |
| 8 | 6 | 0 | -4.496497 | -0.588094 | 0.273637 |
| 9 | 6 | 0 | -2.257355 | 0.102482 | 0.118800 |
| 10 | 8 | 0 | 2.848078 | 1.181260 | 0.704662 |
| 11 | 8 | 0 | 2.723611 | -0.919607 | -0.101631 |
| 12 | 6 | 0 | 4.154321 | -0.998040 | -0.024150 |
| 13 | 7 | 0 | 0.029117 | -2.526234 | -0.740966 |
| 14 | 1 | 0 | -1.899609 | 1.978109 | -0.898166 |
| 15 | 1 | 0 | -4.493541 | -0.602010 | 1.364563 |
| 16 | 1 | 0 | -4.281913 | -1.590332 | -0.100033 |
| 17 | 1 | 0 | -5.460448 | -0.245574 | -0.095600 |
| 18 | 1 | 0 | 4.405851 | -2.005895 | -0.344761 |
| 19 | 1 | 0 | 4.612248 | -0.264383 | -0.687909 |
| 20 | 1 | 0 | 4.488735 | -0.829113 | 0.999452 |
| 21 | 6 | 0 | 0.623225 | 2.601855 | -0.545090 |
| 22 | 1 | 0 | 1.084108 | 3.076981 | 0.320450 |
| 23 | 1 | 0 | 1.414113 | 2.417920 | -1.275266 |
| 24 | 1 | 0 | -0.117133 | 3.280221 | -0.967520 |

**3c**

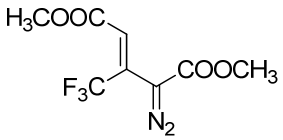



Sum of electronic and zero-point Energies= -720.970659
Sum of electronic and thermal Energies= -720.956308
Sum of electronic and thermal Enthalpies= -720.955363
Sum of electronic and thermal Free Energies= -721.013707

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.117323 | 0.868208 | -0.459865 |
| 2 | 6 | 0 | -0.905126 | -0.001879 | -0.388554 |
| 3 | 6 | 0 | 1.214574 | 0.093224 | -1.121491 |
| 4 | 7 | 0 | -0.539220 | -1.263450 | -0.958150 |
| 5 | 6 | 0 | -2.247169 | 0.227250 | 0.191048 |
| 6 | 8 | 0 | 3.480439 | 0.606044 | -0.476837 |
| 7 | 8 | 0 | 2.251967 | -0.757613 | 0.810510 |
| 8 | 6 | 0 | 3.357338 | -0.896100 | 1.715000 |
| 9 | 6 | 0 | 2.463973 | 0.012752 | -0.247794 |
| 10 | 8 | 0 | -2.546334 | 1.226780 | 0.796616 |
| 11 | 8 | 0 | -3.072638 | -0.789132 | -0.030615 |
| 12 | 6 | 0 | -4.385709 | -0.652895 | 0.524727 |
| 13 | 7 | 0 | 0.637317 | -1.237677 | -1.360819 |
| 14 | 1 | 0 | 1.512738 | 0.522519 | -2.082802 |
| 15 | 1 | 0 | 3.650062 | 0.077932 | 2.107531 |
| 16 | 1 | 0 | 4.202990 | -1.356459 | 1.203651 |
| 17 | 1 | 0 | 3.001112 | -1.539647 | 2.514813 |
| 18 | 1 | 0 | -4.913289 | -1.563760 | 0.253868 |
| 19 | 1 | 0 | -4.329676 | -0.552048 | 1.609174 |
| 20 | 1 | 0 | -4.888018 | 0.218321 | 0.103024 |
| 21 | 6 | 0 | 0.258090 | 2.271824 | 0.005662 |
| 22 | 1 | 0 | -0.713111 | 2.729534 | 0.179927 |
| 23 | 1 | 0 | 0.814530 | 2.288357 | 0.949767 |
| 24 | 1 | 0 | 0.828748 | 2.860206 | -0.715960 |

***s-trans*-1h**

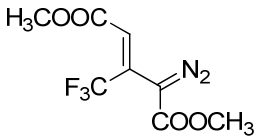



Sum of electronic and zero-point Energies= -1018.716719
Sum of electronic and thermal Energies= -1018.699889
Sum of electronic and thermal Enthalpies= -1018.698945
Sum of electronic and thermal Free Energies= -1018.762757

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.111492 | 0.115862 | 0.116502 |
| 2 | 6 | 0 | -1.350115 | 0.175465 | 0.022444 |
| 3 | 6 | 0 | 0.805565 | -1.018761 | 0.234023 |
| 4 | 7 | 0 | -1.945154 | 1.352747 | -0.071270 |
| 5 | 6 | 0 | -2.253666 | -0.976885 | -0.005646 |
| 6 | 8 | 0 | 2.864323 | -1.346361 | 1.382092 |
| 7 | 8 | 0 | 2.886730 | -1.064224 | -0.841801 |
| 8 | 6 | 0 | 4.316047 | -1.177482 | -0.826810 |
| 9 | 6 | 0 | 2.292846 | -1.136659 | 0.347203 |
| 10 | 8 | 0 | -1.893595 | -2.125665 | 0.061702 |
| 11 | 8 | 0 | -3.531759 | -0.596506 | -0.116703 |
| 12 | 6 | 0 | -4.492562 | -1.659445 | -0.158204 |
| 13 | 7 | 0 | -2.467498 | 2.335229 | -0.152568 |
| 14 | 1 | 0 | 0.274603 | -1.961364 | 0.290073 |
| 15 | 1 | 0 | 4.617924 | -2.132060 | -0.394942 |
| 16 | 1 | 0 | 4.750313 | -0.360371 | -0.249251 |
| 17 | 1 | 0 | 4.626589 | -1.115177 | -1.866622 |
| 18 | 1 | 0 | -5.458469 | -1.173956 | -0.271649 |
| 19 | 1 | 0 | -4.293780 | -2.315280 | -1.005940 |
| 20 | 1 | 0 | -4.461268 | -2.233447 | 0.768015 |
| 21 | 6 | 0 | 0.793826 | 1.463605 | 0.073371 |
| 22 | 9 | 0 | 0.342440 | 2.260659 | 1.058763 |
| 23 | 9 | 0 | 2.115318 | 1.395627 | 0.199384 |
| 24 | 9 | 0 | 0.529626 | 2.101901 | -1.080640 |

***s-cis*-1h**

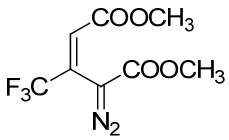



Sum of electronic and zero-point Energies= -1018.712729
Sum of electronic and thermal Energies= -1018.695774
Sum of electronic and thermal Enthalpies= -1018.694830
Sum of electronic and thermal Free Energies= -1018.759052

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.155303 | 0.072278 | 0.021283 |
| 2 | 6 | 0 | 1.185490 | 0.662654 | 0.098502 |
| 3 | 6 | 0 | -1.221981 | 0.796020 | -0.331239 |
| 4 | 7 | 0 | 1.297967 | 1.902947 | 0.524643 |
| 5 | 6 | 0 | 2.406859 | 0.004145 | -0.372271 |
| 6 | 8 | 0 | -2.965665 | -0.797745 | -0.743556 |
| 7 | 8 | 0 | -3.473260 | 1.305871 | -0.156383 |
| 8 | 6 | 0 | -4.863928 | 0.975400 | -0.261550 |
| 9 | 6 | 0 | -2.625974 | 0.307619 | -0.422859 |
| 10 | 8 | 0 | 2.403869 | -1.054360 | -0.942963 |
| 11 | 8 | 0 | 3.499259 | 0.728915 | -0.105777 |
| 12 | 6 | 0 | 4.735936 | 0.168081 | -0.566479 |
| 13 | 7 | 0 | 1.401885 | 2.954404 | 0.888416 |
| 14 | 1 | 0 | -1.089064 | 1.838744 | -0.601095 |
| 15 | 1 | 0 | -5.113050 | 0.165507 | 0.424588 |
| 16 | 1 | 0 | -5.103609 | 0.676142 | -1.282585 |
| 17 | 1 | 0 | -5.403189 | 1.880356 | 0.006416 |
| 18 | 1 | 0 | 5.505401 | 0.878276 | -0.274702 |
| 19 | 1 | 0 | 4.910233 | -0.798614 | -0.094024 |
| 20 | 1 | 0 | 4.717449 | 0.048283 | -1.649863 |
| 21 | 6 | 0 | -0.268995 | -1.382702 | 0.472989 |
| 22 | 9 | 0 | -0.373961 | -2.232736 | -0.543067 |
| 23 | 9 | 0 | 0.797457 | -1.740940 | 1.200722 |
| 24 | 9 | 0 | -1.333426 | -1.556611 | 1.268905 |

***s-trans*-2h**

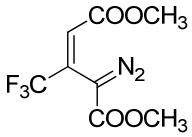



Sum of electronic and zero-point Energies= -1018.721878
Sum of electronic and thermal Energies= -1018.705132
Sum of electronic and thermal Enthalpies= -1018.704188
Sum of electronic and thermal Free Energies= -1018.767618

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.797739 | -0.638987 | -0.051532 |
| 2 | 6 | 0 | 0.498358 | 0.786628 | -0.183874 |
| 3 | 6 | 0 | -0.113100 | -1.612167 | -0.092641 |
| 4 | 7 | 0 | 1.328259 | 1.575532 | -0.841257 |
| 5 | 6 | 0 | -0.679020 | 1.432095 | 0.407770 |
| 6 | 8 | 0 | -1.888669 | -0.646430 | -1.373997 |
| 7 | 8 | 0 | -2.340610 | -2.187282 | 0.190243 |
| 8 | 6 | 0 | -3.736960 | -2.043329 | -0.095004 |
| 9 | 6 | 0 | -1.528788 | -1.392687 | -0.502535 |
| 10 | 8 | 0 | -1.476812 | 0.865123 | 1.109002 |
| 11 | 8 | 0 | -0.739322 | 2.729039 | 0.086488 |
| 12 | 6 | 0 | -1.850081 | 3.449615 | 0.634379 |
| 13 | 7 | 0 | 2.015978 | 2.260567 | -1.391048 |
| 14 | 1 | 0 | 0.157472 | -2.624851 | 0.180872 |
| 15 | 1 | 0 | -3.938817 | -2.284370 | -1.139263 |
| 16 | 1 | 0 | -4.057102 | -1.022416 | 0.115407 |
| 17 | 1 | 0 | -4.244532 | -2.744214 | 0.562776 |
| 18 | 1 | 0 | -1.752166 | 4.465270 | 0.259494 |
| 19 | 1 | 0 | -2.788223 | 3.008693 | 0.296877 |
| 20 | 1 | 0 | -1.808451 | 3.440039 | 1.723874 |
| 21 | 6 | 0 | 2.224855 | -0.984392 | 0.300348 |
| 22 | 9 | 0 | 3.075222 | -0.472659 | -0.611313 |
| 23 | 9 | 0 | 2.578800 | -0.469199 | 1.485028 |
| 24 | 9 | 0 | 2.446806 | -2.297598 | 0.351922 |

***s-cis*-2h**

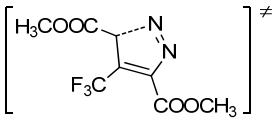



Sum of electronic and zero-point Energies= -1018.721759
Sum of electronic and thermal Energies= -1018.704959
Sum of electronic and thermal Enthalpies= -1018.704014
Sum of electronic and thermal Free Energies= -1018.767738

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.185165 | 0.710347 | 0.107416 |
| 2 | 6 | 0 | -0.636152 | -0.483445 | 0.222222 |
| 3 | 6 | 0 | 1.523203 | 0.774523 | 0.005198 |
| 4 | 7 | 0 | -0.166240 | -1.505409 | 0.920707 |
| 5 | 6 | 0 | -1.982617 | -0.647453 | -0.332608 |
| 6 | 8 | 0 | 2.069014 | -1.515339 | -0.457606 |
| 7 | 8 | 0 | 3.691393 | 0.010383 | -0.215138 |
| 8 | 6 | 0 | 4.656890 | -1.015745 | -0.469767 |
| 9 | 6 | 0 | 2.414116 | -0.379845 | -0.236622 |
| 10 | 8 | 0 | -2.508335 | 0.157511 | -1.054967 |
| 11 | 8 | 0 | -2.536257 | -1.804127 | 0.051164 |
| 12 | 6 | 0 | -3.842931 | -2.065935 | -0.476376 |
| 13 | 7 | 0 | 0.219125 | -2.361512 | 1.516594 |
| 14 | 1 | 0 | 2.014057 | 1.737700 | 0.054985 |
| 15 | 1 | 0 | 4.510822 | -1.436643 | -1.465086 |
| 16 | 1 | 0 | 4.574055 | -1.806609 | 0.276612 |
| 17 | 1 | 0 | 5.626817 | -0.529862 | -0.400331 |
| 18 | 1 | 0 | -4.125254 | -3.040128 | -0.085419 |
| 19 | 1 | 0 | -4.545100 | -1.302591 | -0.140539 |
| 20 | 1 | 0 | -3.814937 | -2.085549 | -1.565999 |
| 21 | 6 | 0 | -0.551831 | 2.045373 | 0.178607 |
| 22 | 9 | 0 | 0.216739 | 2.988772 | 0.749297 |
| 23 | 9 | 0 | -1.663410 | 1.963439 | 0.912746 |
| 24 | 9 | 0 | -0.879134 | 2.505320 | -1.029974 |

**$TS_{s\text{-}cis\text{-}1h \rightarrow 3h}$**



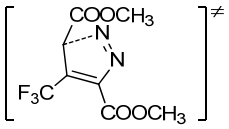

Imaginary Freq. = -514.7018 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.665663
Sum of electronic and thermal Energies= -1018.649792
Sum of electronic and thermal Enthalpies= -1018.648848
Sum of electronic and thermal Free Energies= -1018.709655

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.031900 | 0.178980 | -0.280338 |
| 2 | 6 | 0 | -1.085704 | 1.004638 | -0.163554 |
| 3 | 6 | 0 | 1.297223 | 0.778554 | -0.340599 |
| 4 | 7 | 0 | -0.672393 | 2.314642 | -0.091856 |
| 5 | 6 | 0 | -2.541384 | 0.788891 | 0.011160 |
| 6 | 8 | 0 | 2.466495 | -0.676269 | 1.127018 |
| 7 | 8 | 0 | 3.614656 | 0.616831 | -0.307819 |
| 8 | 6 | 0 | 4.833976 | 0.121199 | 0.255568 |
| 9 | 6 | 0 | 2.492620 | 0.134137 | 0.235293 |
| 10 | 8 | 0 | -3.349608 | 1.664638 | -0.146298 |
| 11 | 8 | 0 | -2.811205 | -0.442973 | 0.412819 |
| 12 | 6 | 0 | -4.200488 | -0.755422 | 0.592220 |
| 13 | 7 | 0 | 0.390730 | 2.739631 | 0.042519 |
| 14 | 1 | 0 | 1.485228 | 1.527383 | -1.108856 |
| 15 | 1 | 0 | 4.908166 | -0.957051 | 0.110929 |
| 16 | 1 | 0 | 4.880426 | 0.349695 | 1.320971 |
| 17 | 1 | 0 | 5.633152 | 0.630966 | -0.276831 |
| 18 | 1 | 0 | -4.223753 | -1.794618 | 0.908727 |
| 19 | 1 | 0 | -4.634630 | -0.111438 | 1.356958 |
| 20 | 1 | 0 | -4.736983 | -0.627864 | -0.348227 |
| 21 | 6 | 0 | -0.128483 | -1.337723 | -0.332408 |
| 22 | 9 | 0 | -1.097107 | -1.662340 | -1.199578 |
| 23 | 9 | 0 | 0.979053 | -1.934127 | -0.779353 |
| 24 | 9 | 0 | -0.426459 | -1.867348 | 0.849140 |

**$TS_{s\text{-}cis\text{-}2h \rightarrow 3h}$**



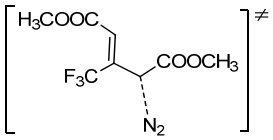

Imaginary Freq. = -488.7595 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.666886
Sum of electronic and thermal Energies= -1018.650760
Sum of electronic and thermal Enthalpies= -1018.649816
Sum of electronic and thermal Free Energies= -1018.712022

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.036383 | 0.392029 | -0.313628 |
| 2 | 6 | 0 | -0.613072 | -0.828845 | -0.307333 |
| 3 | 6 | 0 | 1.407670 | 0.450225 | -0.625383 |
| 4 | 7 | 0 | 0.230417 | -1.818901 | -0.785840 |
| 5 | 6 | 0 | -2.011241 | -1.245952 | -0.035547 |
| 6 | 8 | 0 | 2.194505 | -0.887148 | 1.210328 |
| 7 | 8 | 0 | 3.646744 | 0.207237 | -0.102969 |
| 8 | 6 | 0 | 4.717293 | -0.311092 | 0.694818 |
| 9 | 6 | 0 | 2.419392 | -0.161349 | 0.274720 |
| 10 | 8 | 0 | -2.479730 | -2.262997 | -0.469509 |
| 11 | 8 | 0 | -2.639327 | -0.368062 | 0.729650 |
| 12 | 6 | 0 | -4.035103 | -0.616153 | 0.954316 |
| 13 | 7 | 0 | 1.284441 | -1.693151 | -1.229175 |
| 14 | 1 | 0 | 1.774464 | 1.320971 | -1.155527 |
| 15 | 1 | 0 | 4.709881 | -1.401220 | 0.679862 |
| 16 | 1 | 0 | 4.629214 | 0.041567 | 1.722987 |
| 17 | 1 | 0 | 5.629671 | 0.068856 | 0.241782 |
| 18 | 1 | 0 | -4.373994 | 0.193649 | 1.594546 |
| 19 | 1 | 0 | -4.573514 | -0.605510 | 0.006227 |
| 20 | 1 | 0 | -4.170486 | -1.578687 | 1.447498 |
| 21 | 6 | 0 | -0.756160 | 1.681906 | -0.186356 |
| 22 | 9 | 0 | -1.045276 | 1.953105 | 1.085881 |
| 23 | 9 | 0 | -1.901034 | 1.650657 | -0.877275 |
| 24 | 9 | 0 | -0.053440 | 2.714891 | -0.664818 |

**TS*s-trans*-1h→carbene**



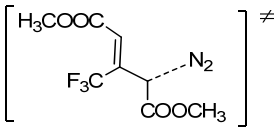

Imaginary Freq. = -257.9076 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.664411
Sum of electronic and thermal Energies= -1018.646689
Sum of electronic and thermal Enthalpies= -1018.645745
Sum of electronic and thermal Free Energies= -1018.711909

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.062131 | 0.050367 | -0.301093 |
| 2 | 6 | 0 | 1.321660 | 0.121393 | -0.709784 |
| 3 | 6 | 0 | -0.672465 | -1.124488 | -0.072265 |
| 4 | 7 | 0 | 1.974375 | 1.677004 | 0.474465 |
| 5 | 6 | 0 | 2.256075 | -0.935589 | -0.344767 |
| 6 | 8 | 0 | -2.739828 | -2.070280 | -0.756557 |
| 7 | 8 | 0 | -2.710134 | -0.643927 | 0.977287 |
| 8 | 6 | 0 | -4.139446 | -0.732750 | 1.068482 |
| 9 | 6 | 0 | -2.154761 | -1.332762 | -0.012815 |
| 10 | 8 | 0 | 2.123654 | -2.026067 | -0.858820 |
| 11 | 8 | 0 | 3.266531 | -0.591949 | 0.448757 |
| 12 | 6 | 0 | 4.262694 | -1.607204 | 0.649954 |
| 13 | 7 | 0 | 2.469249 | 2.629224 | 0.669247 |
| 14 | 1 | 0 | -0.087402 | -2.037942 | -0.053797 |
| 15 | 1 | 0 | -4.443936 | -1.765291 | 1.240951 |
| 16 | 1 | 0 | -4.595006 | -0.362372 | 0.149354 |
| 17 | 1 | 0 | -4.418179 | -0.106755 | 1.911993 |
| 18 | 1 | 0 | 5.010154 | -1.153514 | 1.295710 |
| 19 | 1 | 0 | 3.823547 | -2.479845 | 1.133489 |
| 20 | 1 | 0 | 4.705996 | -1.896841 | -0.302645 |
| 21 | 6 | 0 | -0.864225 | 1.341197 | -0.393636 |
| 22 | 9 | 0 | -0.234527 | 2.272174 | -1.112929 |
| 23 | 9 | 0 | -1.065806 | 1.860223 | 0.826773 |
| 24 | 9 | 0 | -2.067082 | 1.160467 | -0.955046 |

**$TS_{s\text{-}cis\text{-}1h \rightarrow carbene}$**



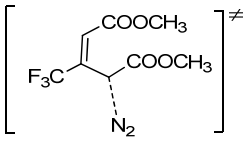

Imaginary Freq. = -269.3058 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.666692
Sum of electronic and thermal Energies= -1018.649290
Sum of electronic and thermal Enthalpies= -1018.648346
Sum of electronic and thermal Free Energies= -1018.712879

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.078573 | -0.160667 | -0.051356 |
| 2 | 6 | 0 | -1.249944 | -0.201057 | -0.594330 |
| 3 | 6 | 0 | 0.644354 | 0.996505 | 0.341171 |
| 4 | 7 | 0 | -2.204013 | -1.578636 | 0.607627 |
| 5 | 6 | 0 | -2.171188 | 0.920845 | -0.468334 |
| 6 | 8 | 0 | 2.521915 | 1.696049 | 1.589527 |
| 7 | 8 | 0 | 2.839144 | 0.889208 | -0.483731 |
| 8 | 6 | 0 | 4.259433 | 1.014699 | -0.315793 |
| 9 | 6 | 0 | 2.104113 | 1.228169 | 0.565155 |
| 10 | 8 | 0 | -1.904505 | 1.956976 | -1.039307 |
| 11 | 8 | 0 | -3.317536 | 0.688546 | 0.167416 |
| 12 | 6 | 0 | -4.285584 | 1.746475 | 0.096906 |
| 13 | 7 | 0 | -2.792616 | -2.460566 | 0.862062 |
| 14 | 1 | 0 | 0.022982 | 1.871483 | 0.501153 |
| 15 | 1 | 0 | 4.593683 | 0.383335 | 0.508210 |
| 16 | 1 | 0 | 4.524963 | 2.053170 | -0.116848 |
| 17 | 1 | 0 | 4.694341 | 0.681252 | -1.254097 |
| 18 | 1 | 0 | -5.157113 | 1.375647 | 0.630217 |
| 19 | 1 | 0 | -3.900611 | 2.646057 | 0.577204 |
| 20 | 1 | 0 | -4.536012 | 1.961999 | -0.941795 |
| 21 | 6 | 0 | 0.914456 | -1.412995 | -0.243574 |
| 22 | 9 | 0 | 1.954339 | -1.446653 | 0.601797 |
| 23 | 9 | 0 | 0.193491 | -2.519170 | -0.010123 |
| 24 | 9 | 0 | 1.391809 | -1.516021 | -1.485250 |

**$TS_{s\text{-}trans\text{-}2h \rightarrow carbene}$**



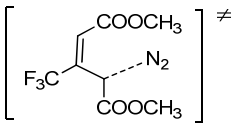

Imaginary Freq. = -226.7068 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.666194
Sum of electronic and thermal Energies= -1018.648587
Sum of electronic and thermal Enthalpies= -1018.647643
Sum of electronic and thermal Free Energies= -1018.713551

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.226560 | -0.722622 | -0.018258 |
| 2 | 6 | 0 | -0.357927 | 0.446587 | 0.591890 |
| 3 | 6 | 0 | 1.542617 | -0.792155 | -0.287121 |
| 4 | 7 | 0 | -2.076459 | -0.325629 | 1.492744 |
| 5 | 6 | 0 | -0.981961 | 1.447696 | -0.283336 |
| 6 | 8 | 0 | 2.115319 | 1.339309 | 0.598497 |
| 7 | 8 | 0 | 3.735058 | -0.106211 | 0.019524 |
| 8 | 6 | 0 | 4.711314 | 0.852239 | 0.440038 |
| 9 | 6 | 0 | 2.461034 | 0.274855 | 0.152200 |
| 10 | 8 | 0 | -0.291180 | 1.980063 | -1.117635 |
| 11 | 8 | 0 | -2.237434 | 1.784389 | 0.001761 |
| 12 | 6 | 0 | -2.769357 | 2.865779 | -0.778047 |
| 13 | 7 | 0 | -2.795634 | -0.446764 | 2.302992 |
| 14 | 1 | 0 | 1.955363 | -1.635680 | -0.823540 |
| 15 | 1 | 0 | 4.602061 | 1.062652 | 1.504422 |
| 16 | 1 | 0 | 4.602140 | 1.777745 | -0.126617 |
| 17 | 1 | 0 | 5.677796 | 0.395560 | 0.241823 |
| 18 | 1 | 0 | -3.788282 | 3.001988 | -0.424916 |
| 19 | 1 | 0 | -2.185217 | 3.771397 | -0.614815 |
| 20 | 1 | 0 | -2.765030 | 2.608767 | -1.837567 |
| 21 | 6 | 0 | -0.655680 | -1.871459 | -0.471409 |
| 22 | 9 | 0 | -1.090592 | -2.601324 | 0.566967 |
| 23 | 9 | 0 | -1.737409 | -1.419264 | -1.119016 |
| 24 | 9 | 0 | -0.019542 | -2.708480 | -1.290380 |

**$TS_{s\text{-}cis\text{-}2h \rightarrow carbene}$**



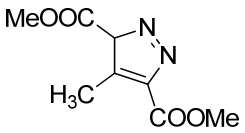

Imaginary Freq. = -309.1751 $cm^{-1}$

Sum of electronic and zero-point Energies= -1018.667214
Sum of electronic and thermal Energies= -1018.649473
Sum of electronic and thermal Enthalpies= -1018.648529
Sum of electronic and thermal Free Energies= -1018.714990

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.207480 | 0.783443 | 0.024092 |
| 2 | 6 | 0 | -0.154933 | -0.595842 | -0.279387 |
| 3 | 6 | 0 | 1.501288 | 1.083736 | 0.188332 |
| 4 | 7 | 0 | -0.206326 | -1.382116 | 1.573670 |
| 5 | 6 | 0 | -1.514115 | -0.873596 | -0.725746 |
| 6 | 8 | 0 | 2.838373 | -0.669486 | 1.053725 |
| 7 | 8 | 0 | 3.092078 | -0.054046 | -1.091720 |
| 8 | 6 | 0 | 4.094592 | -1.070374 | -1.263243 |
| 9 | 6 | 0 | 2.540501 | 0.006622 | 0.106818 |
| 10 | 8 | 0 | -1.837729 | -0.398932 | -1.793646 |
| 11 | 8 | 0 | -2.248538 | -1.726123 | -0.019218 |
| 12 | 6 | 0 | -3.507023 | -2.082460 | -0.609650 |
| 13 | 7 | 0 | 0.126823 | -2.016424 | 2.396433 |
| 14 | 1 | 0 | 1.841484 | 2.079420 | 0.459777 |
| 15 | 1 | 0 | 3.652937 | -2.054738 | -1.107937 |
| 16 | 1 | 0 | 4.912493 | -0.914599 | -0.559849 |
| 17 | 1 | 0 | 4.443177 | -0.965763 | -2.286940 |
| 18 | 1 | 0 | -3.970192 | -2.772656 | 0.090922 |
| 19 | 1 | 0 | -4.128847 | -1.196559 | -0.739416 |
| 20 | 1 | 0 | -3.350252 | -2.566711 | -1.573735 |
| 21 | 6 | 0 | -0.830428 | 1.875577 | 0.192216 |
| 22 | 9 | 0 | -1.212019 | 2.404694 | -0.972641 |
| 23 | 9 | 0 | -1.928559 | 1.397176 | 0.796157 |
| 24 | 9 | 0 | -0.372969 | 2.887846 | 0.946788 |

**3h**




Sum of electronic and zero-point Energies= -1018.720253
Sum of electronic and thermal Energies= -1018.704203
Sum of electronic and thermal Enthalpies= -1018.703259
Sum of electronic and thermal Free Energies= -1018.766095

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.068349 | 0.200205 | -0.529896 |
| 2 | 6 | 0 | -1.009405 | -0.564996 | -0.331055 |
| 3 | 6 | 0 | 1.127355 | -0.707436 | -1.042509 |
| 4 | 7 | 0 | -0.706652 | -1.924738 | -0.667995 |
| 5 | 6 | 0 | -2.352257 | -0.157412 | 0.165483 |
| 6 | 8 | 0 | 3.453757 | -1.175759 | -0.639953 |
| 7 | 8 | 0 | 2.164050 | -0.467136 | 1.057332 |
| 8 | 6 | 0 | 3.288622 | -0.544142 | 1.950610 |
| 9 | 6 | 0 | 2.405451 | -0.808484 | -0.201453 |
| 10 | 8 | 0 | -2.610317 | 0.975102 | 0.472133 |
| 11 | 8 | 0 | -3.189027 | -1.179986 | 0.216451 |
| 12 | 6 | 0 | -4.513512 | -0.873577 | 0.677916 |
| 13 | 7 | 0 | 0.471074 | -2.027295 | -1.052119 |
| 14 | 1 | 0 | 1.430367 | -0.481076 | -2.071312 |
| 15 | 1 | 0 | 4.076571 | 0.128709 | 1.612387 |
| 16 | 1 | 0 | 3.662721 | -1.566827 | 1.991825 |
| 17 | 1 | 0 | 2.910676 | -0.232761 | 2.920472 |
| 18 | 1 | 0 | -5.056585 | -1.814161 | 0.645777 |
| 19 | 1 | 0 | -4.475204 | -0.485614 | 1.696095 |
| 20 | 1 | 0 | -4.978890 | -0.138858 | 0.020624 |
| 21 | 6 | 0 | 0.271644 | 1.666507 | -0.290244 |
| 22 | 9 | 0 | 0.108805 | 1.996217 | 0.988711 |
| 23 | 9 | 0 | 1.529519 | 2.004842 | -0.631861 |
| 24 | 9 | 0 | -0.547857 | 2.418170 | -1.025284 |