# Supporting Information

## NHC-Catalyzed β-Specific Addition of N-Based Nucleophiles to Allenoates

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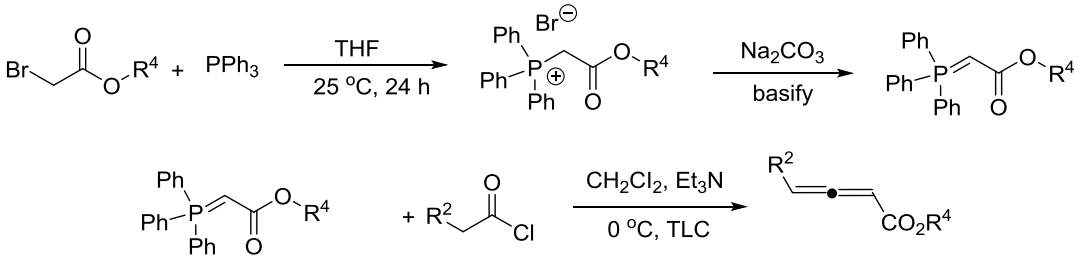
# 1. General Information

Common reagents and materials were purchased from commercial sources and purified by recrystallization or distillation. Melting points were determined in open capillaries and were uncorrected. IR spectra were taken on a FT-IR-Tensor 27 spectrometer in KBr pellets and reported in $cm^{-1}$. $^1H$ NMR spectra were measured on a Bruker DPX 400 MHz spectrometer in $CDCl_3$ with chemical shift ($\delta$) given in ppm relative to TMS as internal standard. Highresolution mass spectra (HRMS) were obtained on a micrOTOF-QⅡ HRMS/MS instrument (Bruker) with the technique of electrospray ionization. Optical rotation values were measured with instruments operating at $\lambda$ = 589 nm, corresponding to the sodium D line at the temperatures indicated. TLC was carried out on $SiO_2$ (silica gel 60 F254, Merck), and the spots were located with UV light.

# 2. Synthesis of Allenoates (2a-2d and 2f-2h)

Allenoates **2a-2d** and **2f-2h** were prepared according to the literature[1].

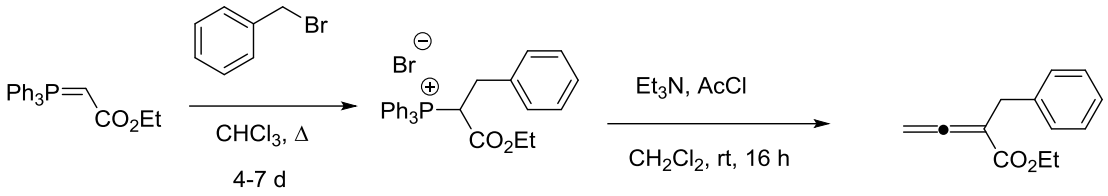
**2a-2d and 2f-2h:**




To a solution of $PPh_3$ (26.2 g, 100 mmol) in THF (150 mL), bromoacetate (100 mmol, 1.0 equiv.) was added over 20 minutes. The reaction mixture was stirred at room temperature for 24 hours and the precipitate filtered, washed with cold $Et_2O$ and dried. The collected phosphonium salt was dissolved in $CH_2Cl_2$ (100 mL) and saturated aqueous $Na_2CO_3$ (150 mL) was added. The mixture was stirred at room temperature for 2 hours and separated the organic layer, then extracted water layer with $CH_2Cl_2$ (20 mL), washed the combined organic layer with saturated aqueous NaCl (50 mL), and dried with $Na_2SO_4$. The $Na_2SO_4$ was filtered and washed with $CH_2Cl_2$. The filtrate was evaporated to 100 mL and directly engaged in the next step.

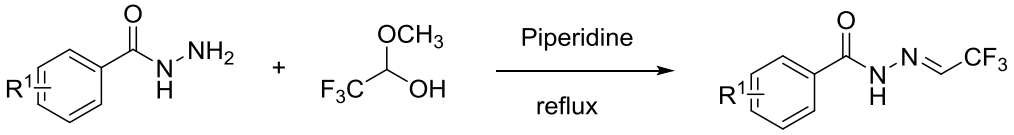
To the solution of stabilized ylide, and triethylamine (14 mL, 100 mmol, 1 equiv.) at 0 °C , alkyl chloride (10 mL, 110 mmol, 1.1 equiv.) in solution in $CH_2Cl_2$ (20 mL) was added dropwise. After completion of the reaction (TLC), the solution was concentrated to afford a gummy residue. This was treated with Pet-EtOAc 20: 1 (petro ether: ethyl acetate =20: 1, 250 mL, 30-60 °C boiling range Pet) and silica gel (100-200 section, 100 g), stirred vigorously for 1 hour. The mixture was filtered and washed with Pet-EtOAc 20: 1, filtrate evaporated and to a flash column chromatography (eluent Pet-EtOAc 20: 1, 30-60 °C boiling range Pet) to afford the pure product **2a-2d** and **2f-2h** as colorless or yellow oil.

**2e:**



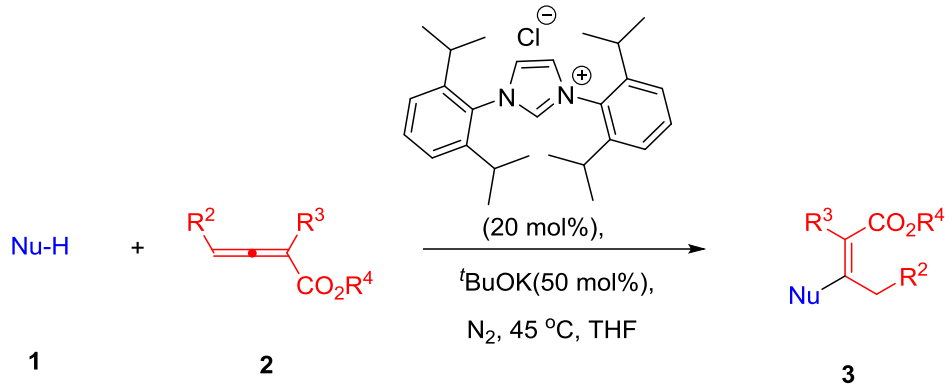

A solution of (carbethoxymethylene)triphenylphosphorane (80 g, 230 mmol) and the benzyl bromide (250 mmol, 1.1 equiv) in $CHCl_3$ (500 mL) was heated under reflux for 4−7 days until TLC (hexanes/EtOAc, 2:1) indicated the complete disappearance of the phosphorane. The mixture was concentrated and the crude oily foam was co-evaporated with $CH_2Cl_2$. The resultant crude phosphonium salt was dissolved in $CH_2Cl_2$ (500 mL) and $Et_3N$ (64 mL, 460 mmol, 2 equiv) was added, followed by stirring for 30 min. AcCl (16.35 mL, 230 mmol, 1 equiv) was then slowly added over 30 min with vigorous stirring. The resultant suspension was stirred for 16 h and concentrated. The thick slurry was stirred with $Et_2O$ (300 mL) for 2 h and then filtered over a pad of silica gel. The residue on the filter was washed with $Et_2O$ and the combined organic fractions were concentrated. Column chromatography of the crude oil (hexanes/$Et_2O$, 40:1–20:1) afforded the allenoate (**2e**).

## 3. Synthesis of trifluoromethylated acylhydrazone (1h-1n)



To a solution of 2,2,2-trifluoro-1-methoxyethan-1-ol (0.65 g, 5 mmol) in THF (20 mL), piperidine (0.3 g, 3.5 mmol.) was added and stirred at room temperature for 1 hours. Acylhydrazine (5 mmol) was then added and the reaction mixture was heated under reflux for 6-12 hours until TLC indicated the complete disappearance of the acylhydrazine. After the reaction, solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (petro ether: ethyl acetate = 5:1) to afford products **1h-1n**[2].

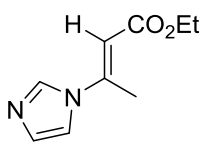
## 4. General Procedure for the Syntheses of Products




An oven-dried 10 mL Schlenk tube equipped with a magnetic stir bar was charged with imidazolium salt **A** (0.04 mmol), $^{t}$BuOK (0.1 mmol), and pronucleophile **1** (0.20 mmol). Freshly distilled THF (2 mL), allenoates **2** (0.30 mmol) ware added into the mixture with a syringe. Then tube was closed with a septum, evacuated, and refilled with nitrogen. The mixture was stirred at 45 °C until completion (monitored by TLC). After removal of the solvent under reduced pressure, the resulted crude residue was purified by column chromatography (silicagel, mixtures of petroleum ether/ethyl acetate, 1:1-10:1, v/v) to afford the desired product **3**.

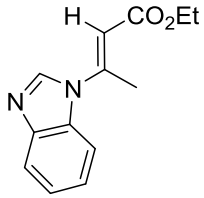
## 5. Characterization Data of Products

**Ethyl (E)-3-(1H-imidazol-1-yl) but-2-enoate (3aa)**



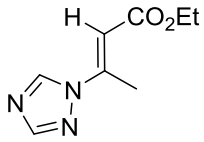
White solid (27.4 mg, 76% yield), m.p.: 62.1-64.8 ºC, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.25 (s, 1H), 7.15 (s, 1H), 6.01 (d, J = 0.9 Hz, 1H), 4.23 (q, J = 7.1 Hz, 2H), 2.72 (d, J = 0.9 Hz, 3H), 1.32 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.03, 147.77, 135.17, 130.92, 116.45, 107.27, 60.47, 16.48, 14.26. HRMS (ESI) calcd for $[C_9H_{13}N_2O_2, M+H]^+$ : 181.0972, found: 181.0951.

**Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3ba)**



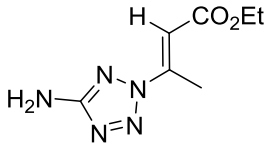
White solid (41.0 mg, 89% yield), m.p.: 57.3-60.7 ºC, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.88–7.79 (m, 1H), 7.70–7.58 (m, 1H), 7.42–7.30 (m, 2H), 6.20 (d, J = 1.0 Hz, 1H), 4.27 (q, J = 7.1 Hz, 2H), 2.83 (d, J = 1.0 Hz, 3H), 1.35 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.10, 148.35, 144.57, 141.07, 132.25, 124.29, 123.54, 121.03, 112.12, 111.28, 60.55, 18.29, 14.29. HRMS (ESI) calcd for $[C_{13}H_{15}N_2O_2, M+H]^+$ : 231.1128, found: 231.1112.

**Ethyl (E)-3-(1H-1,2,4-triazol-1-yl) but-2-enoate (3ca)**



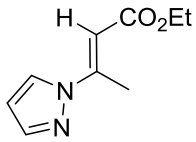
Clear oil (29.7 mg, 82% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.04 (s, 1H), 6.61 (d, J = 0.9 Hz, 1H), 4.24 (q, J = 7.1 Hz, 2H), 2.77 (d, J = 0.9 Hz, 3H), 1.32 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.02, 152.69, 146.28, 141.65, 108.61, 60.58, 15.02, 14.23. HRMS (ESI) calcd for $[C_8H_{12}N_3O_2, M+H]^+$ : 182.0924, found: 182.0918.

**Ethyl (E)-3-(5-amino-2H-tetrazol-2-yl) but-2-enoate (3da)**



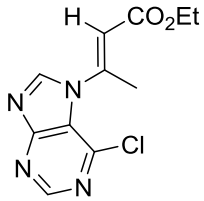
White solid (22.1 mg, 56% yield), m.p.: 105.3-108.4 ºC, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 6.84 – 6.67 (m, 1H), 4.63 (s, 2H), 4.25 (q, J = 7.1 Hz, 2H), 2.86 (d, J = 0.9 Hz, 3H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.86, 165.78, 146.66, 109.37, 60.70, 14.26, 14.22.. HRMS (ESI) calcd for $[C_7H_{12}N_5O_2, M+H]^+$ : 198.0986, found: 198.0976.

**Ethyl (E)-3-(1H-pyrazol-1-yl) but-2-enoate (3ea)**



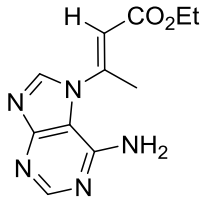
Clear oil (13.3 mg, 37% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.81 (m, 1H), 7.68 (d, J = 1.5 Hz, 1H), 6.49 (d, J = 0.9 Hz, 1H), 6.43 (dd, J = 2.6, 1.7 Hz, 1H), 4.21 (q, J = 7.1 Hz, 2H), 2.77 (d, J = 0.9 Hz, 3H), 1.31 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.91, 149.84, 142.07, 127.36, 108.42, 105.01, 60.09, 15.11, 14.30. HRMS (ESI) calcd for $[C_9H_{13}N_2O_2, M+H]^+$ : 181.0972, found: 181.0957.

**Ethyl (E)-3-(6-chloro-7H-purin-7-yl) but-2-enoate (3fa)**



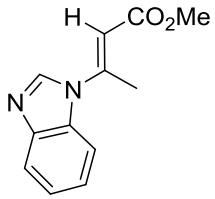
White solid (45.9 mg, 86% yield), m.p.: 142.8-144.3 °C, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.38 (s, 1H), 6.97 (d, J = 1.0 Hz, 1H), 4.29 (q, J = 7.1 Hz, 2H), 2.91 (d, J = 1.0 Hz, 3H), 1.36 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.67, 152.63, 152.00, 151.44, 145.78, 143.00, 132.74, 113.64, 60.86, 17.13, 14.25. HRMS (ESI) calcd for $[C_{11}H_{12}ClN_4O_2, M+H]^+$ : 267.0643, found: 267.0627.

**Ethyl (E)-3-(6-amino-7H-purin-7-yl) but-2-enoate (3ga)**



White solid (21.3 mg, 43% yield), m.p.: 164.6-166.9 °C, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.05 (s, 1H), 7.02 (s, 1H), 5.84 (s, 2H), 4.26 (q, J = 7.1 Hz, 2H), 2.87 (s, 3H), 1.34 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.27, 155.80, 153.69, 150.13, 146.54, 138.47, 120.68, 112.16, 60.56, 17.05, 14.28. HRMS (ESI) calcd for $[C_{11}H_{14}N_5O_2, M+H]^+$ : 248.1142, found: 248.1134.

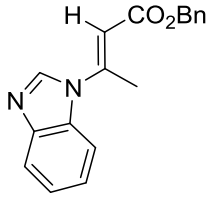
**Methyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bb)**



White solid (40.7 mg, 94% yield), m.p.: 68.2-69.8 °C, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.89 – 7.80 (m, 1H), 7.66 – 7.62 (m, 1H), 7.42 – 7.30 (m, 2H), 6.22 (d, J = 1.3 Hz, 1H), 3.81 (s, 3H), 2.83 (d, J = 0.9 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ

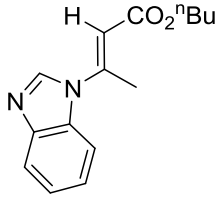
166.52, 148.64, 144.60, 141.04, 132.23, 124.33, 123.58, 121.06, 112.11, 110.66, 51.65, 18.28. HRMS (ESI) calcd for [$C_{12}H_{13}N_2O_2$, M+H]$^+$ : 217.0972, found: 217.0965.

**Benzyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bc)**



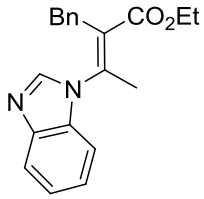
White solid (42.7 mg, 73% yield), m.p.: 26.5-28.2 $^o$C, $^1$H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.87 – 7.80 (m, 1H), 7.65-7.61 (m, 1H), 7.45 – 7.30 (m, 7H), 6.26 (d, J = 1.0 Hz, 1H), 5.25 (s, 2H), 2.84 (d, J = 1.0 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.89, 148.99, 144.59, 141.02, 135.72, 132.17, 128.66, 128.41, 124.34, 123.60, 121.05, 112.17, 110.58, 66.40, 18.34. HRMS (ESI) calcd for [$C_{18}H_{17}N_2O_2$, M+H]$^+$ : 293.1285, found: 293.1275.

**Butyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bd)**



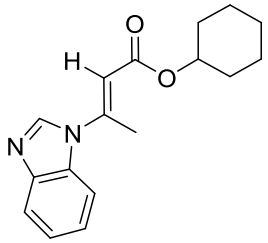
Yellow oil (32.03 mg, 62% yield), $^1$H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.86–7.81 (m, 1H), 7.67 – 7.59 (m, 1H), 7.43 – 7.30 (m, 2H), 6.20 (s, 1H), 4.21 (t, J = 6.7 Hz, 2H), 2.82 (s, 3H), 1.75 – 1.63 (m, 2H), 1.50 – 1.38 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.20, 148.32, 144.56, 141.08, 132.23, 124.26, 123.51, 121.01, 112.11, 111.25, 64.46, 30.68, 19.20, 18.28, 13.75. HRMS (ESI) calcd for [$C_{15}H_{19}N_2O_2$, M+H]$^+$ : 259.1441, found: 259.1434.

**Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl)-2-benzylbut-2-enoate(3be)**



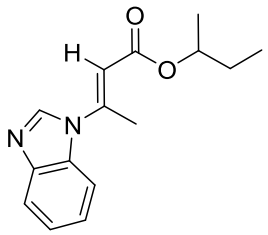
Clear oil (35.9 mg, 56% yield), $^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.83 – 7.76 (m, 1H), 7.38 – 7.23 (m, 8H), 3.93 (s, 2H), 3.66 (q, J = 7.1 Hz, 2H), 2.35 (s, 3H), 0.54 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 167.05, 143.32, 141.93, 137.50, 135.89, 133.61, 131.28, 128.78, 128.20, 126.78, 123.49, 122.49, 120.39, 110.29, 61.10, 35.76, 20.08, 13.17. HRMS (ESI) calcd for [$C_{20}H_{21}N_2O_2$, M+H]$^+$ : 321.1598, found: 321.1580.

**Cyclohexyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bf)**



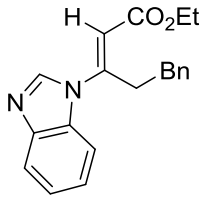
Clear oil (36.4 mg, 64% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.87 – 7.81 (m, 1H), 7.67 – 7.61 (m, 1H), 7.41 – 7.31 (m, 2H), 6.18 (d, J = 1.0 Hz, 1H), 4.93– 4.86 (m, 1H), 2.82 (d, J = 0.9 Hz, 3H), 1.99 – 1.89 (m, 2H), 1.83 – 1.71 (m, 2H), 1.53 – 1.22 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.64, 148.09, 144.64, 141.19, 132.36, 124.32, 123.56, 121.08, 112.20, 112.14, 73.12, 31.83, 25.45, 23.92, 18.40. HRMS (ESI) calcd for $[C_{17}H_{21}N_2O_2, M+H]^+$ : 285.1598, found: 285.1588.

**Sec-butyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bg)**



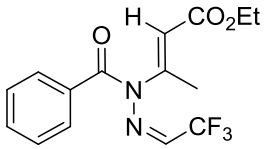
Clear oil (30.0 mg, 58% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.86 – 7.82 (m, 1H), 7.66 – 7.62 (m, 1H), 7.43 – 7.31 (m, 2H), 6.19 (d, J = 1.0 Hz, 1H), 5.02 – 4.94 (m, 1H), 2.83 (d, J = 0.9 Hz, 3H), 1.73– 1.58 (m, 2H), 1.30 (d, J = 6.3 Hz, 3H), 0.96 (t, J = 7.5 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.80, 148.10, 144.57, 141.10, 132.28, 124.25, 123.49, 121.01, 112.11, 111.92, 72.57, 28.87, 19.56, 18.31, 9.78. HRMS (ESI) calcd for $[C_{15}H_{19}N_2O_2, M+H]^+$ : 259.1441, found: 259.1437.

**Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl)-5-phenylpent-2-enoate (3bh)**



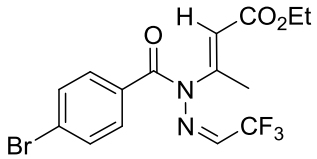
Clear oil (55.7 mg, 87% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.83 – 7.77 (m, 1H), 7.45 – 7.22 (m, 8H), 6.12 (t, J = 7.8 Hz, 1H), 4.07 (q, J = 7.1 Hz, 2H), 3.70 – 3.61 (m, 4H), 1.14 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.03, 143.59, 142.59, 138.33, 133.63, 130.90, 128.85, 128.54, 128.34, 126.77, 123.40, 122.49, 120.48, 110.47, 61.51, 36.40, 33.98, 13.96. HRMS (ESI) calcd for $[C_{20}H_{21}N_2O_2, M+H]^+$ : 321.1598, found: 321.1579.

**Ethyl (E)-3-(1-benzoyl-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but-2-enoate (5aa)**



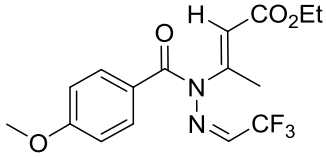
Clear oil (44.6 mg, 68% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 2H), 7.56 – 7.51 (m, 1H), 7.46 – 7.41 (m, 2H), 7.05 (q, J = 3.6 Hz, 1H), 6.00 (d, J = 1.3 Hz, 1H), 4.26 (q, J = 7.1 Hz, 2H), 2.39 (d, J = 1.3 Hz, 3H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.28, 164.55, 149.05, 132.42, 131.93, 130.21, 127.94 (q, J = 39.6 Hz), 127.85, 124.91, 120.13 (q, J = 271.5 Hz), 61.02, 16.68, 14.15. HRMS (ESI) calcd for $[C_{15}H_{15}F_3N_2O_3Na, M+Na]^+$ : 351.0927, found: 351.0910.

**Ethyl (E)-3-(1-(4-bromobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-Enoate (5ba)**



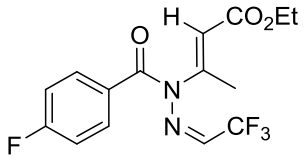
White solid (52.1 mg, 64% yield), m.p.: 164.6-166.9 ºC, $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.5 Hz, 2H), 7.58 (d, J = 8.5 Hz, 2H), 7.04 (q, J = 3.4 Hz, 1H), 5.99 (s, 1H), 4.26 (q, J = 7.1 Hz, 2H), 2.38 (s, 3H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.27, 164.44, 148.63, 131.86, 131.18, 128.29 (q, J = 39.7 Hz), 126.88, 125.17, 120.04 (q, J = 271.6 Hz), 61.10, 16.64, 14.14. HRMS (ESI) calcd for $[C_{15}H_{14}BrF_3N_2O_3Na, M+Na]^+$ : 429.0032, found: 429.0013.

**Ethyl (E)-3-(1-(4-methoxybenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but-2-enoate (5ca)**



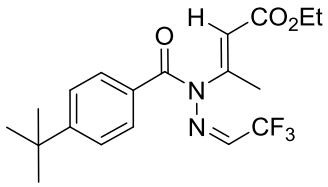
Clear oil (23.6 mg, 33% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.81 (m, 2H), 7.03 (q, J = 3.6 Hz, 1H), 6.96 – 6.91 (m, 2H), 5.97 (d, J = 1.3 Hz, 1H), 4.25 (q, J = 7.1 Hz, 2H), 3.87 (s, 3H), 2.38 (d, J = 1.3 Hz, 3H), 1.32 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.38, 164.66, 162.69, 149.51, 132.82, 127.41 (q, J = 39.5 Hz), 124.44, 124.28, 120.26 (q, J = 271.4 Hz), 113.21, 60.95, 55.43, 16.71, 14.15. HRMS (ESI) calcd for $[C_{16}H_{17}F_3N_2O_4Na, M+Na]^+$ : 381.1033, found: 381.1021.

**Ethyl (E)-3-(1-(4-fluorobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5da)**



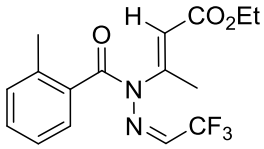
Clear oil (49.9 mg, 72% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.79 (m, 2H), 7.16 – 7.09 (m, 2H), 7.04 (q, J = 3.6 Hz, 1H), 6.00 (d, J = 1.3 Hz, 1H), 4.26 (q, J = 7.1 Hz, 2H), 2.38 (d, J = 1.3 Hz, 3H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.02, 164.87 (d, J = 253.6 Hz), 164.50, 148.85, 133.00 (d, J = 9.1 Hz), 128.40 (d, J = 3.3 Hz), 128.04 (q, J = 39.7 Hz), 125.06, 120.11 (q, J = 271.6 Hz), 115.08 (d, J = 21.9 Hz), 61.08, 16.65, 14.15. HRMS (ESI) calcd for [$C_{15}H_{14}F_4N_2O_3Na$, M+Na]$^+$ : 369.0833, found: 369.0810.

**Ethyl (E)-3-(1-(4-(tert-butyl)benzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl ) but-2-enoate (5ea)**



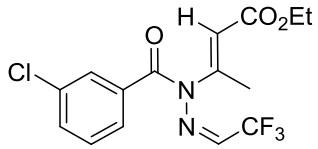
Clear oil (56.9 mg, 74% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.48 – 7.44 (m, 2H), 7.05 (q, J = 3.7 Hz, 1H), 5.98 (d, J = 1.3 Hz, 1H), 4.25 (q, J = 7.1 Hz, 2H), 2.38 (d, J = 1.3 Hz, 3H), 1.35 (s, 9H), 1.32 (t, J = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.92, 164.61, 155.72, 149.34, 130.44, 129.32, 127.68 (q, J = 39.6 Hz), 124.88, 124.68, 120.24 (q, J = 271.5 Hz), 60.96, 35.05, 31.10, 16.71, 14.15. HRMS (ESI) calcd for [$C_{19}H_{23}F_3N_2O_3Na$, M+Na]$^+$ : 407.1553, found: 407.1535.

**Ethyl (E)-3-(1-(2-methylbenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5fa)**



Clear oil (30.8 mg, 45% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 1H), 7.29 – 7.26 (m, 1H), 7.22 (t, J = 7.1 Hz, 2H), 7.03 (q, J = 3.6 Hz, 1H), 6.01 (d, J = 1.3 Hz, 1H), 4.25 (q, J = 7.1 Hz, 2H), 2.40 (d, J = 1.2 Hz, 3H), 2.29 (s, 3H), 1.32 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 171.26, 164.44, 148.62, 135.45, 134.00, 130.16, 130.12, 128.41 (q, J = 39.7 Hz), 127.49, 125.38, 125.31, 119.96 (q, J = 271.6 Hz), 61.08, 19.44, 16.72, 14.14. HRMS (ESI) calcd for [$C_{16}H_{17}F_3N_2O_3Na$, M+Na]$^+$ : 365.1083, found: 365.1071.

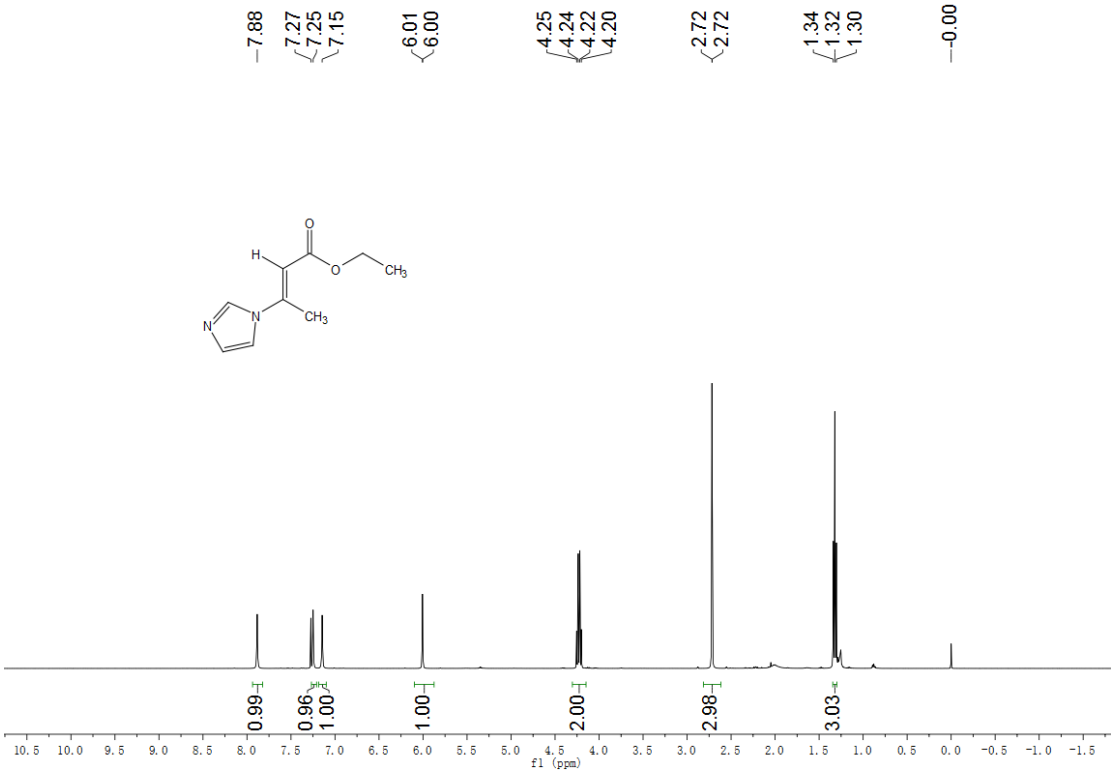
**Ethyl (E)-3-(1-(3-chlorobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5ga)**

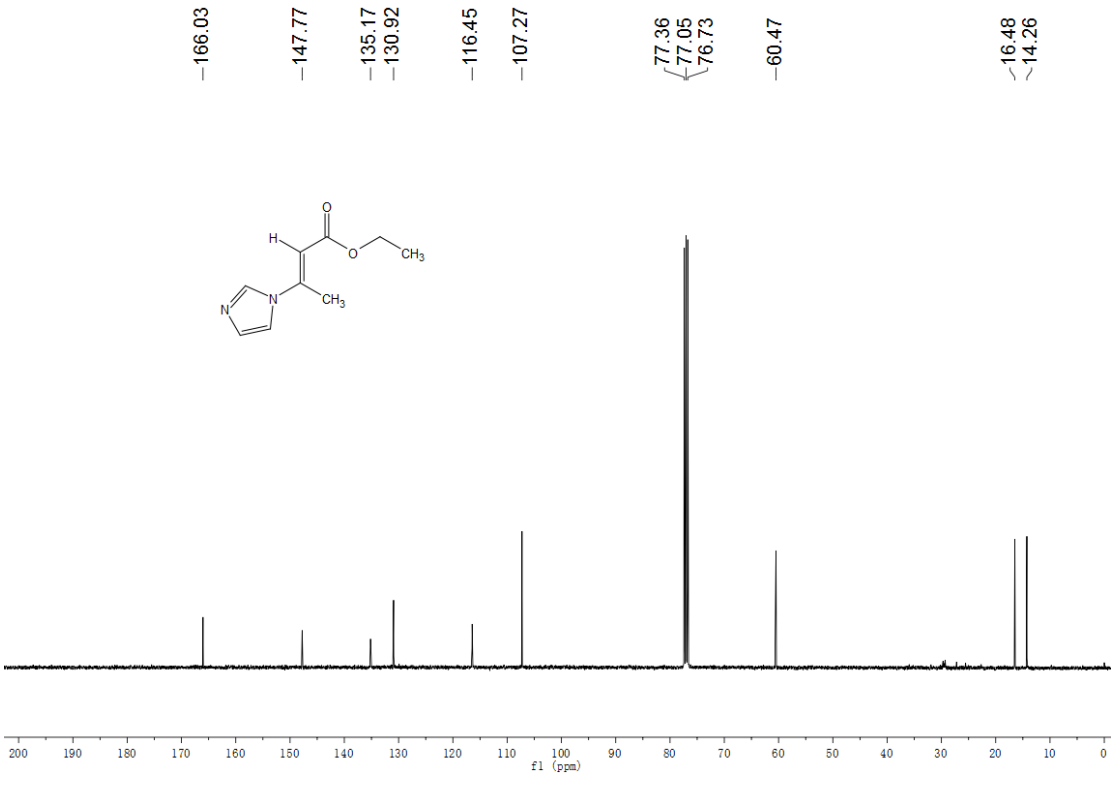



Clear oil (37.7 mg, 52% yield), $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.76 (t, J = 1.8 Hz, 1H), 7.63 (dt, J = 7.8, 1.3 Hz, 1H), 7.51 –7.49 (m, 1H), 7.37 (t, J = 7.9 Hz, 1H), 7.05 (q, J = 3.6 Hz, 1H), 6.00 (d, J = 1.3 Hz, 1H), 4.26 (q, J = 7.1 Hz, 2H), 2.38 (d, J = 1.3 Hz, 3H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 167.88, 164.41, 148.49, 134.09, 134.01, 131.89, 130.31, 129.12, 128.45 (q, J = 39.8 Hz), 128.29, 125.28, 120.02 (q, J = 271.7 Hz), 61.11, 16.62, 14.14. HRMS (ESI) calcd for $[C_{15}H_{14}ClF_3N_2O_3Na, M+Na]^+$ : 385.0537, found: 385.0519.

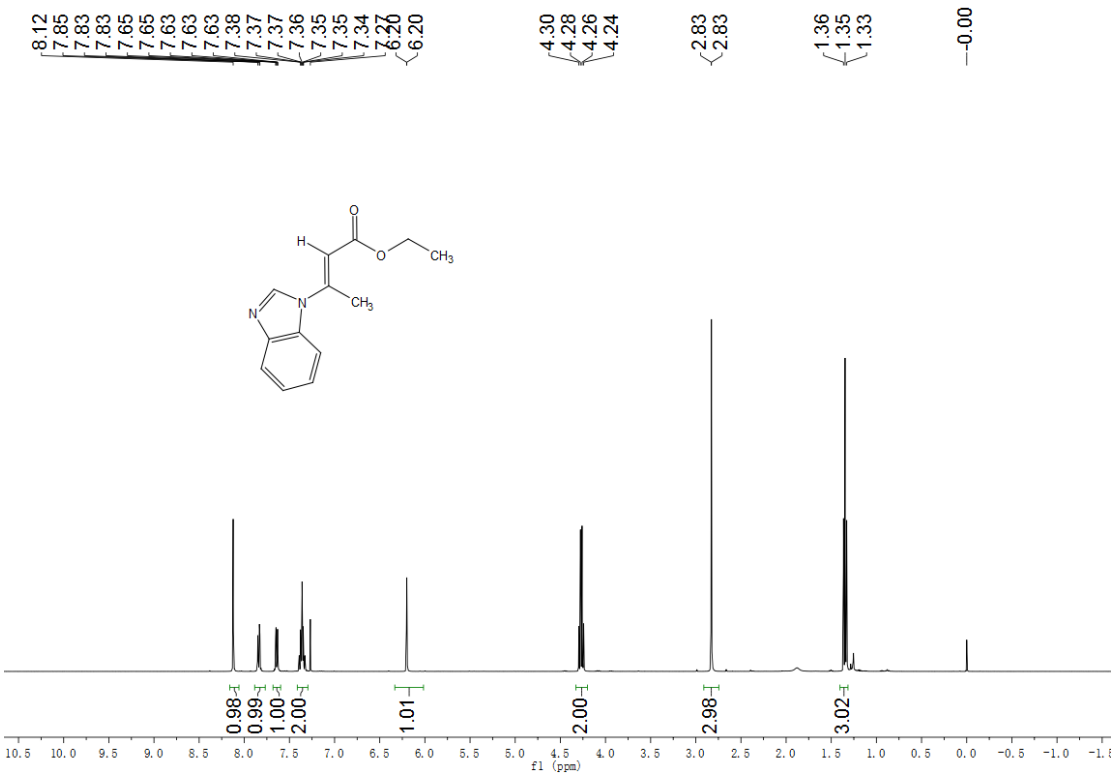
# 6. Copies of $^{1}$H NMR and $^{13}$C NMR Spectra of Products

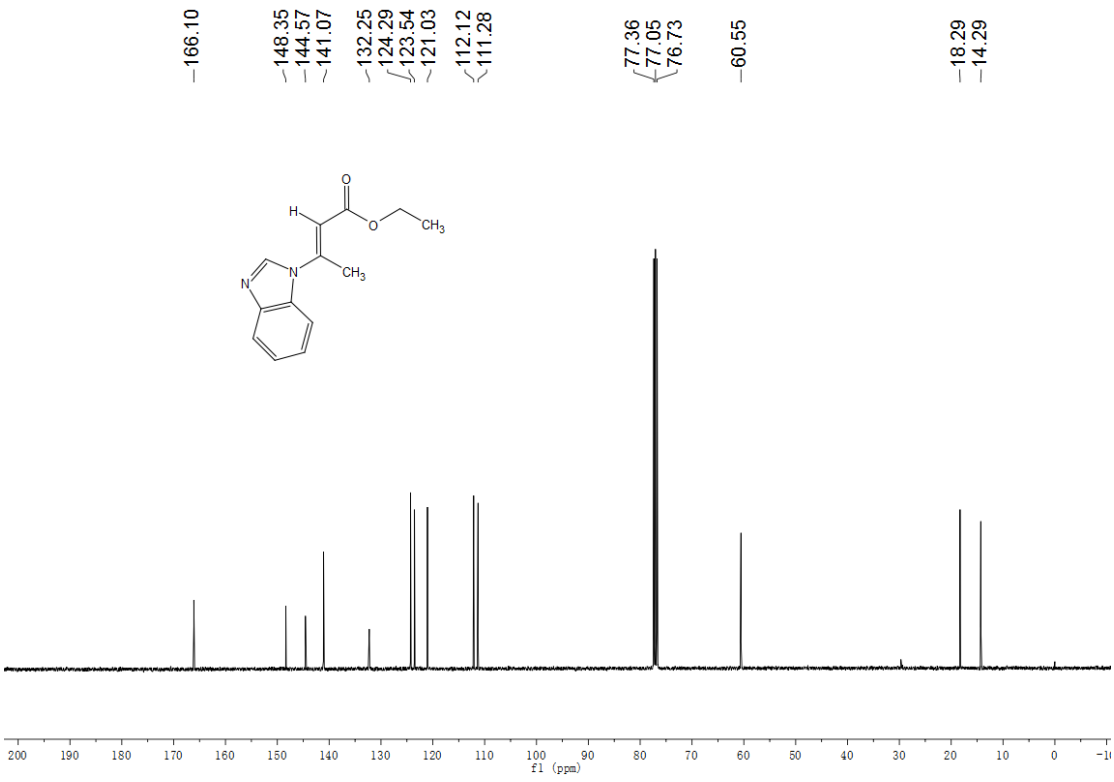
## Ethyl (E)-3-(1H-imidazol-1-yl) but-2-enoate (3aa)



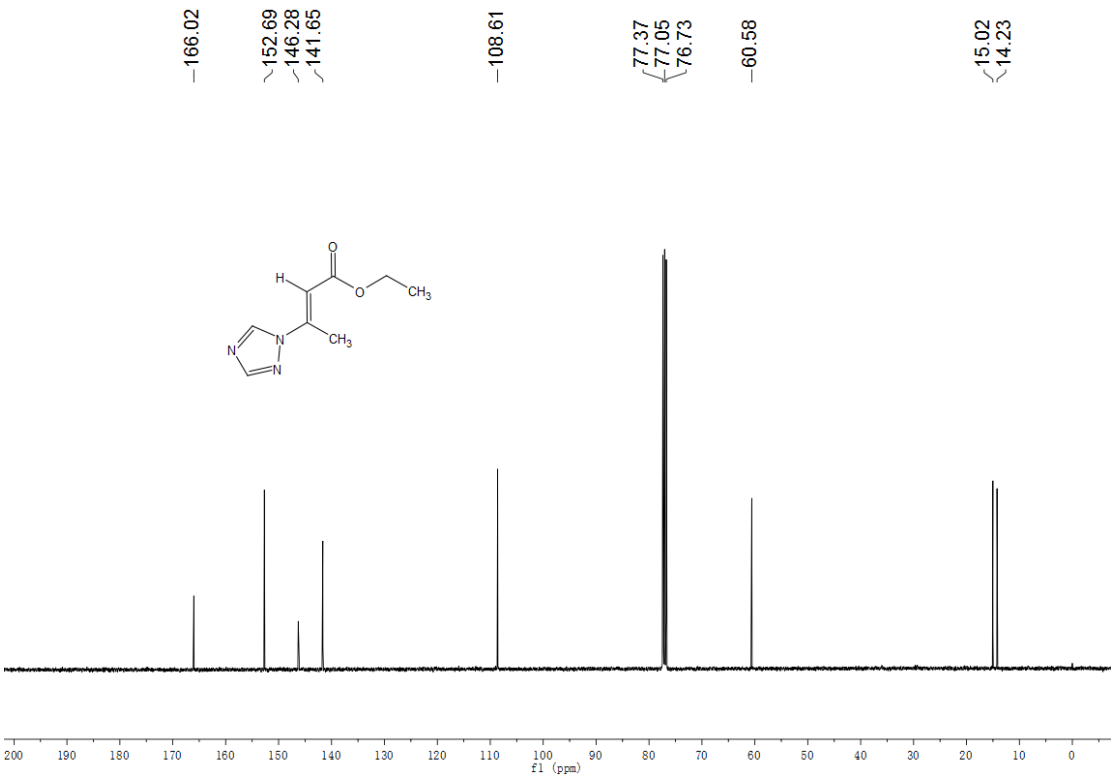



## Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3ba)

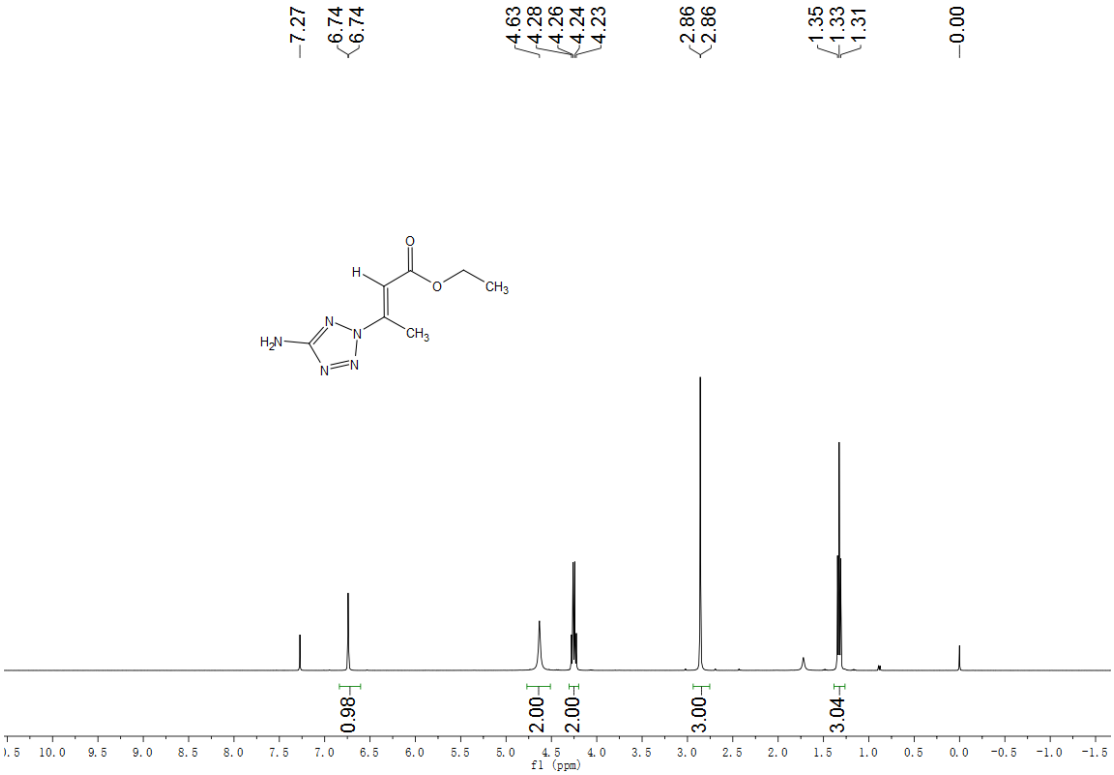


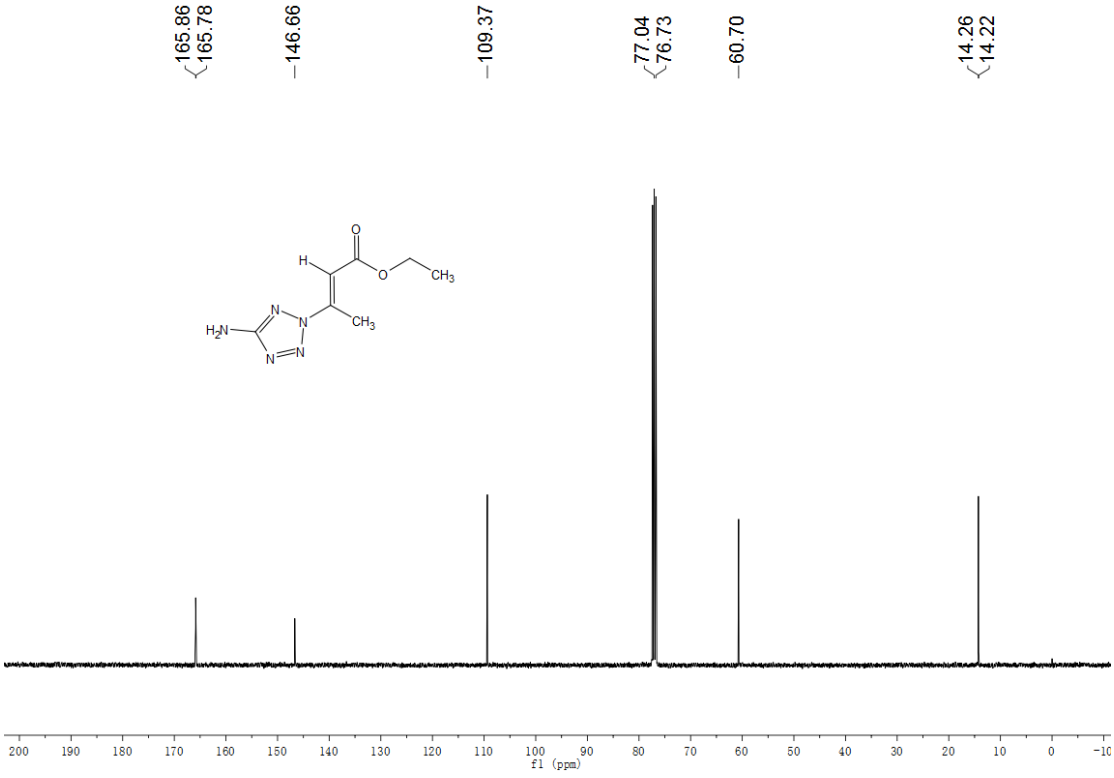



## Ethyl (E)-3-(1H-1,2,4-triazol-1-yl) but-2-enoate (3ca)

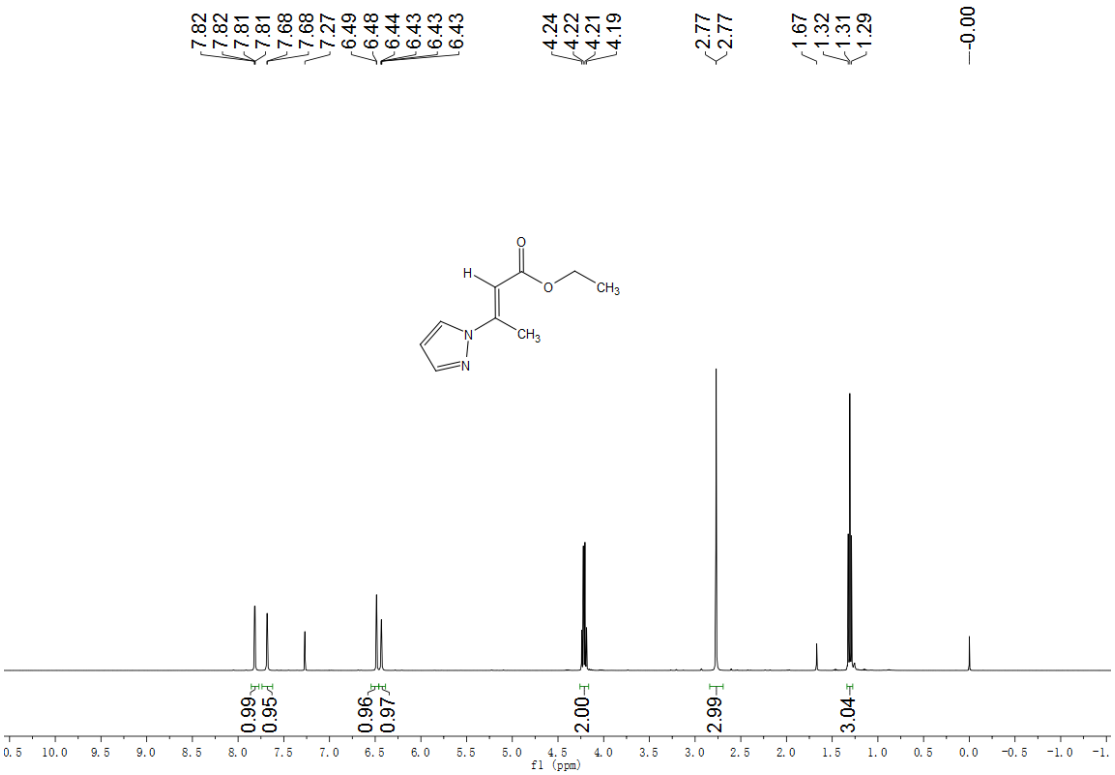



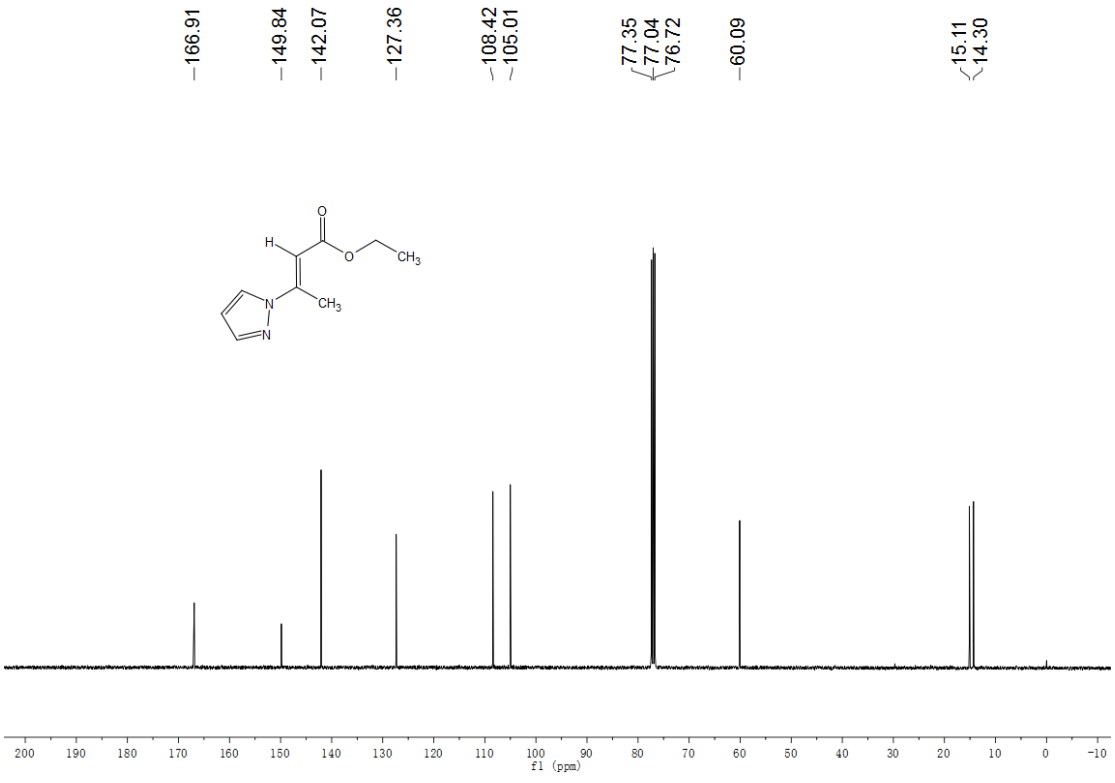
## Ethyl (E)-3-(5-amino-2H-tetrazol-2-yl) but-2-enoate (3da)



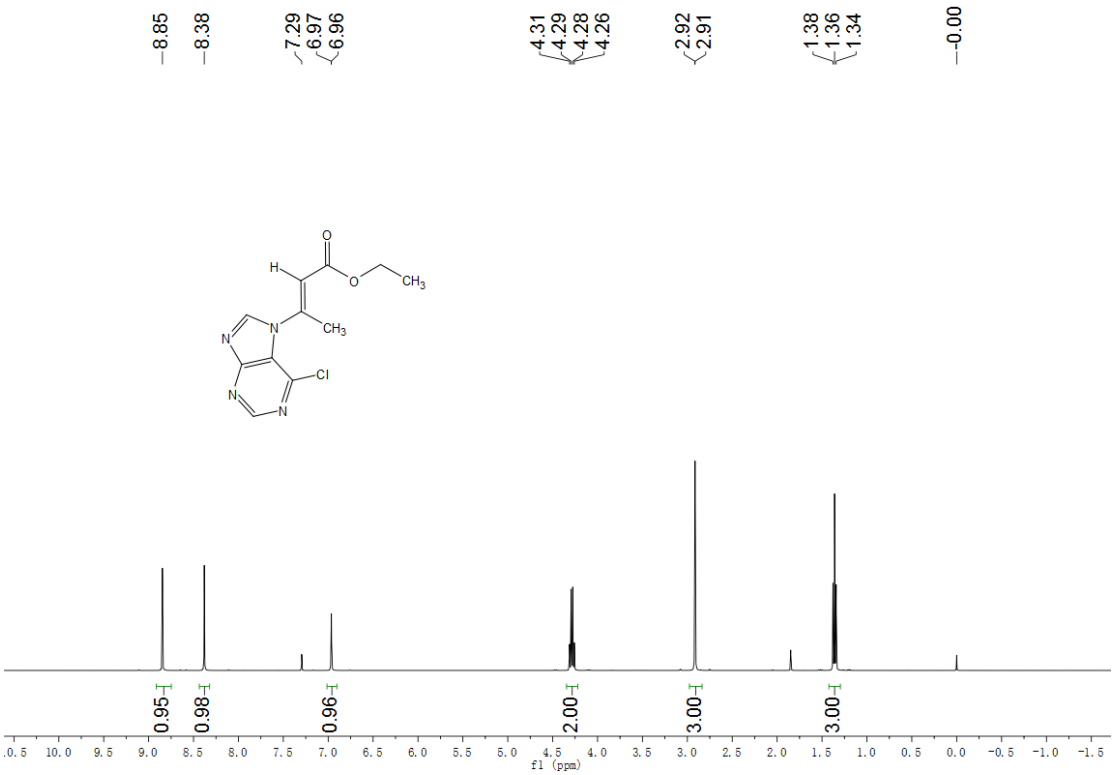



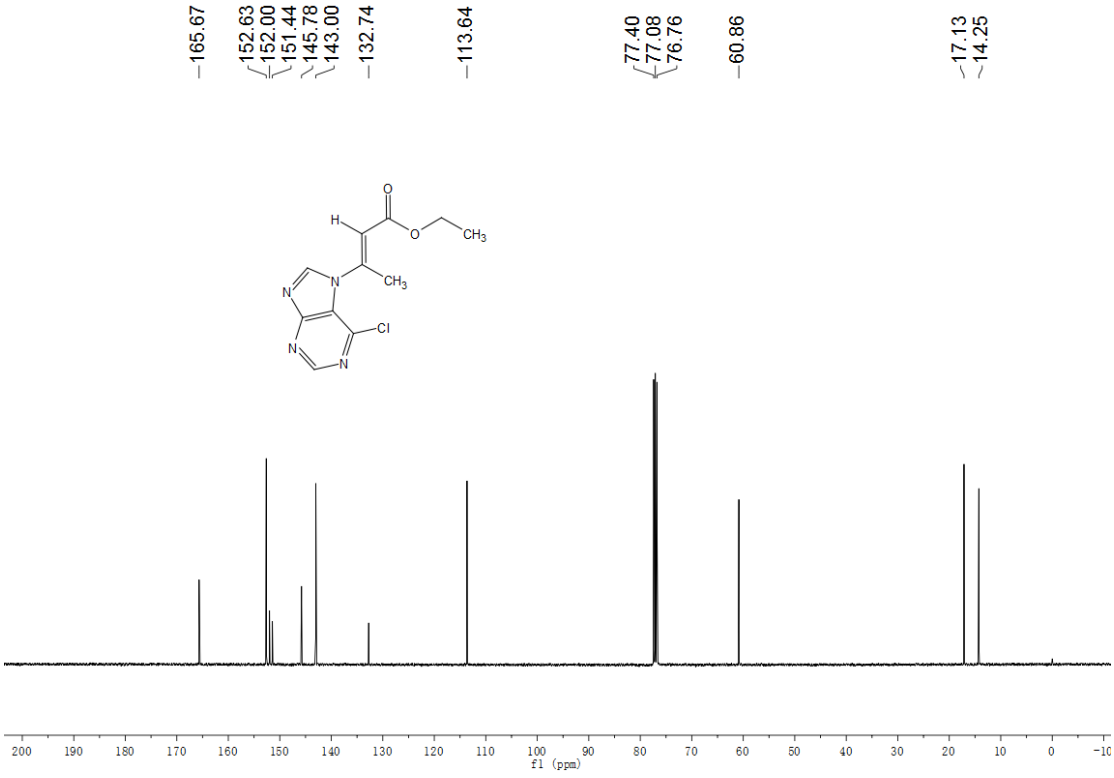
## Ethyl (E)-3-(1H-pyrazol-1-yl) but-2-enoate (3ea)



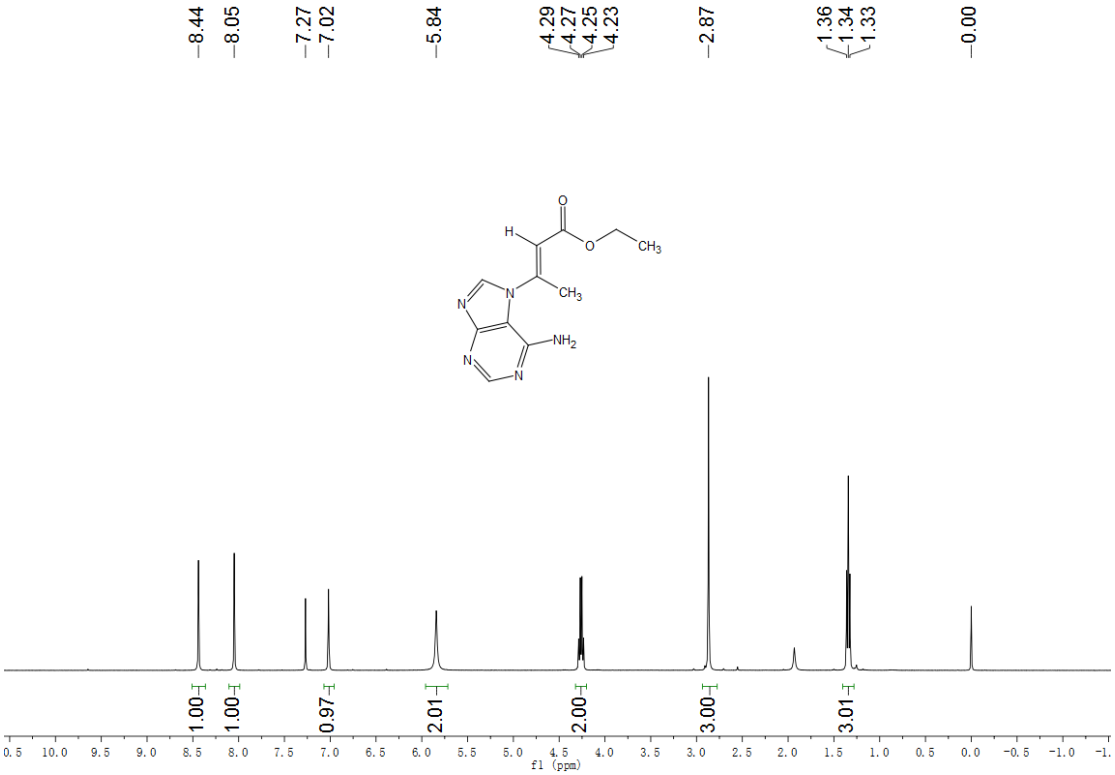



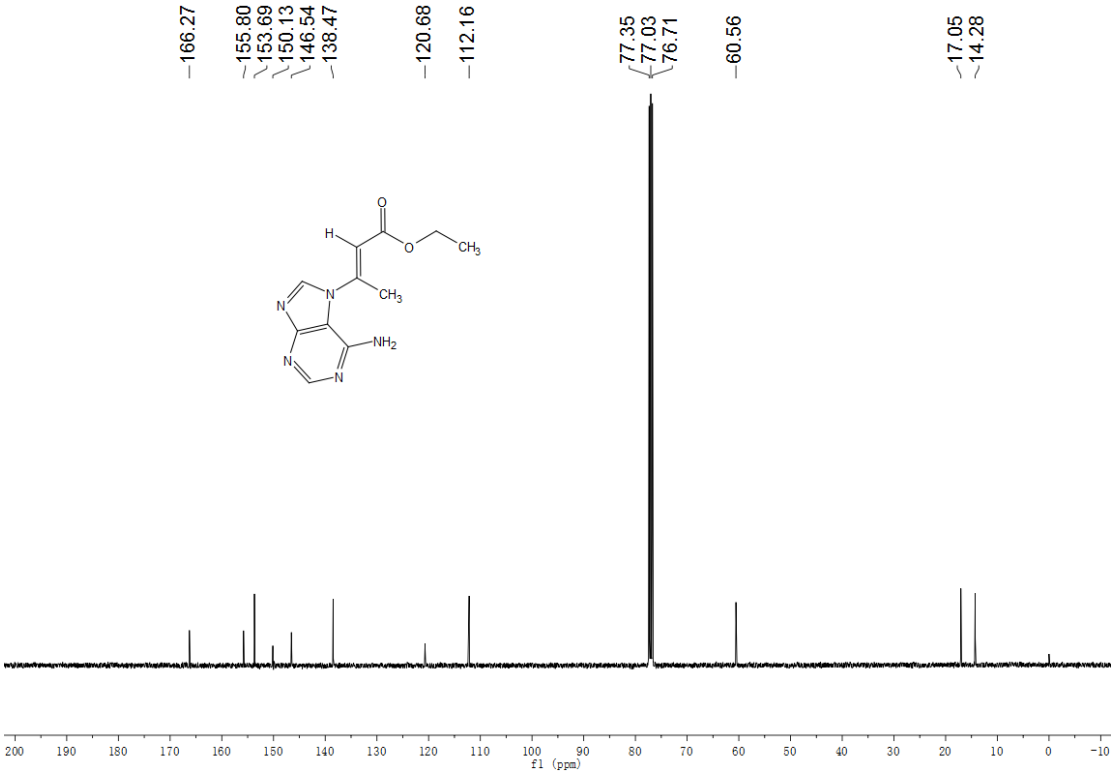
## Ethyl (E)-3-(6-chloro-7H-purin-7-yl) but-2-enoate (3fa)



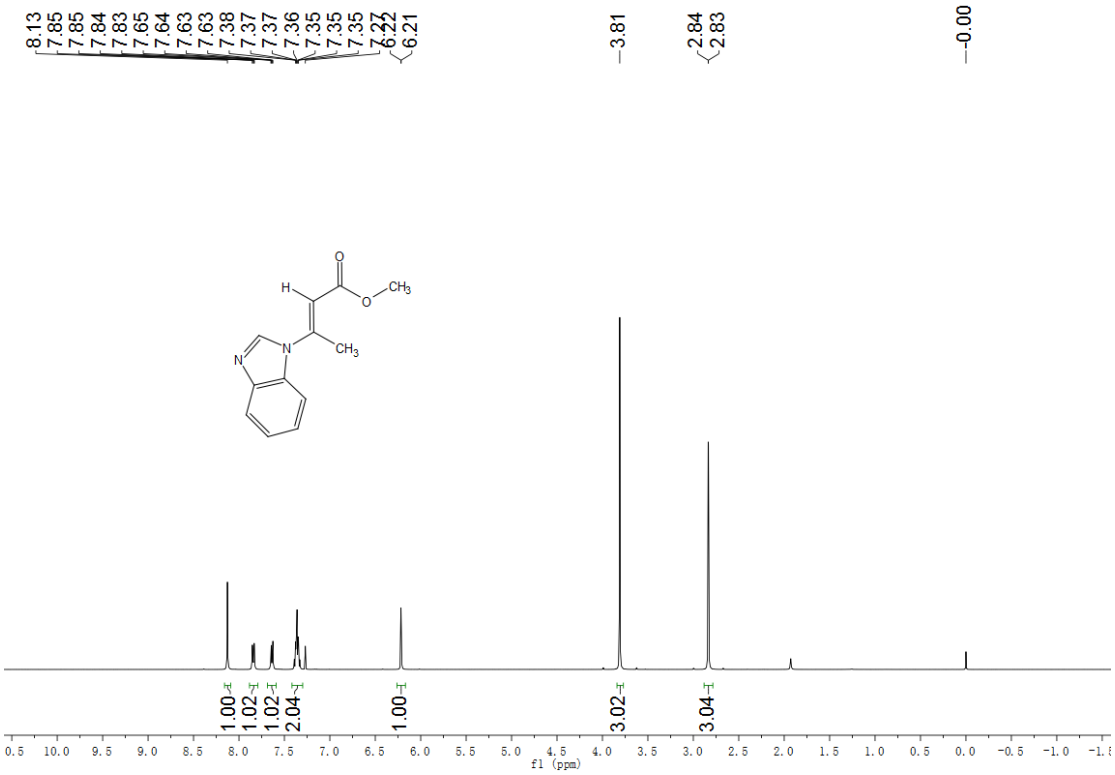



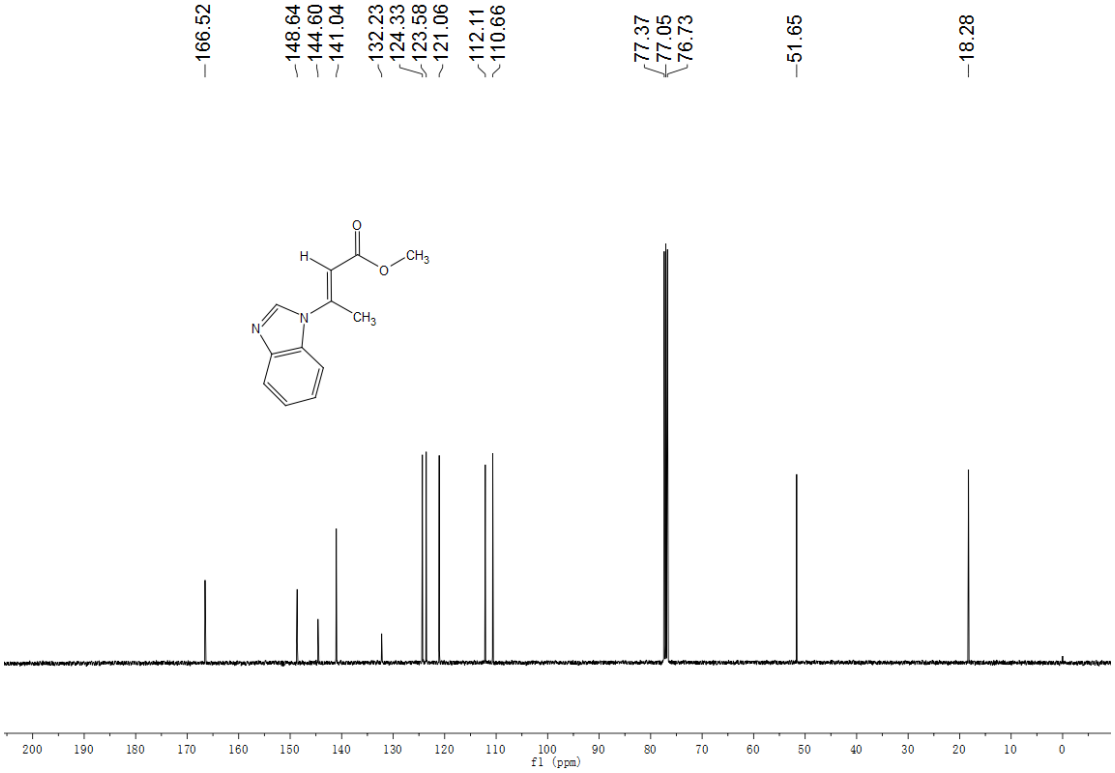
## Ethyl (E)-3-(6-amino-7H-purin-7-yl) but-2-enoate (3ga)



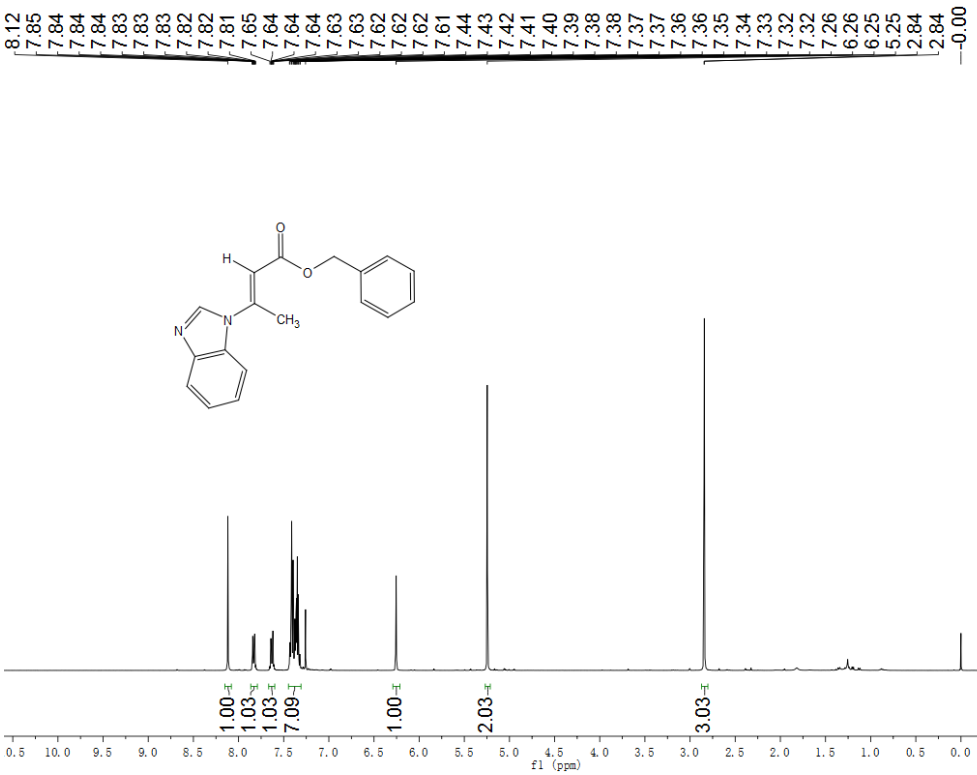



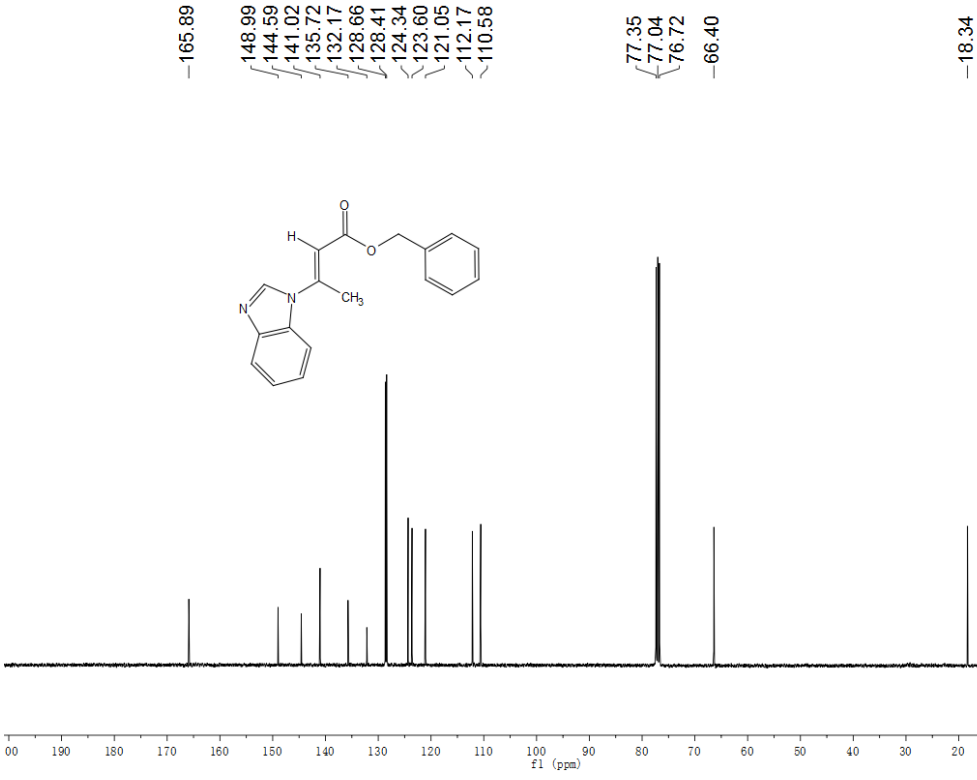
## Methyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bb)



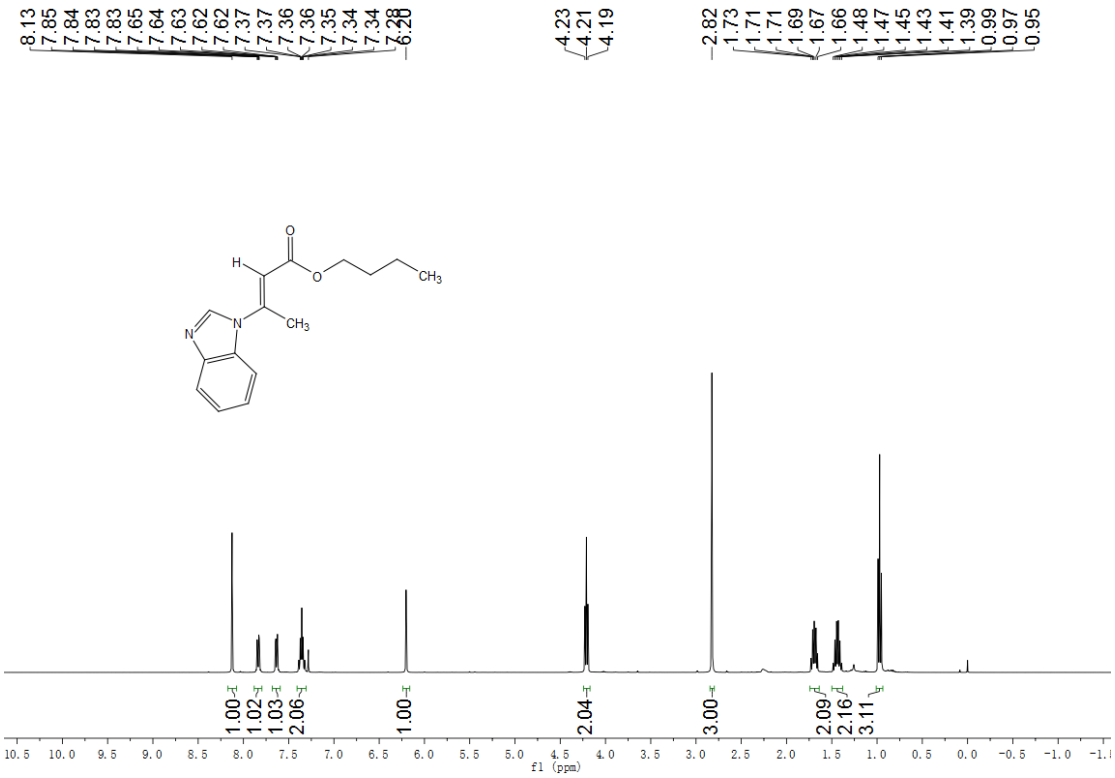



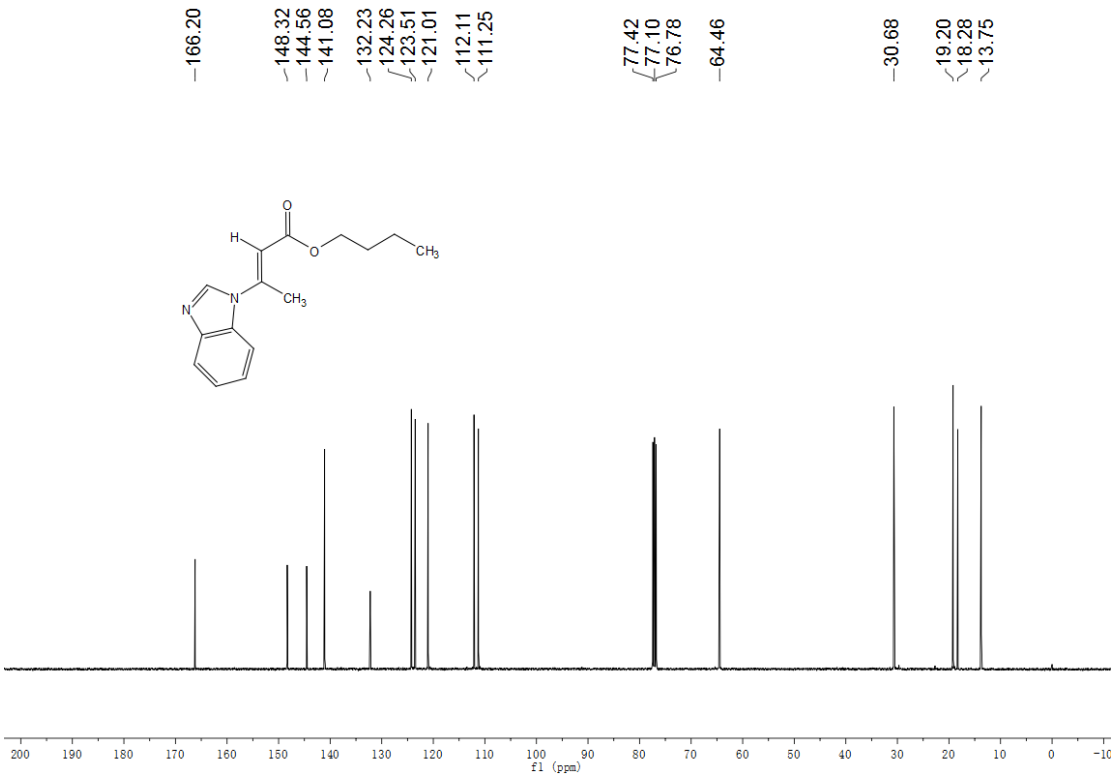
## Benzyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bc)



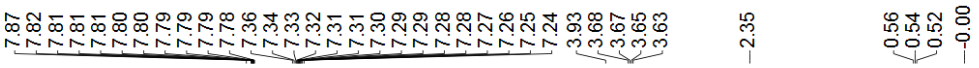



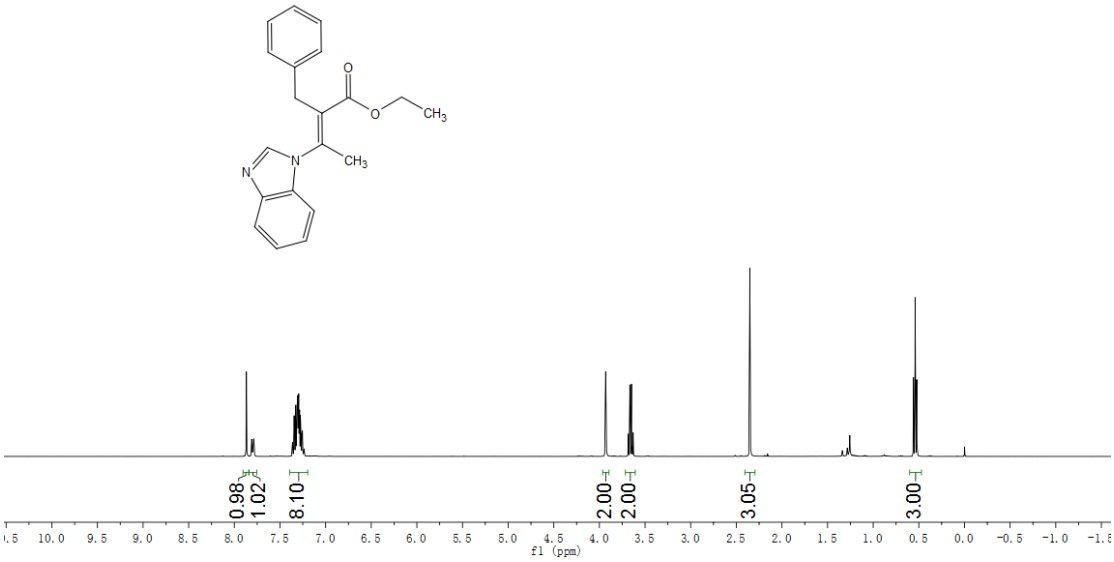
## Butyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bd)

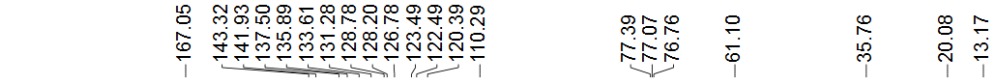


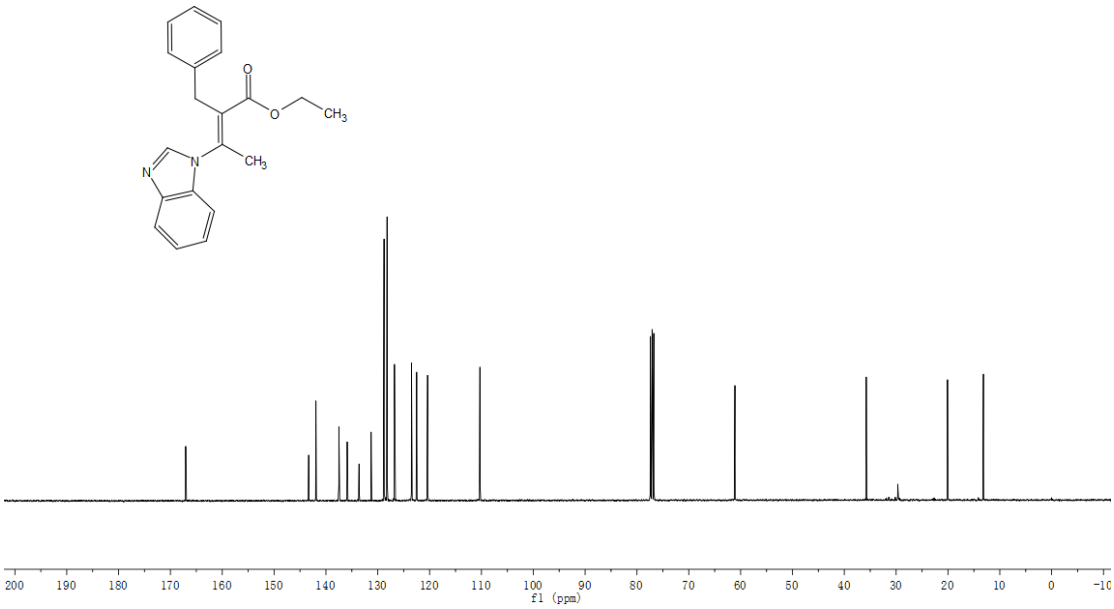



## Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl)-2-benzylbut-2-enoate(3be)



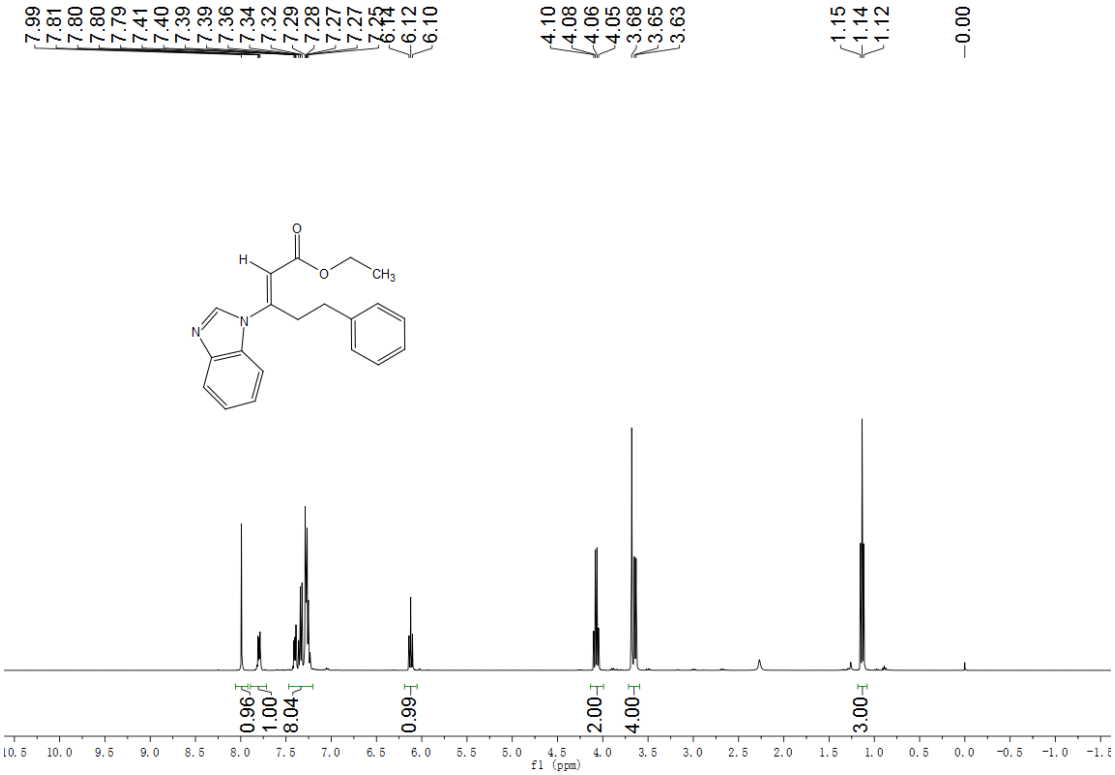



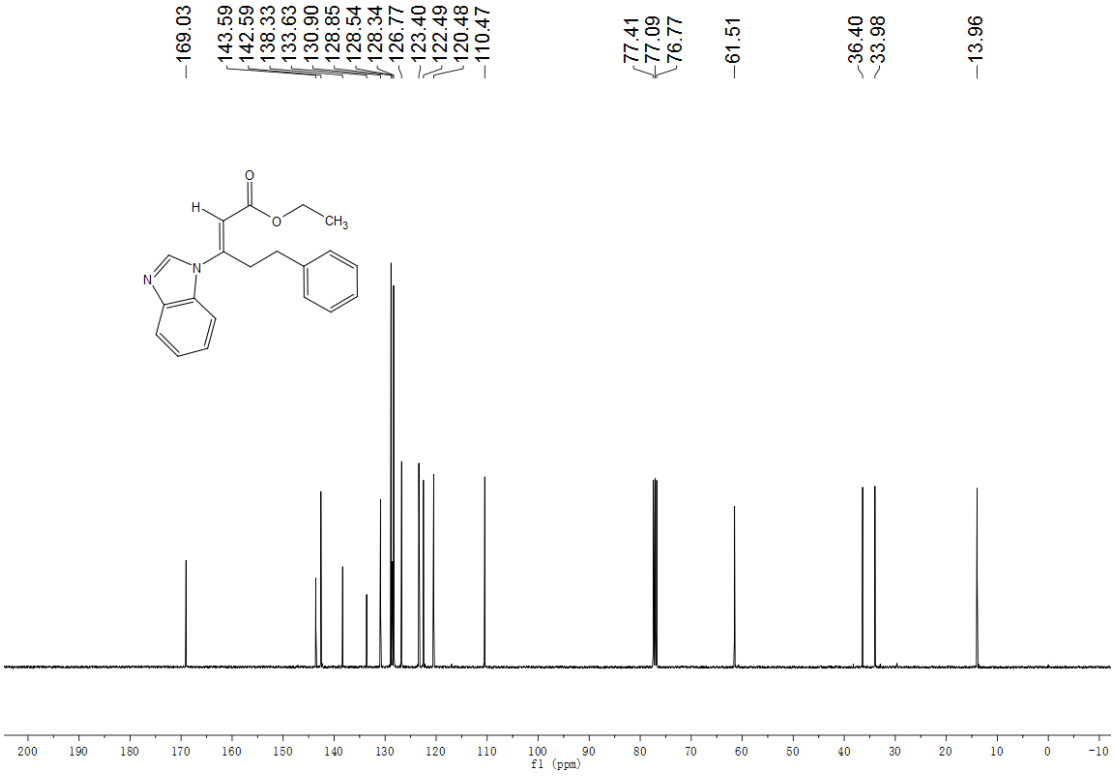



## Cyclohexyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bf)

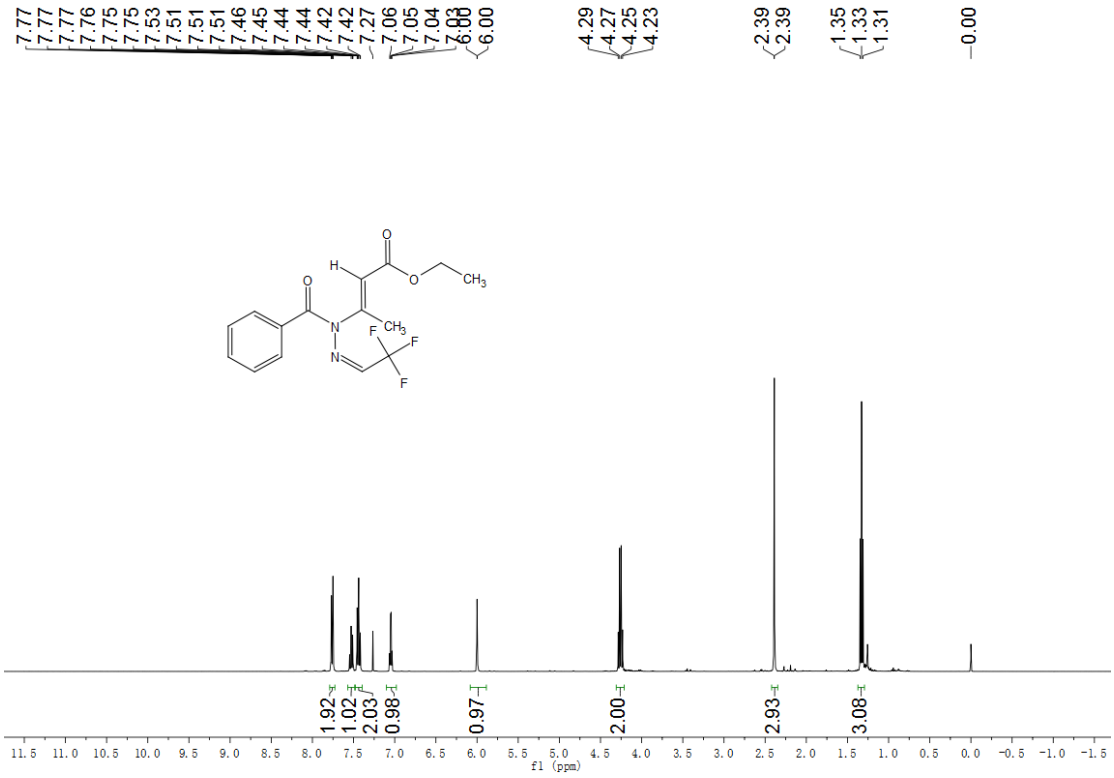
## Sec-butyl (E)-3-(1H-benzo[d]imidazol-1-yl) but-2-enoate (3bg)

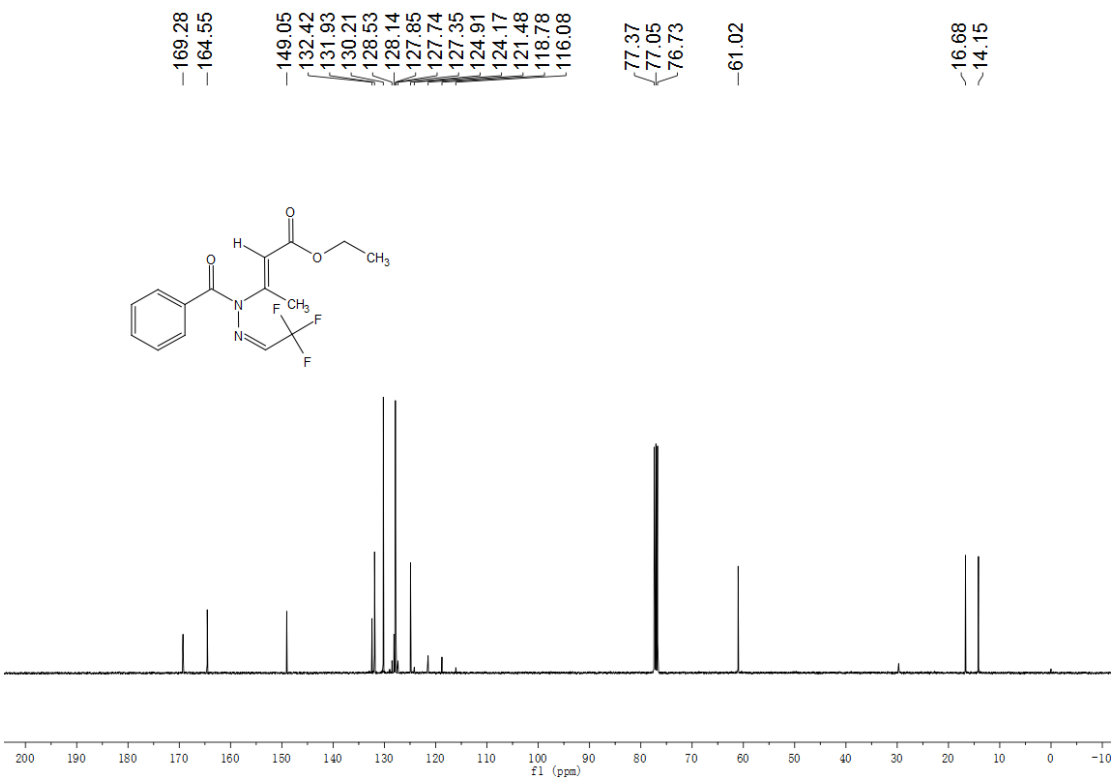
## Ethyl (E)-3-(1H-benzo[d]imidazol-1-yl)-5-phenylpent-2-enoate (3bh)



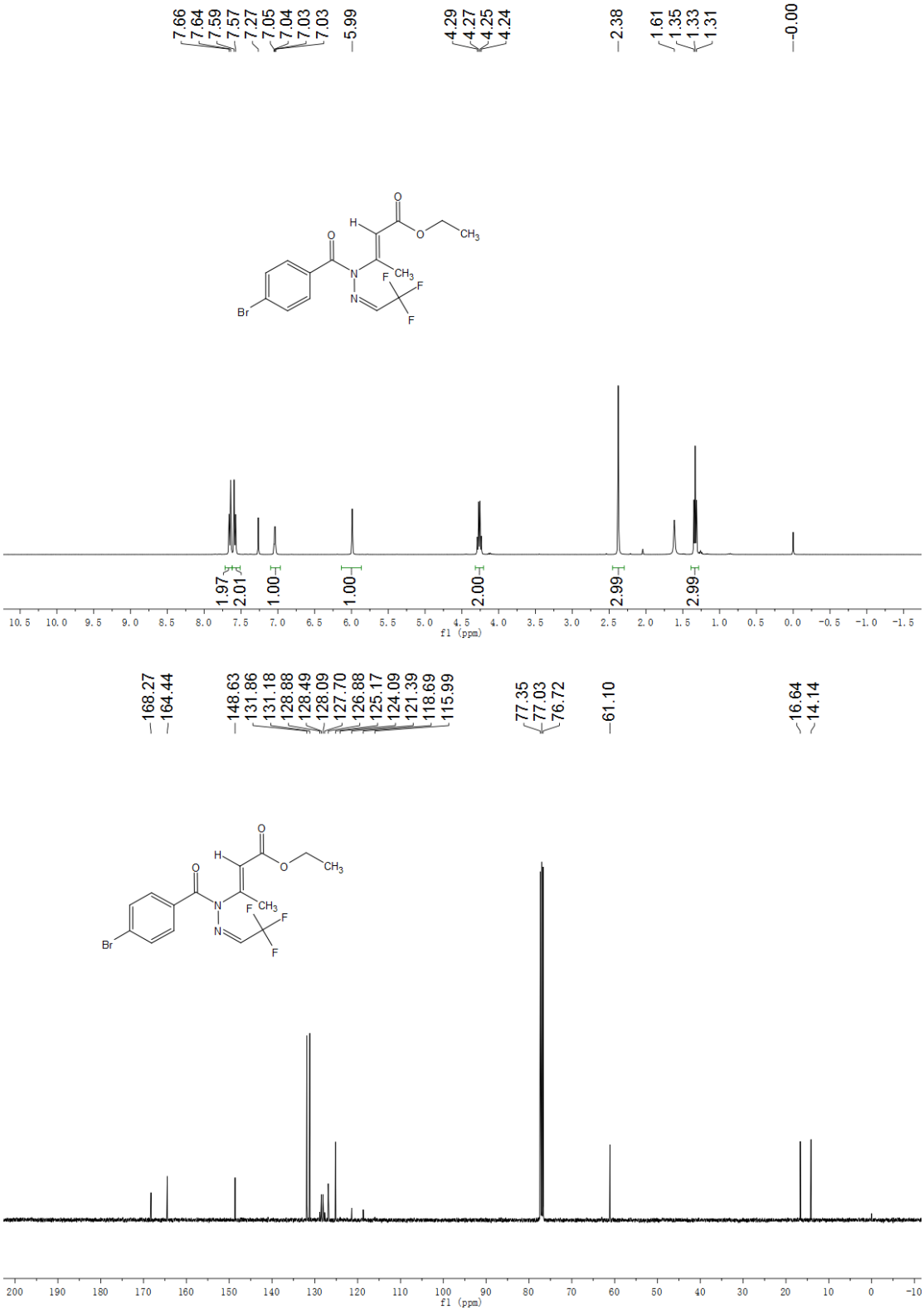



**Ethyl (E)-3-(1-benzoyl-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but-2-enoate (5aa)**

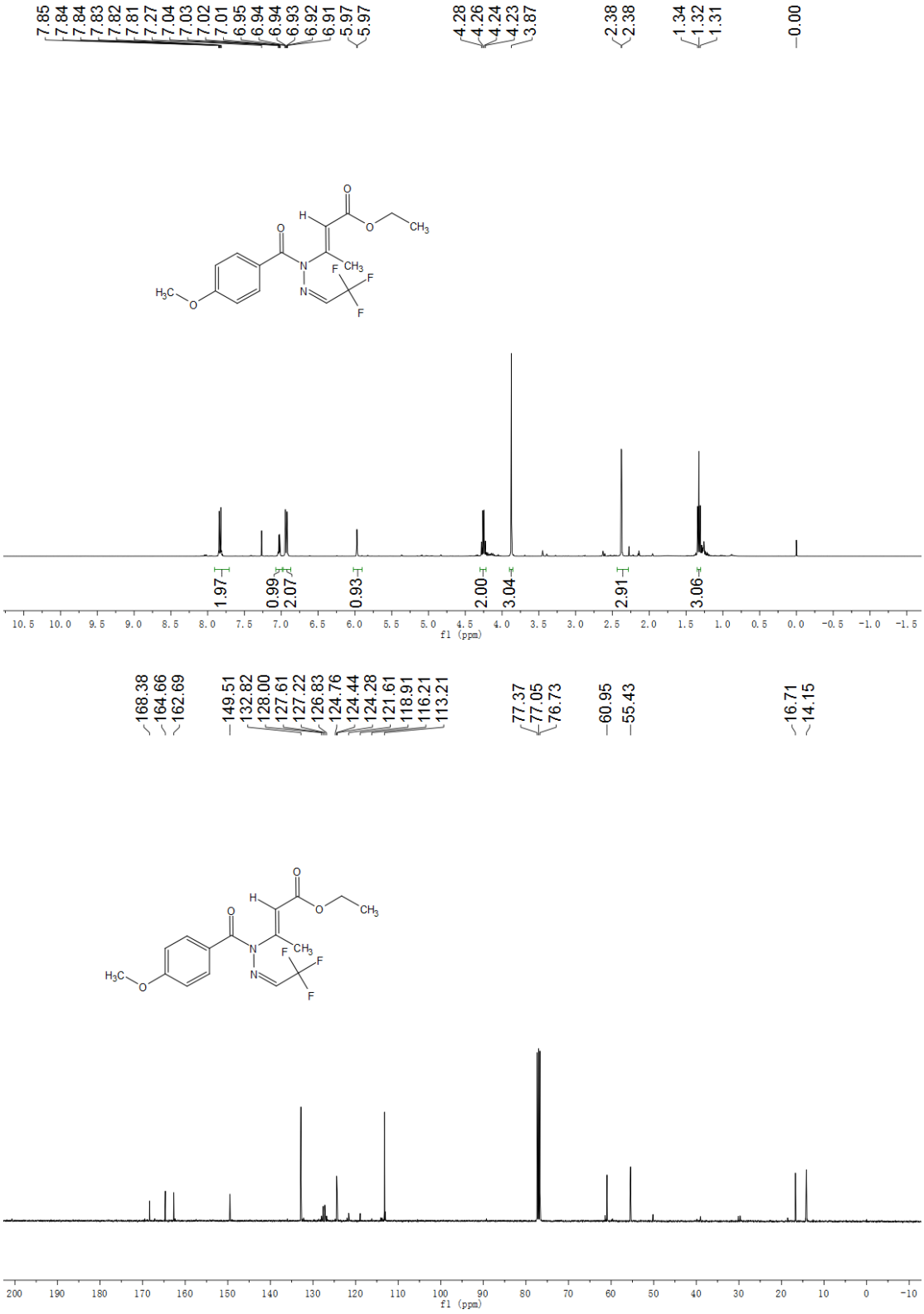


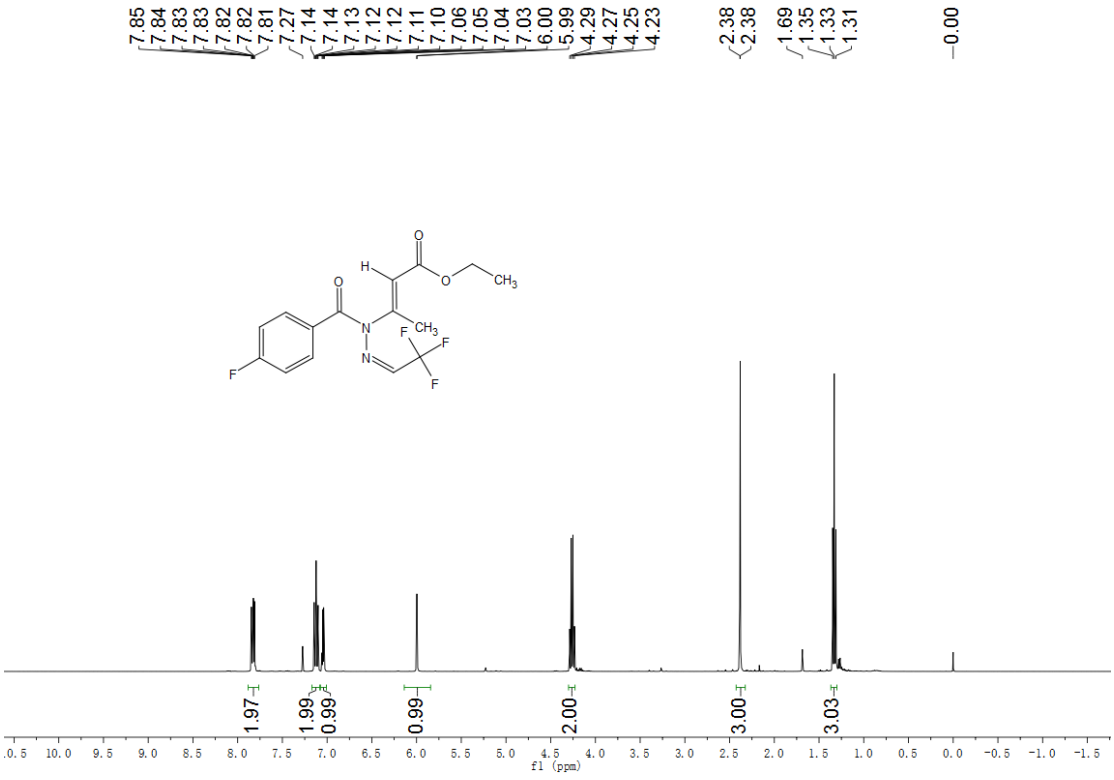
**Ethyl (E)-3-(1-(4-bromobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-Enoate (5ba)**

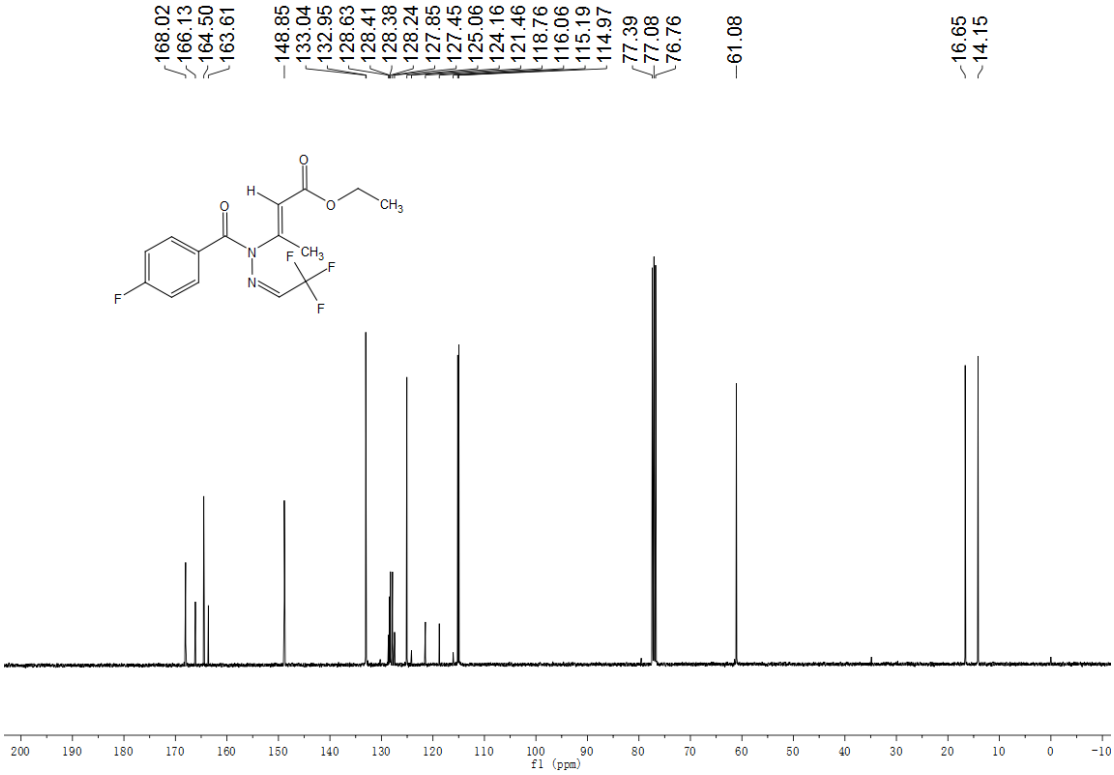


**Ethyl (E)-3-(1-(4-methoxybenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but-2-enoate (5ca)**

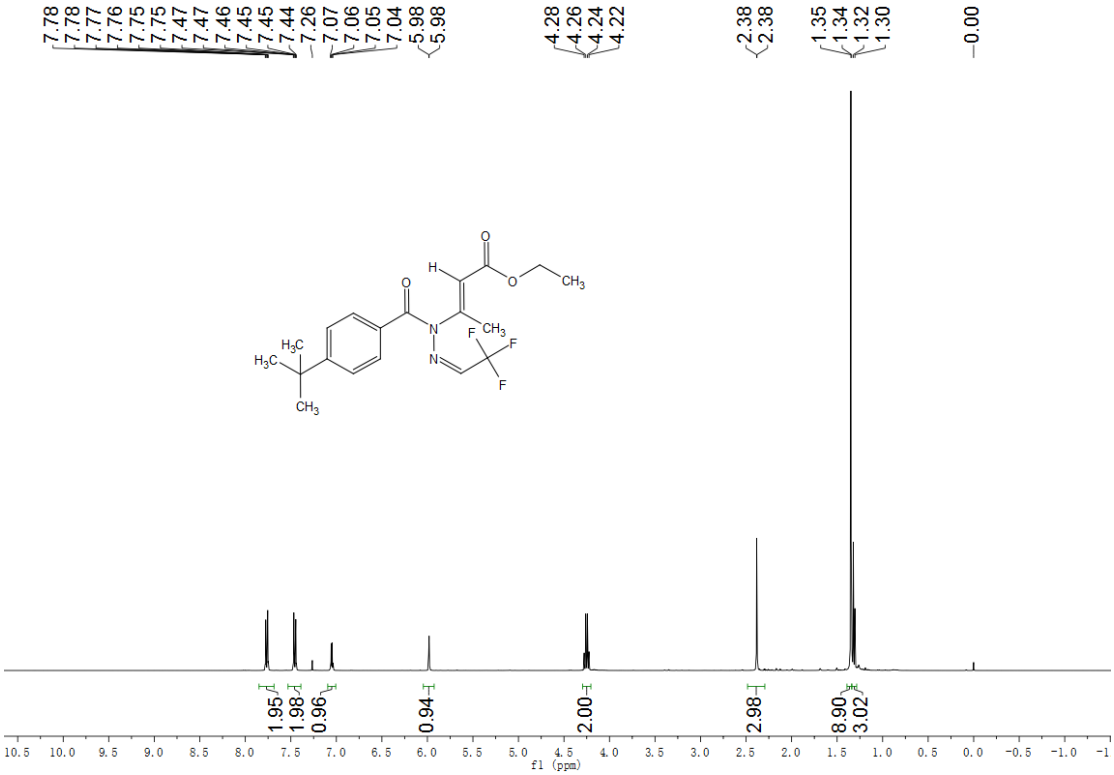


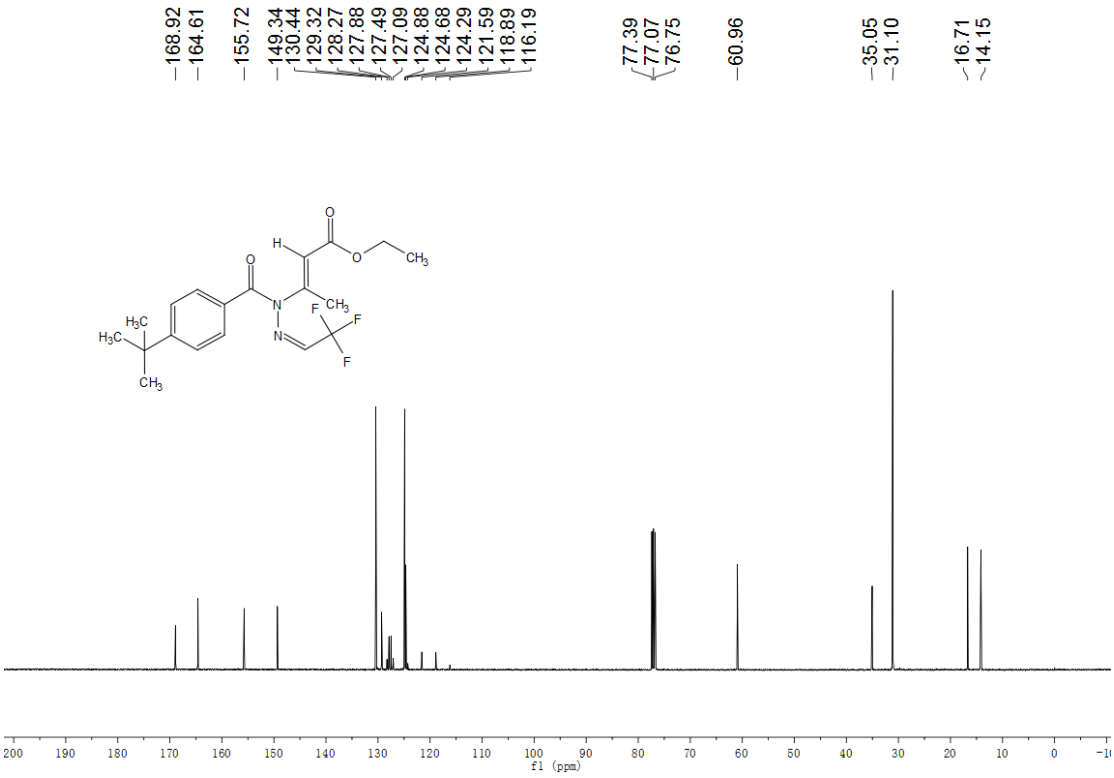
**Ethyl (E)-3-(1-(4-fluorobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5da)**



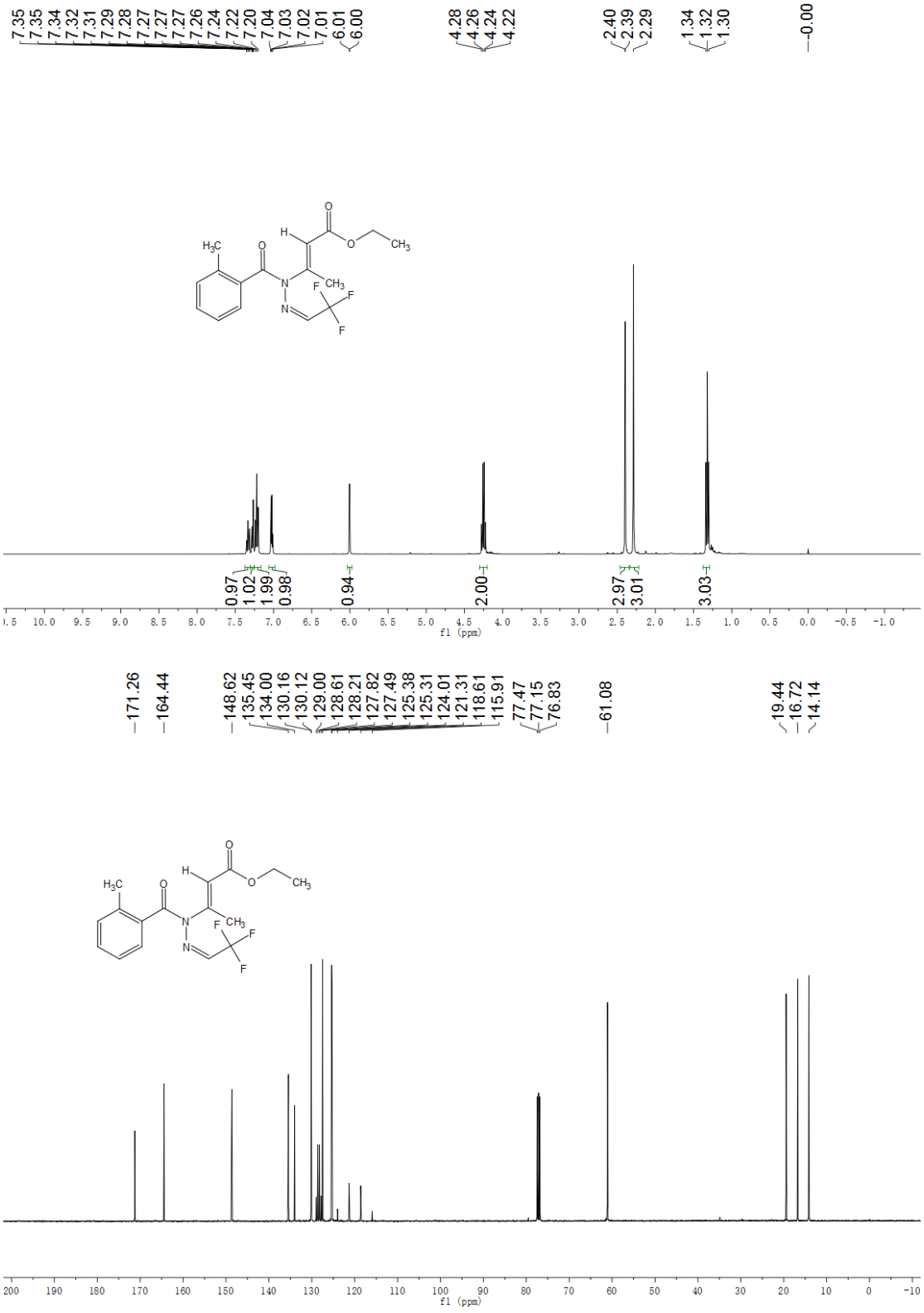



**Ethyl (E)-3-(1-(4-(tert-butyl)benzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl ) but-2-enoate (5ea)**

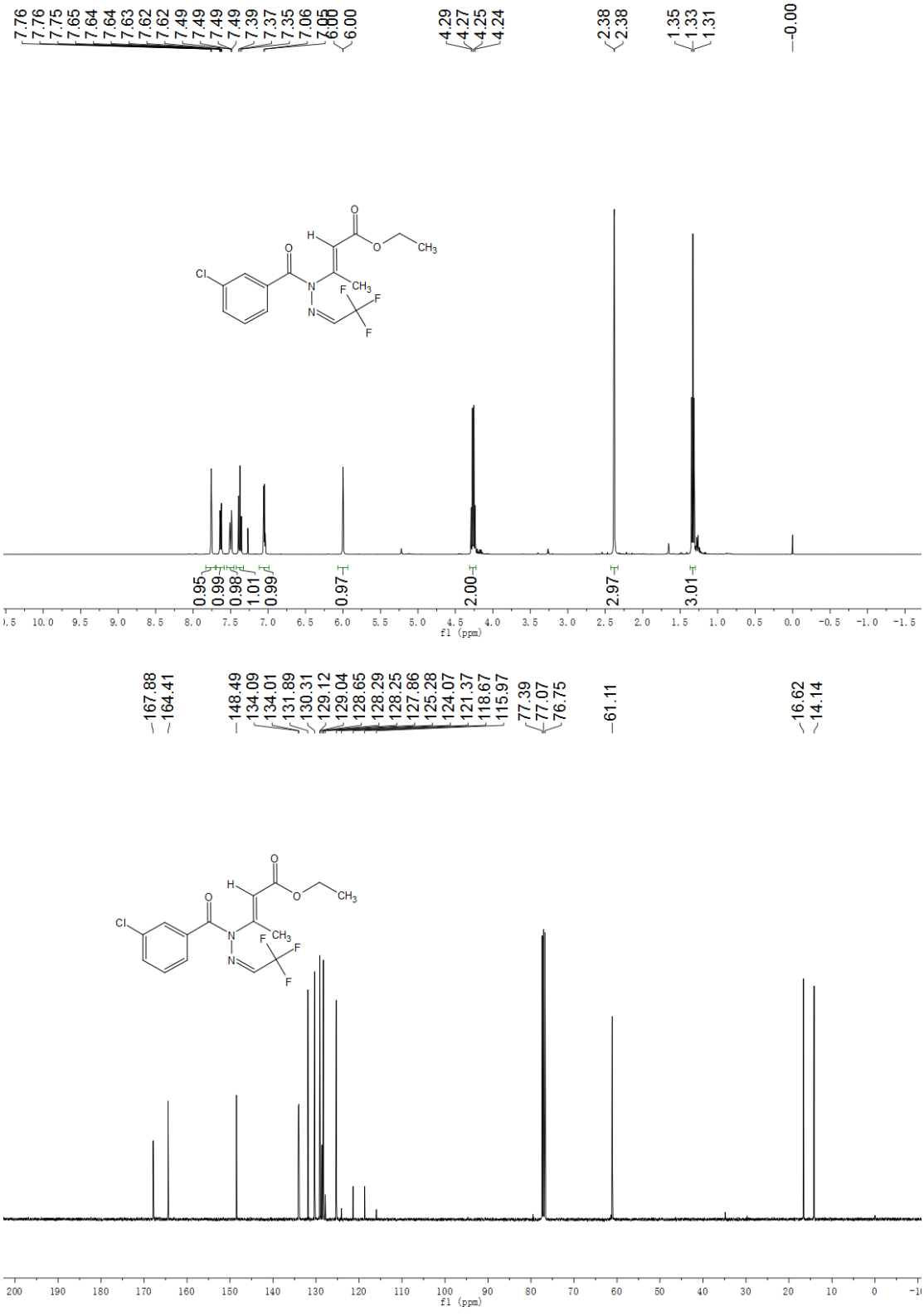


**Ethyl (E)-3-(1-(2-methylbenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5fa)**



**Ethyl (E)-3-(1-(3-chlorobenzoyl)-2-((Z)-2,2,2-trifluoroethylidene)hydrazinyl) but -2-enoate (5ga)**



**7. Copies of $^1$H NMR Spectra of control experiments** (Nuclear Magnetic Resonance (NMR) was employed to determine the amount of samples with 1,3,5-trimethoxybenzene (0.1 mmol) as internal standard.)

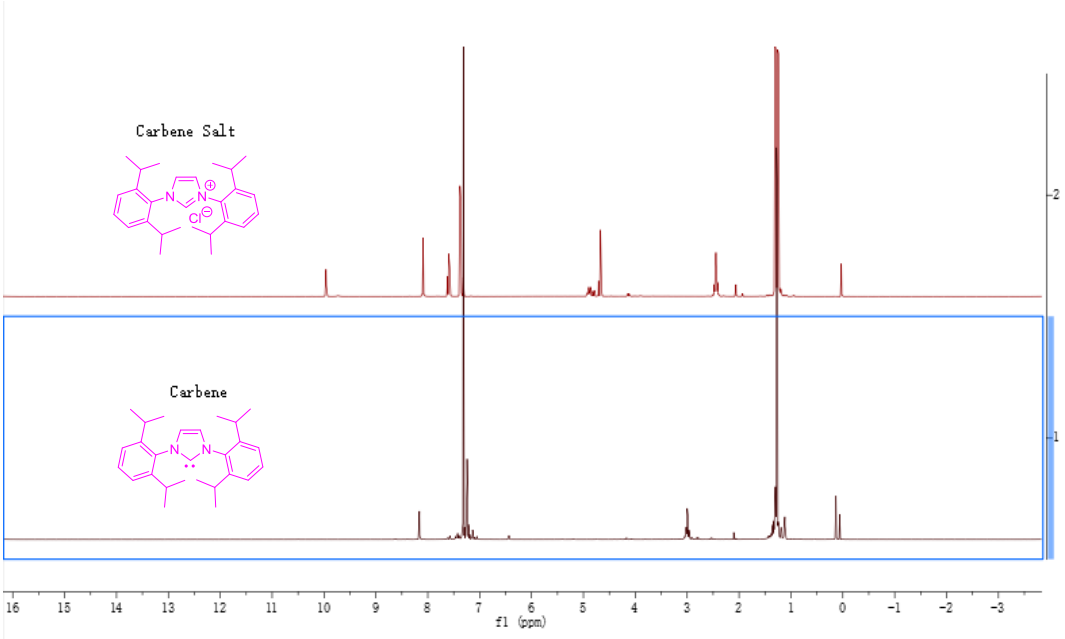



Figure S1. $^1$H NMR of NHC precatalyst and NHC (After adding the base, the characteristic peak of the carbene salt disappeared at 9.93).

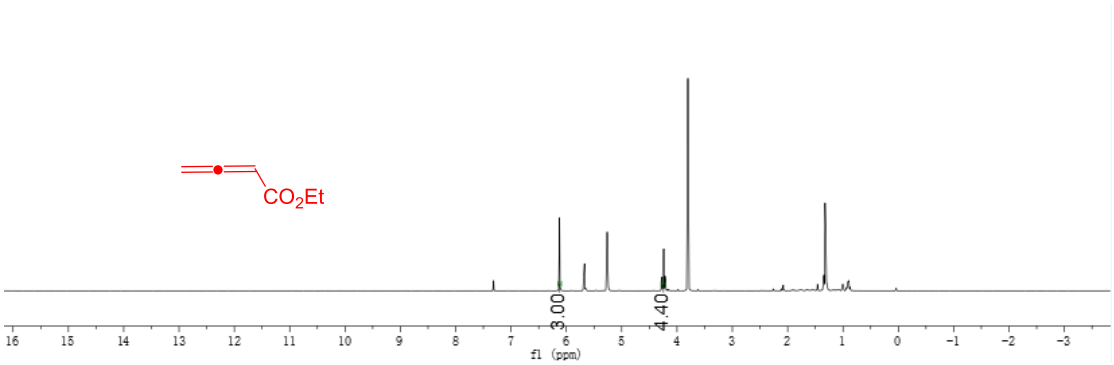



Figure S2. 0.22 mmol of allenoate in $CDCl_3$ (4.40÷2×0.1 mmol=0.22 mmol. The resonance signal at 6.08 are three hydrogen on the benzene ring of 1,3,5-trimethoxybenzene. The chemical shift of $CH_2$ in 2,3-butadienoic acid, ethyl ester is 4.21).

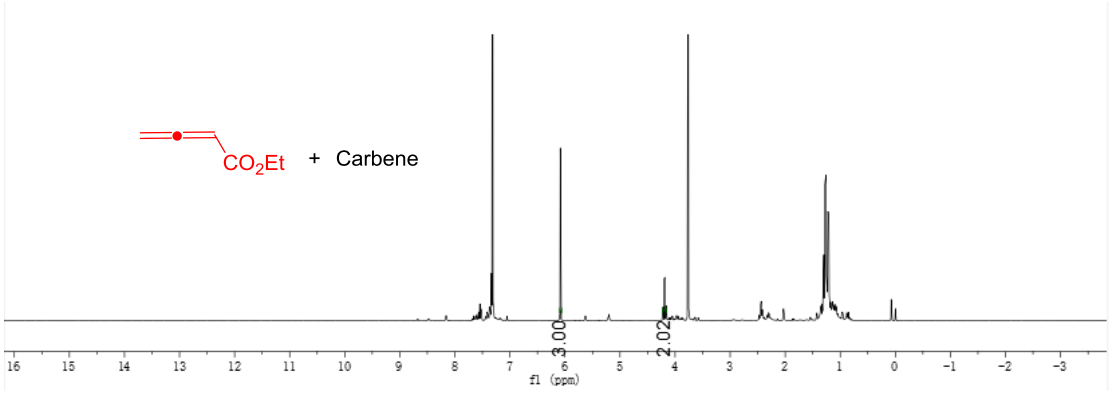



Figure S3. After adding carbene, the amount of allenoate was decreased by 54.5% (Compared with Figure 2).

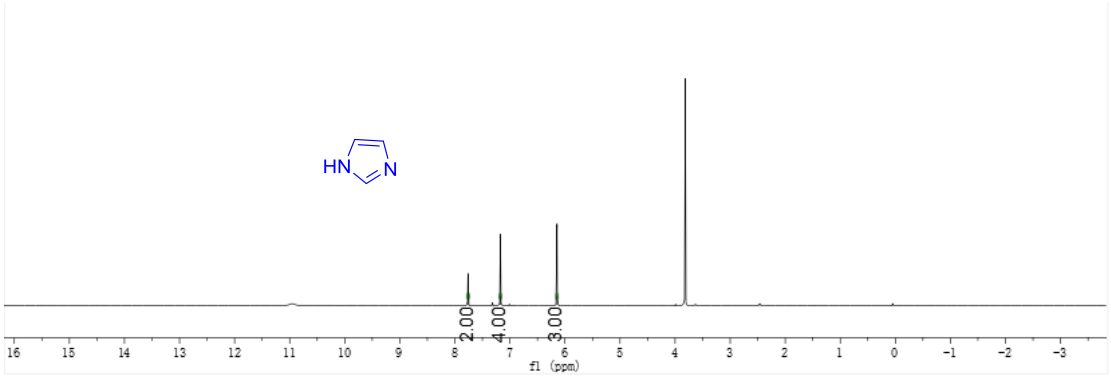



Figure S4. 0.2 mmol of imidazole (2.00÷1×0.1 mmol=0.2 mmol. Resonance signal at 7.70 and 6.08 are the characteristic peaks of imidazole and 1,3,5-trimethoxybenzene, respectively).

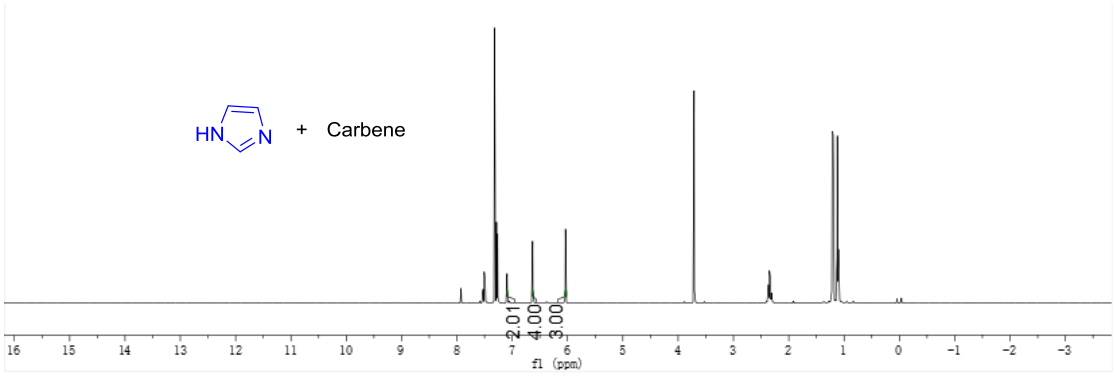



Figure S5. The addition of carbene had no effect on the amount of imidazole (Compared with Figure 4).

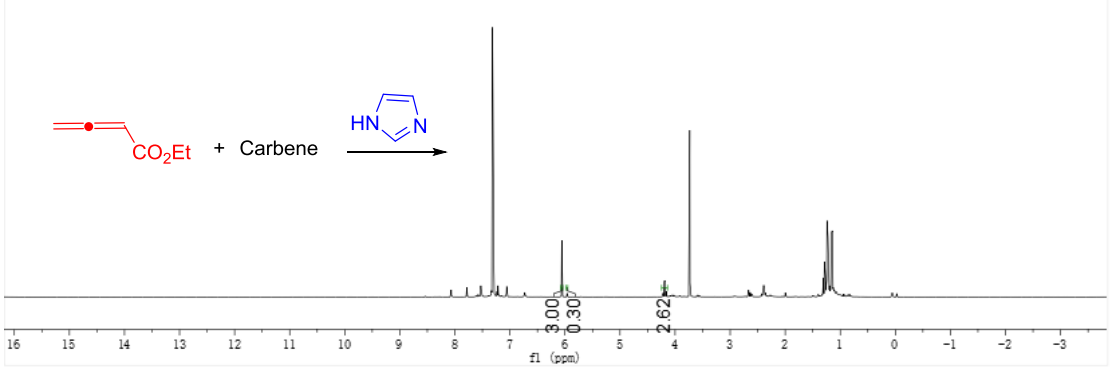



Figure S6. The intermediate generated from 2,3-butadienoic acid, ethyl ester and NHC was

added to the solution of imidazole to furnish the product in 15% of yield (0.30÷2×100%=15%. The resonance signal with an area of 0.3 is the characteristic peak of the product **3aa**.).

## 8. Computational Methods:

The DFT calculations were performed using the Gaussian16 program[3]. All structures were optimized at the M06-2X[4]/6-31G** level, and the corresponding vibrational frequencies were calculated at the same level. The structures discussed in this paper were fully optimized in THF solvent using the integral equation formalism polarizable continuum model (IEF-PCM)[5]. Then, frequency calculations at the same level of theory were carried out to identify all of the stationary points as minima (zero imaginary frequency) or transition state (only one frequency), and to provide free energies.

## 9. References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5. (a) B. Mennucci, J. Tomasi, *J. Chem. Phys.*, 1997, **106**, 5151–5158. (b) V. Barone, M. Cossi, *J. Phys. Chem. A.*, 1998, **102**, 1995–2001.

# 10. Geometrical Coordinates of the Listed Complexes

**R1**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.129225 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.138126 |
| Thermal correction to Enthalpy= | | | 0.139070 |
| Thermal correction to Gibbs Free Energy= | | | 0.094625 |
| Sum of electronic and zero-point Energies= | | | -383.566001 |
| Sum of electronic and thermal Energies= | | | -383.557099 |
| Sum of electronic and thermal Enthalpies= | | | -383.556155 |
| Sum of electronic and thermal Free Energies= | | | -383.600600 |
| C | -2.50043700 | -0.40404900 | 0.00002500 |
| C | -3.73923800 | -0.00923300 | 0.00001100 |
| C | -1.24950700 | -0.80048100 | 0.00002900 |
| H | -4.26899900 | 0.16259900 | 0.93212800 |
| H | -4.26902100 | 0.16246700 | -0.93211900 |
| H | -0.98902400 | -1.85400700 | -0.00001200 |
| C | -0.14470200 | 0.19091000 | -0.00013700 |
| O | -0.27235000 | 1.39458300 | -0.00005700 |
| O | 1.04261200 | -0.43077000 | -0.00003400 |
| C | 2.19431200 | 0.43037000 | 0.00000100 |
| C | 3.41869000 | -0.45727500 | 0.00012600 |
| H | 2.15209100 | 1.07293300 | 0.88398000 |
| H | 2.15220600 | 1.07284600 | -0.88404600 |
| H | 4.32054600 | 0.15867800 | 0.00015400 |
| H | 3.43263800 | -1.09369600 | 0.88760500 |
| H | 3.43275400 | -1.09378400 | -0.88728800 |

Frequencies

| | | |
|---|---|---|
| 35.1984 | 76.0478 | 108.3652 |
| 157.1202 | 207.7926 | 275.5214 |
| 360.5844 | 379.5371 | 417.0370 |
| 480.2358 | 488.6015 | 776.2149 |
| 794.0610 | 812.7023 | 902.1691 |
| 904.1000 | 916.3516 | 994.8691 |
| 997.3740 | 1083.1534 | 1131.1330 |
| 1155.8722 | 1189.2129 | 1243.2876 |
| 1300.8313 | 1374.4048 | 1409.3517 |
| 1442.4795 | 1484.0945 | 1499.3662 |
| 1505.1594 | 1532.3861 | 1841.5772 |
| 2097.0143 | 3091.6218 | 3101.6509 |
| 3148.8094 | 3166.2409 | 3177.6689 |
| 3180.0487 | 3229.8002 | 3254.0549 |

**R2**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.072349 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.076015 |
| Thermal correction to Enthalpy= | | | 0.076959 |
| Thermal correction to Gibbs Free Energy= | | | 0.046127 |
| Sum of electronic and zero-point Energies= | | | -226.063879 |
| Sum of electronic and thermal Energies= | | | -226.060213 |
| Sum of electronic and thermal Enthalpies= | | | -226.059269 |
| Sum of electronic and thermal Free Energies= | | | -226.090101 |
| C | -0.59175200 | 0.99164700 | 0.00007500 |
| C | -1.13930400 | -0.26363800 | 0.00009100 |
| C | 0.97728700 | -0.55161300 | -0.00002200 |
| N | 0.76527400 | 0.78897800 | -0.00004400 |
| H | 1.47659100 | 1.50431200 | -0.00012700 |
| H | -1.02666100 | 1.97784400 | 0.00015100 |
| H | -2.18682700 | -0.52830300 | 0.00016800 |
| H | 1.97075800 | -0.97690300 | -0.00008000 |
| N | -0.15259600 | -1.22259700 | -0.00009500 |

Frequencies

| | | |
|---|---|---|
| 589.4033 | 663.3912 | 694.9569 |
| 757.6677 | 842.8545 | 895.5639 |
| 916.4790 | 947.4608 | 1093.3841 |
| 1122.7820 | 1164.1256 | 1197.4830 |
| 1297.6225 | 1405.4341 | 1483.6063 |
| 1550.0496 | 1607.1373 | 3268.6574 |
| 3280.6221 | 3302.5422 | 3676.2638 |

**R2$^{-}$**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.058791 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.062264 |
| Thermal correction to Enthalpy= | | | 0.063208 |
| Thermal correction to Gibbs Free Energy= | | | 0.032711 |
| Sum of electronic and zero-point Energies= | | | -225.570145 |
| Sum of electronic and thermal Energies= | | | -225.566671 |
| Sum of electronic and thermal Enthalpies= | | | -225.565727 |
| Sum of electronic and thermal Free Energies= | | | -225.596224 |
| C | 0.89802200 | -0.69326700 | 0.00007700 |
| C | 0.89963900 | 0.69167700 | 0.00007500 |
| C | -1.09842700 | 0.00109800 | -0.00002400 |
| N | -0.39349500 | -1.14344200 | -0.00006300 |
| H | 1.74144900 | -1.37621400 | 0.00014400 |
| H | 1.74410300 | 1.37326400 | 0.00014100 |
| H | -2.18650700 | 0.00203300 | -0.00010300 |
| N | -0.39142800 | 1.14399500 | -0.00007300 |

Frequencies

| | | |
|---|---|---|
| 678.6931 | 716.4774 | 785.9705 |
| 829.5275 | 841.8683 | 937.0371 |
| 951.8252 | 1115.8713 | 1129.1672 |
| 1225.4610 | 1266.0808 | 1304.9718 |
| 1368.8587 | 1522.6209 | 1539.2200 |
| 3173.1100 | 3196.4083 | 3222.8860 |

**NHC**

| | |
|---|---|
| Zero-point correction= | 0.575239 (Hartree/Particle) |
| Thermal correction to Energy= | 0.604926 |
| Thermal correction to Enthalpy= | 0.605871 |
| Thermal correction to Gibbs Free Energy= | 0.514591 |
| Sum of electronic and zero-point Energies= | -1158.994197 |
| Sum of electronic and thermal Energies= | -1158.964510 |
| Sum of electronic and thermal Enthalpies= | -1158.963566 |
| Sum of electronic and thermal Free Energies= | -1159.054845 |

| | | | |
|---|---|---|---|
| C | 0.04603400 | 0.02921700 | -0.32474700 |
| C | 0.70090800 | -0.02020200 | 1.88556300 |
| C | -0.65170500 | -0.01086500 | 1.87203800 |
| N | -1.01679300 | 0.01933800 | 0.53183500 |
| H | 1.40925800 | -0.04174000 | 2.69918600 |
| H | -1.37663400 | -0.02011400 | 2.67133000 |
| N | 1.09513600 | 0.00412500 | 0.55235400 |
| C | -2.37747100 | 0.01946100 | 0.08751100 |
| C | -3.01819700 | -1.21142000 | -0.11295200 |
| C | -3.01629500 | 1.24764100 | -0.13061000 |
| C | -4.35174400 | -1.18907000 | -0.52669200 |
| C | -4.34808000 | 1.22091600 | -0.55049600 |
| C | -5.01333500 | 0.01504300 | -0.74157900 |
| H | -4.87642200 | -2.12713300 | -0.68584100 |
| H | -4.86825600 | 2.15734300 | -0.73306700 |
| H | -6.04947100 | 0.01340700 | -1.06514200 |
| C | 2.46751600 | -0.01311400 | 0.13574000 |
| C | 3.08658500 | -1.25340600 | -0.07908900 |
| C | 3.13510100 | 1.20901100 | -0.03080900 |
| C | 4.41789500 | -1.24638100 | -0.50063800 |
| C | 4.46544100 | 1.16607300 | -0.45339500 |
| C | 5.09946500 | -0.04895700 | -0.68914300 |
| H | 4.92919900 | -2.18622100 | -0.68122600 |
| H | 5.01321600 | 2.09153800 | -0.59764500 |
| H | 6.13415700 | -0.06288700 | -1.01732000 |
| C | -2.29670100 | 2.57386100 | 0.04549200 |
| C | -3.00349100 | 3.46147100 | 1.07506200 |
| C | -2.15928100 | 3.29109900 | -1.30233500 |

| | | | |
|---|---|---|---|
| H | -1.28603200 | 2.36866100 | 0.41334600 |
| H | -3.07979800 | 2.95861700 | 2.04337000 |
| H | -2.45058200 | 4.39512300 | 1.21428800 |
| H | -4.01567100 | 3.71916400 | 0.74699100 |
| H | -1.62155100 | 2.66591800 | -2.02064100 |
| H | -3.14265400 | 3.52683600 | -1.72298300 |
| H | -1.61048100 | 4.23008600 | -1.18083700 |
| C | -2.30563700 | -2.53584500 | 0.10420800 |
| C | -2.33148200 | -3.39526200 | -1.16429300 |
| C | -2.91036200 | -3.28865100 | 1.29453800 |
| H | -1.25610700 | -2.32473900 | 0.33372500 |
| H | -1.87712900 | -2.86331000 | -2.00471300 |
| H | -1.77566400 | -4.32380100 | -1.00192300 |
| H | -3.35553400 | -3.66432000 | -1.44272100 |
| H | -2.85665500 | -2.68887500 | 2.20779000 |
| H | -3.96256200 | -3.52882400 | 1.10880600 |
| H | -2.37517600 | -4.22729300 | 1.46639800 |
| C | 2.31276500 | -2.55135600 | 0.08747000 |
| C | 3.18968500 | -3.72065900 | 0.54012400 |
| C | 1.58238200 | -2.89640300 | -1.21859500 |
| H | 1.55266800 | -2.38727000 | 0.86046100 |
| H | 3.77768700 | -3.46496200 | 1.42611500 |
| H | 2.56051200 | -4.58189500 | 0.78102800 |
| H | 3.87970300 | -4.03455700 | -0.24938700 |
| H | 0.92070400 | -2.07860200 | -1.51700700 |
| H | 2.30888900 | -3.06960400 | -2.02014400 |
| H | 0.98610100 | -3.80667900 | -1.09404700 |
| C | 2.41188800 | 2.52820600 | 0.18724500 |
| C | 1.69028700 | 2.94682500 | -1.10180000 |
| C | 3.33374800 | 3.64679700 | 0.67676700 |
| H | 1.64857100 | 2.36441700 | 0.95696000 |
| H | 0.99677500 | 2.16589800 | -1.42587100 |
| H | 1.12972400 | 3.87398500 | -0.94195800 |
| H | 2.41977900 | 3.12050700 | -1.90050500 |
| H | 3.91743000 | 3.33762500 | 1.54849000 |
| H | 4.02992000 | 3.96431600 | -0.10587500 |
| H | 2.73817100 | 4.52095900 | 0.95374500 |

Frequencies

| | | |
|---|---|---|
| 16.9312 | 22.1862 | 38.0723 |
| 46.3540 | 49.8213 | 59.8376 |
| 68.1936 | 70.4002 | 80.0791 |
| 90.1314 | 98.6530 | 131.0675 |
| 134.1690 | 144.4637 | 152.8661 |
| 167.8745 | 220.9608 | 233.8312 |

| | | |
|---|---|---|
| 243.3591 | 247.9270 | 251.7365 |
| 255.3097 | 262.2085 | 267.7514 |
| 277.3549 | 282.2794 | 288.0050 |
| 296.1408 | 297.7172 | 305.0284 |
| 305.4643 | 314.5912 | 322.0593 |
| 325.5494 | 338.8092 | 403.4684 |
| 409.9927 | 428.8877 | 444.7232 |
| 447.6346 | 456.4538 | 484.2659 |
| 527.1684 | 531.7569 | 565.4063 |
| 579.8548 | 589.6726 | 596.6359 |
| 625.4473 | 647.4996 | 649.5038 |
| 651.6225 | 682.8708 | 687.3004 |
| 742.6764 | 743.7404 | 759.3947 |
| 787.0875 | 795.7641 | 829.9341 |
| 833.3006 | 833.5310 | 837.6173 |
| 843.8687 | 914.2785 | 919.3657 |
| 925.8794 | 931.1166 | 935.9628 |
| 938.3100 | 940.6035 | 949.2550 |
| 960.9415 | 967.6728 | 968.1410 |
| 968.4943 | 973.0529 | 976.8100 |
| 980.8500 | 983.9984 | 1009.1955 |
| 1013.6601 | 1070.8644 | 1075.4116 |
| 1083.8911 | 1089.0258 | 1092.6974 |
| 1098.1603 | 1102.5814 | 1139.0022 |
| 1146.0633 | 1148.1822 | 1149.6521 |
| 1152.7054 | 1157.7767 | 1181.2774 |
| 1183.9291 | 1190.5383 | 1191.3202 |
| 1209.8108 | 1214.3115 | 1248.1358 |
| 1282.4695 | 1286.1784 | 1291.3032 |
| 1291.7083 | 1311.6643 | 1320.6308 |
| 1323.2462 | 1337.7464 | 1343.0904 |
| 1344.7470 | 1346.8226 | 1356.5858 |
| 1363.9136 | 1380.8072 | 1396.1601 |
| 1396.8544 | 1402.6966 | 1403.8944 |
| 1404.3401 | 1407.2312 | 1422.9381 |
| 1423.9506 | 1426.3694 | 1426.8460 |
| 1435.4656 | 1450.5225 | 1490.4439 |
| 1492.6018 | 1494.6312 | 1494.9067 |
| 1496.1777 | 1497.3784 | 1500.0244 |
| 1500.6155 | 1507.6757 | 1508.2435 |
| 1510.1814 | 1512.2898 | 1514.4766 |
| 1517.0669 | 1520.8047 | 1523.1164 |
| 1530.4389 | 1531.5565 | 1536.1781 |
| 1544.5308 | 1633.6831 | 1679.7774 |

| | | |
|---|---|---|
| 1681.7127 | 1683.7741 | 1685.4609 |
| 3049.1953 | 3051.6667 | 3055.4954 |
| 3059.1735 | 3059.7192 | 3062.2973 |
| 3066.7091 | 3068.3730 | 3087.8288 |
| 3088.3724 | 3097.3731 | 3105.3557 |
| 3131.5515 | 3132.8174 | 3134.6686 |
| 3139.1530 | 3139.6598 | 3142.1295 |
| 3143.1139 | 3144.1787 | 3145.8590 |
| 3146.8211 | 3147.1249 | 3148.2168 |
| 3151.8972 | 3152.4450 | 3156.8545 |
| 3158.6331 | 3197.6259 | 3201.7096 |
| 3208.2302 | 3217.8474 | 3227.2376 |
| 3229.6384 | 3278.3596 | 3300.4999 |

**$TS_I$**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.706606 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.745048 |
| Thermal correction to Enthalpy= | | | 0.745992 |
| Thermal correction to Gibbs Free Energy= | | | 0.637725 |
| Sum of electronic and zero-point Energies= | | | -1542.554075 |
| Sum of electronic and thermal Energies= | | | -1542.515634 |
| Sum of electronic and thermal Enthalpies= | | | -1542.514690 |
| Sum of electronic and thermal Free Energies= | | | -1542.622957 |
| C | -0.06469600 | 0.75201100 | -1.65368900 |
| C | -0.82611400 | -0.02804000 | -2.39175300 |
| C | 0.55177800 | 1.93314500 | -1.44557800 |
| H | -0.99496500 | 0.26113000 | -3.42605200 |
| H | -1.30176200 | -0.92474800 | -2.01683300 |
| H | 1.62893300 | 2.00007500 | -1.33603700 |
| C | -0.17318800 | 3.18424800 | -1.32212600 |
| O | 0.35170600 | 4.27101200 | -1.12449000 |
| O | -1.51272000 | 3.06579400 | -1.50579700 |
| C | -2.25148000 | 4.29044500 | -1.54155400 |
| C | -3.56835900 | 4.01030500 | -2.23533900 |
| H | -1.67102000 | 5.04574000 | -2.07668300 |
| H | -2.40266700 | 4.65085400 | -0.51766600 |
| H | -4.17312600 | 4.91976800 | -2.26722600 |
| H | -3.39316900 | 3.67221300 | -3.25939700 |
| H | -4.13612700 | 3.23652500 | -1.71254900 |
| C | 0.21391900 | -0.62872600 | 0.14480400 |
| C | -0.03352300 | -2.01046200 | 1.94470900 |
| C | 1.27617000 | -1.68585700 | 1.86404100 |
| N | 1.39813500 | -0.83954100 | 0.76687100 |
| H | -0.57677100 | -2.61494700 | 2.65420000 |

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|---|---|---|---|
| H | 2.12385200 | -1.97183900 | 2.46693300 |
| N | -0.65945700 | -1.35340400 | 0.89056000 |
| C | 2.64157900 | -0.25230800 | 0.34989800 |
| C | 2.95741200 | 1.03778200 | 0.80695900 |
| C | 3.48068300 | -0.99602900 | -0.48886800 |
| C | 4.17622500 | 1.57927400 | 0.39592700 |
| C | 4.68793700 | -0.40838900 | -0.87579600 |
| C | 5.03297100 | 0.86320700 | -0.43545600 |
| H | 4.45598500 | 2.57602300 | 0.71942600 |
| H | 5.36150700 | -0.94956900 | -1.53272600 |
| H | 5.97439900 | 1.30481600 | -0.74708000 |
| C | -2.07523300 | -1.37579100 | 0.64979100 |
| C | -2.65702200 | -2.57266200 | 0.20020200 |
| C | -2.80622700 | -0.19424800 | 0.86771500 |
| C | -4.03592600 | -2.56855700 | -0.02446000 |
| C | -4.18086600 | -0.24942000 | 0.62589900 |
| C | -4.78862900 | -1.42064700 | 0.18804800 |
| H | -4.52834400 | -3.47050700 | -0.36948900 |
| H | -4.78900300 | 0.63467700 | 0.77785200 |
| H | -5.85878200 | -1.43678100 | 0.00754700 |
| C | 3.06788900 | -2.35872200 | -1.02011100 |
| C | 4.22714900 | -3.35771200 | -1.05612900 |
| C | 2.43912300 | -2.20049900 | -2.41103800 |
| H | 2.30090900 | -2.76665900 | -0.35262100 |
| H | 4.71884300 | -3.43671700 | -0.08256300 |
| H | 3.85417300 | -4.34721300 | -1.33487000 |
| H | 4.98043000 | -3.07368500 | -1.79728300 |
| H | 1.59021300 | -1.51050100 | -2.38209700 |
| H | 3.17753500 | -1.80429300 | -3.11660400 |
| H | 2.09113800 | -3.16822800 | -2.78656100 |
| C | 2.00957500 | 1.80314900 | 1.71768300 |
| C | 2.12009800 | 3.32072600 | 1.56380900 |
| C | 2.23171200 | 1.40742800 | 3.18456400 |
| H | 0.98757300 | 1.51937300 | 1.43532600 |
| H | 2.01510000 | 3.63405100 | 0.52214500 |
| H | 1.32040700 | 3.79956200 | 2.13743300 |
| H | 3.07062400 | 3.69613300 | 1.95755300 |
| H | 2.08071700 | 0.33740900 | 3.34799800 |
| H | 3.25234200 | 1.65982100 | 3.49205500 |
| H | 1.53631800 | 1.95074000 | 3.83204700 |
| C | -1.81244000 | -3.81330800 | -0.07311900 |
| C | -0.97080300 | -3.63735900 | -1.34601700 |
| C | -2.63715400 | -5.09734100 | -0.16944600 |
| H | -1.11599500 | -3.93985100 | 0.76251700 |

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|---|---|---|---|
| H | -0.28606800 | -2.78772200 | -1.26886600 |
| H | -0.37543900 | -4.53685200 | -1.53206100 |
| H | -1.62317100 | -3.47673100 | -2.21155900 |
| H | -3.28618900 | -5.23070600 | 0.70059300 |
| H | -3.26151800 | -5.10420800 | -1.06860600 |
| H | -1.96581500 | -5.95764900 | -0.23095300 |
| C | -2.13174400 | 1.09143200 | 1.33976500 |
| C | -1.59444100 | 0.97104000 | 2.77464100 |
| C | -3.04150800 | 2.31543200 | 1.24914100 |
| H | -1.28414400 | 1.27649500 | 0.66905500 |
| H | -0.83006700 | 0.19733500 | 2.87745100 |
| H | -1.14614700 | 1.92278300 | 3.07968000 |
| H | -2.41062100 | 0.74372700 | 3.46886200 |
| H | -3.45560800 | 2.43437900 | 0.24537600 |
| H | -3.86706100 | 2.25909200 | 1.96720600 |
| H | -2.45925300 | 3.21156600 | 1.48270300 |

Frequencies

| | | |
|---|---|---|
| -243.9112 | 25.4867 | 34.9711 |
| 39.0144 | 44.9466 | 46.9565 |
| 57.8708 | 65.0958 | 66.3173 |
| 74.6805 | 79.1074 | 83.3546 |
| 91.7408 | 96.5753 | 99.8004 |
| 111.1277 | 120.0497 | 133.4922 |
| 138.3171 | 139.9684 | 148.9160 |
| 154.2825 | 156.5894 | 171.7349 |
| 177.7862 | 200.7633 | 218.4546 |
| 223.3789 | 234.9713 | 237.1179 |
| 248.5405 | 255.5539 | 263.6853 |
| 276.3176 | 282.4794 | 285.2668 |
| 289.2846 | 300.3151 | 306.1404 |
| 306.9860 | 312.9379 | 319.1222 |
| 321.5327 | 336.2550 | 338.3821 |
| 355.5521 | 371.4767 | 373.0857 |
| 391.1471 | 395.6103 | 418.5195 |
| 423.6889 | 442.6197 | 445.3752 |
| 448.9695 | 452.5969 | 472.1330 |
| 531.3477 | 547.1260 | 554.0113 |
| 559.3245 | 571.9455 | 577.4069 |
| 589.7907 | 591.8786 | 601.2443 |
| 628.3859 | 651.6823 | 658.6748 |
| 682.7622 | 704.2899 | 710.9856 |
| 743.7436 | 758.7613 | 776.5158 |
| 779.1913 | 784.0574 | 788.8994 |
| 806.0963 | 816.2537 | 820.0036 |

| | | |
|---|---|---|
| 827.6964 | 831.7180 | 834.4669 |
| 884.7629 | 885.1656 | 890.7989 |
| 912.4373 | 917.0740 | 927.4592 |
| 930.5108 | 932.5398 | 935.3978 |
| 935.6775 | 942.9967 | 959.9299 |
| 964.8168 | 967.5303 | 975.0455 |
| 977.2482 | 977.7801 | 979.7225 |
| 983.5597 | 987.6929 | 996.2458 |
| 1007.8428 | 1012.0063 | 1077.1003 |
| 1080.9936 | 1088.8750 | 1091.2365 |
| 1093.6567 | 1100.8567 | 1103.9238 |
| 1113.4976 | 1128.9877 | 1138.1184 |
| 1143.6352 | 1149.4372 | 1151.2022 |
| 1152.5388 | 1156.2989 | 1163.4526 |
| 1175.1419 | 1180.6193 | 1188.6422 |
| 1188.8475 | 1193.0857 | 1211.9684 |
| 1213.8758 | 1251.7874 | 1277.6460 |
| 1284.8063 | 1290.8789 | 1291.9914 |
| 1301.3192 | 1312.1540 | 1315.3904 |
| 1321.4369 | 1329.4804 | 1331.3020 |
| 1341.0692 | 1343.7233 | 1347.1216 |
| 1347.2676 | 1356.8255 | 1366.6666 |
| 1377.2016 | 1378.9663 | 1395.5307 |
| 1400.8992 | 1403.8977 | 1407.4172 |
| 1408.0892 | 1409.7591 | 1420.1402 |
| 1422.4076 | 1428.6862 | 1431.8697 |
| 1434.6207 | 1441.1649 | 1457.5133 |
| 1459.8682 | 1491.2432 | 1491.4900 |
| 1492.6516 | 1493.6551 | 1494.4526 |
| 1496.0899 | 1496.5626 | 1499.2866 |
| 1502.0027 | 1503.2438 | 1509.0443 |
| 1509.7169 | 1510.4006 | 1512.0988 |
| 1518.3772 | 1518.8307 | 1519.3862 |
| 1520.3717 | 1525.8771 | 1528.3764 |
| 1529.7652 | 1536.2955 | 1537.5930 |
| 1638.6955 | 1676.9195 | 1678.5410 |
| 1681.4724 | 1683.4102 | 1770.1516 |
| 1931.4975 | 3056.1115 | 3058.4192 |
| 3058.7593 | 3060.1465 | 3063.1537 |
| 3063.5162 | 3066.7930 | 3066.8613 |
| 3079.2528 | 3085.0329 | 3085.3604 |
| 3087.6653 | 3088.2843 | 3094.8497 |
| 3130.0794 | 3134.2505 | 3136.6542 |
| 3138.7327 | 3139.5652 | 3140.7718 |

| | | |
|---|---|---|
| 3140.9351 | 3143.4464 | 3147.0423 |
| 3148.9031 | 3150.3286 | 3151.0847 |
| 3154.8630 | 3157.2206 | 3165.0183 |
| 3165.6731 | 3167.9411 | 3169.1386 |
| 3171.3443 | 3172.7798 | 3204.8495 |
| 3205.9171 | 3217.7193 | 3219.6856 |
| 3225.0741 | 3228.9423 | 3232.0685 |
| 3278.5031 | 3293.5257 | 3326.6734 |

**I**

| | |
|---|---|
| Zero-point correction= | 0.709054 (Hartree/Particle) |
| Thermal correction to Energy= | 0.748039 |
| Thermal correction to Enthalpy= | 0.748983 |
| Thermal correction to Gibbs Free Energy= | 0.637326 |
| Sum of electronic and zero-point Energies= | -1542.616380 |
| Sum of electronic and thermal Energies= | -1542.577395 |
| Sum of electronic and thermal Enthalpies= | -1542.576451 |
| Sum of electronic and thermal Free Energies= | -1542.688108 |

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|---|---|---|---|
| C | 0.04092700 | -0.48700300 | -0.82416800 |
| C | -0.15183700 | 0.06699400 | -2.05398000 |
| C | 0.41440000 | -1.77986600 | -0.35982500 |
| H | -0.03356400 | -0.51448300 | -2.95719300 |
| H | -0.41066800 | 1.11631900 | -2.14640500 |
| H | 0.44531700 | -1.95266000 | 0.70838800 |
| C | 0.78830000 | -2.89851400 | -1.13716400 |
| O | 1.15207800 | -4.00111800 | -0.70982500 |
| O | 0.73310800 | -2.67541900 | -2.49430300 |
| C | 1.16035000 | -3.76046200 | -3.30987700 |
| C | 1.00169800 | -3.32997700 | -4.75352800 |
| H | 0.56112300 | -4.64943000 | -3.08734400 |
| H | 2.20193700 | -4.00881700 | -3.07786900 |
| H | 1.32191700 | -4.12990400 | -5.42586500 |
| H | -0.04313100 | -3.09289900 | -4.96944300 |
| H | 1.60540700 | -2.44200300 | -4.95832400 |
| C | -0.14666900 | 0.45162600 | 0.30817300 |
| C | -1.06318100 | 1.67888700 | 1.92688000 |
| C | 0.28160900 | 1.84947300 | 1.99019200 |
| N | 0.83063500 | 1.07488900 | 0.98459300 |
| H | -1.86506100 | 2.08433500 | 2.52242400 |
| H | 0.89709500 | 2.44731700 | 2.64286600 |
| N | -1.30653700 | 0.80895500 | 0.87860100 |
| C | 2.23369900 | 1.00359000 | 0.65270300 |
| C | 2.72231000 | 1.89853900 | -0.30857500 |
| C | 3.02995100 | 0.05911900 | 1.31170400 |

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|---|---|---|---|
| C | 4.08647100 | 1.83582800 | -0.59775400 |
| C | 4.38707500 | 0.03802300 | 0.98307100 |
| C | 4.90968700 | 0.91570600 | 0.04043300 |
| H | 4.50764100 | 2.51732300 | -1.33022600 |
| H | 5.04217700 | -0.67505800 | 1.47378800 |
| H | 5.96767000 | 0.88210800 | -0.19900900 |
| C | -2.60629700 | 0.32122500 | 0.48469400 |
| C | -3.06813700 | -0.86781500 | 1.06257900 |
| C | -3.33951600 | 1.07069500 | -0.44365300 |
| C | -4.33877500 | -1.30401100 | 0.68018400 |
| C | -4.60480600 | 0.59298400 | -0.78684900 |
| C | -5.09890300 | -0.58248300 | -0.23212100 |
| H | -4.73766400 | -2.21943000 | 1.10629000 |
| H | -5.20970000 | 1.14723200 | -1.49773100 |
| H | -6.08420400 | -0.93883400 | -0.51469400 |
| C | 2.48824100 | -0.87022600 | 2.38376800 |
| C | 2.94338200 | -0.39226400 | 3.76930600 |
| C | 2.89792200 | -2.32796900 | 2.14883500 |
| H | 1.39400300 | -0.82466800 | 2.35857900 |
| H | 2.61560500 | 0.63251500 | 3.96800300 |
| H | 2.53434300 | -1.04205000 | 4.54827200 |
| H | 4.03548100 | -0.41803800 | 3.84361700 |
| H | 2.58604600 | -2.67945900 | 1.16166000 |
| H | 3.98115400 | -2.45406900 | 2.24274400 |
| H | 2.42836900 | -2.96564100 | 2.90407900 |
| C | 1.84268300 | 2.93794000 | -0.98081800 |
| C | 2.04152300 | 2.96502900 | -2.49872000 |
| C | 2.09700000 | 4.32100600 | -0.36718000 |
| H | 0.79508100 | 2.67761800 | -0.79473400 |
| H | 1.90892600 | 1.96758600 | -2.92523600 |
| H | 1.31140300 | 3.63955200 | -2.95581900 |
| H | 3.03829000 | 3.32980000 | -2.76455200 |
| H | 1.91058200 | 4.31952300 | 0.71085700 |
| H | 3.13580000 | 4.62599900 | -0.53040200 |
| H | 1.44534500 | 5.06844400 | -0.82896100 |
| C | -2.27428900 | -1.64039500 | 2.10207700 |
| C | -2.15305600 | -3.12513800 | 1.74807200 |
| C | -2.90462500 | -1.45128000 | 3.48825400 |
| H | -1.25891600 | -1.23105600 | 2.13950500 |
| H | -1.70058200 | -3.25187700 | 0.76144900 |
| H | -1.51831700 | -3.62807300 | 2.48378900 |
| H | -3.12958900 | -3.61936100 | 1.76020200 |
| H | -2.94600000 | -0.39373200 | 3.76532600 |
| H | -3.92601100 | -1.84522600 | 3.50309200 |

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|---|---|---|---|
| H | -2.32340900 | -1.98418100 | 4.24618600 |
| C | -2.82314500 | 2.37202500 | -1.03162500 |
| C | -3.50920100 | 3.56780600 | -0.35794100 |
| C | -3.00060200 | 2.42649900 | -2.55196800 |
| H | -1.74973500 | 2.44198700 | -0.82249500 |
| H | -3.34337100 | 3.56765600 | 0.72333100 |
| H | -3.12475900 | 4.50723700 | -0.76535600 |
| H | -4.58931900 | 3.53552800 | -0.53398400 |
| H | -2.57612200 | 1.53889500 | -3.02799300 |
| H | -4.05713700 | 2.49389600 | -2.82839500 |
| H | -2.49876700 | 3.31192000 | -2.95282800 |

Frequencies

| | | |
|---|---|---|
| 17.4024 | 21.6603 | 25.4952 |
| 36.4956 | 45.2569 | 48.0907 |
| 50.2040 | 57.8615 | 62.8565 |
| 74.0718 | 75.8971 | 84.0378 |
| 91.0784 | 95.7288 | 97.9959 |
| 112.7029 | 120.2111 | 124.4506 |
| 131.3745 | 133.2655 | 146.9234 |
| 166.9201 | 171.5663 | 188.6320 |
| 216.8148 | 224.4724 | 227.5427 |
| 230.1019 | 241.4883 | 242.8752 |
| 249.1476 | 260.1153 | 263.2752 |
| 267.7722 | 268.9262 | 270.9957 |
| 274.0751 | 281.3918 | 290.9568 |
| 295.7433 | 299.6899 | 306.4562 |
| 318.2311 | 320.5319 | 331.2385 |
| 335.1647 | 365.1028 | 387.7812 |
| 419.5142 | 426.9038 | 442.1312 |
| 447.3168 | 450.9792 | 461.6555 |
| 475.2063 | 499.3491 | 531.9479 |
| 546.2989 | 564.8985 | 569.3743 |
| 588.7574 | 597.0008 | 625.8237 |
| 628.2474 | 649.2321 | 650.0601 |
| 651.2369 | 679.2822 | 684.1607 |
| 687.7005 | 717.4961 | 741.2469 |
| 759.7962 | 762.9108 | 768.4070 |
| 770.0995 | 772.2543 | 788.7843 |
| 794.0118 | 806.5087 | 812.5072 |
| 830.1369 | 833.7335 | 834.1190 |
| 835.9307 | 878.2114 | 892.5665 |
| 914.5250 | 915.5111 | 925.4786 |
| 934.2534 | 935.9800 | 941.5863 |
| 943.4153 | 944.6054 | 967.9943 |

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|---|---|---|
| 968.7522 | 969.6995 | 973.3281 |
| 975.0483 | 977.5226 | 980.4131 |
| 986.9297 | 1014.1065 | 1015.2256 |
| 1020.0638 | 1061.4168 | 1072.0411 |
| 1075.5285 | 1084.0212 | 1086.6960 |
| 1109.7789 | 1124.3356 | 1127.2520 |
| 1140.3440 | 1144.9651 | 1146.9215 |
| 1148.3688 | 1149.0049 | 1160.2460 |
| 1166.6603 | 1169.9941 | 1183.4878 |
| 1185.5201 | 1188.0403 | 1193.7475 |
| 1195.9477 | 1209.5930 | 1212.2791 |
| 1250.7605 | 1254.9977 | 1283.3566 |
| 1289.9255 | 1293.1908 | 1296.5613 |
| 1307.1345 | 1307.8919 | 1324.8474 |
| 1328.6819 | 1332.4353 | 1335.7556 |
| 1340.7344 | 1341.9707 | 1360.7350 |
| 1372.9163 | 1390.1923 | 1391.5008 |
| 1392.8706 | 1394.7372 | 1404.4696 |
| 1405.9289 | 1406.6219 | 1407.9224 |
| 1418.9621 | 1424.8319 | 1425.9427 |
| 1427.2942 | 1428.3329 | 1429.0257 |
| 1446.7259 | 1485.3351 | 1490.2760 |
| 1492.1017 | 1493.6304 | 1493.7212 |
| 1494.2857 | 1496.3848 | 1497.3012 |
| 1498.5380 | 1499.5816 | 1504.8274 |
| 1505.2779 | 1508.1951 | 1509.2149 |
| 1509.3594 | 1512.0293 | 1512.5294 |
| 1513.3218 | 1514.3613 | 1520.6693 |
| 1532.0808 | 1533.7747 | 1536.0143 |
| 1538.3161 | 1555.1232 | 1571.4511 |
| 1632.7944 | 1647.4007 | 1677.7220 |
| 1682.1780 | 1689.2623 | 1690.9552 |
| 1722.0680 | 3057.3452 | 3057.6598 |
| 3060.0453 | 3060.6204 | 3063.5781 |
| 3064.1334 | 3064.2890 | 3067.3045 |
| 3075.3114 | 3082.3705 | 3084.3550 |
| 3088.6267 | 3093.4793 | 3094.6366 |
| 3122.7037 | 3137.8500 | 3138.4472 |
| 3138.7537 | 3139.5210 | 3140.8869 |
| 3142.3578 | 3142.7676 | 3142.8604 |
| 3144.7126 | 3146.4123 | 3148.9817 |
| 3154.0407 | 3154.3308 | 3156.7920 |
| 3163.3586 | 3163.8280 | 3165.6046 |
| 3168.8672 | 3183.2159 | 3205.0499 |

| | | |
|---|---|---|
| 3210.1060 | 3216.9832 | 3222.1380 |
| 3228.5250 | 3234.6340 | 3239.0564 |
| 3289.9964 | 3303.3923 | 3335.1726 |

**$TS_{II}$**

| | |
|---|---|
| Zero-point correction= | 0.778682 (Hartree/Particle) |
| Thermal correction to Energy= | 0.821869 |
| Thermal correction to Enthalpy= | 0.822813 |
| Thermal correction to Gibbs Free Energy= | 0.702782 |
| Sum of electronic and zero-point Energies= | -1768.681874 |
| Sum of electronic and thermal Energies= | -1768.638687 |
| Sum of electronic and thermal Enthalpies= | -1768.637743 |
| Sum of electronic and thermal Free Energies= | -1768.757774 |

| | | | |
|---|---|---|---|
| C | 0.21660900 | -0.45074200 | -0.56058700 |
| C | -0.45390500 | 0.02212800 | -1.75484500 |
| C | 0.30154200 | -1.69315600 | -0.01199400 |
| H | -1.74972400 | -0.07661000 | -1.47353300 |
| H | -0.17294800 | 1.03954600 | -2.03282300 |
| H | 0.78912400 | -1.82817700 | 0.94697200 |
| C | -0.33908100 | -2.91578700 | -0.50217800 |
| O | -0.33337000 | -3.96123500 | 0.12558200 |
| O | -0.99141700 | -2.76258800 | -1.66152200 |
| C | -1.87848500 | -3.83021900 | -2.03300000 |
| C | -2.73522900 | -3.32762300 | -3.17355000 |
| H | -2.48596500 | -4.09367000 | -1.16232400 |
| H | -1.28266100 | -4.70509500 | -2.31165900 |
| H | -3.40159700 | -4.12610000 | -3.50939100 |
| H | -3.33806700 | -2.47542700 | -2.84735100 |
| H | -2.11197900 | -3.02172100 | -4.01820200 |
| C | 0.79837700 | 0.61233700 | 0.29583900 |
| C | 0.97856400 | 2.32546600 | 1.69886200 |
| C | 2.23267200 | 1.95651900 | 1.33329200 |
| N | 2.09904000 | 0.88732200 | 0.46474600 |
| H | 0.62479400 | 3.09442800 | 2.36672700 |
| H | 3.20137500 | 2.34835400 | 1.59919700 |
| N | 0.10315800 | 1.48163600 | 1.04054500 |
| C | 3.18981700 | 0.20133000 | -0.18777000 |
| C | 3.57946200 | 0.64566100 | -1.45713100 |
| C | 3.80891900 | -0.85678200 | 0.49136100 |
| C | 4.65971600 | -0.00935100 | -2.05232600 |
| C | 4.88318400 | -1.47587500 | -0.14923200 |
| C | 5.30535300 | -1.05642100 | -1.40588300 |
| H | 5.00004000 | 0.30822400 | -3.03309800 |
| H | 5.39655500 | -2.29558600 | 0.34364400 |

| | | | |
|---|---|---|---|
| H | 6.14335600 | -1.55123500 | -1.88563300 |
| C | -1.33064900 | 1.43583100 | 1.22914800 |
| C | -1.82935600 | 0.54252900 | 2.18789800 |
| C | -2.13365000 | 2.28011900 | 0.45537200 |
| C | -3.21320300 | 0.51339900 | 2.35840000 |
| C | -3.51076900 | 2.21193000 | 0.67133500 |
| C | -4.04482200 | 1.33498900 | 1.60598000 |
| H | -3.64597500 | -0.16654100 | 3.08574000 |
| H | -4.17367500 | 2.84143300 | 0.08615200 |
| H | -5.11974300 | 1.28344200 | 1.74442100 |
| C | 3.38368100 | -1.30207300 | 1.88008300 |
| C | 4.38953800 | -0.80338200 | 2.92620300 |
| C | 3.21179100 | -2.82236100 | 1.97480000 |
| H | 2.41601900 | -0.84106100 | 2.11068300 |
| H | 4.48604300 | 0.28569100 | 2.89999600 |
| H | 4.07146000 | -1.09833800 | 3.92998500 |
| H | 5.37831100 | -1.23479400 | 2.74036600 |
| H | 2.53455000 | -3.20432200 | 1.20585400 |
| H | 4.17190500 | -3.33605600 | 1.86875800 |
| H | 2.80356500 | -3.08660900 | 2.95448800 |
| C | 2.90497900 | 1.80685500 | -2.16696200 |
| C | 2.48012900 | 1.43052600 | -3.58990700 |
| C | 3.82720900 | 3.03276600 | -2.17241600 |
| H | 1.99758100 | 2.07596900 | -1.61466800 |
| H | 1.85138200 | 0.53653300 | -3.58899500 |
| H | 1.91338100 | 2.25182400 | -4.03766300 |
| H | 3.34960000 | 1.24161600 | -4.22686700 |
| H | 4.09376500 | 3.33364000 | -1.15533100 |
| H | 4.75269000 | 2.81365300 | -2.71443800 |
| H | 3.33507700 | 3.87577800 | -2.66528500 |
| C | -0.92920300 | -0.30872500 | 3.06889800 |
| C | -1.36033900 | -1.77756900 | 3.11410200 |
| C | -0.87513500 | 0.28706800 | 4.48232500 |
| H | 0.08902800 | -0.27989000 | 2.66341100 |
| H | -1.37614800 | -2.22614900 | 2.11733000 |
| H | -0.65771900 | -2.34825400 | 3.72913300 |
| H | -2.35388000 | -1.88953900 | 3.55793200 |
| H | -0.52621500 | 1.32375600 | 4.46302600 |
| H | -1.86963300 | 0.27315800 | 4.94001000 |
| H | -0.19973200 | -0.29455500 | 5.11633000 |
| C | -1.55848900 | 3.25911700 | -0.55290800 |
| C | -1.61343200 | 4.68763800 | 0.00409100 |
| C | -2.27120100 | 3.17400200 | -1.90552600 |
| H | -0.50492100 | 3.00556800 | -0.72013300 |

| | | | |
|---|---|---|---|
| H | -1.06482000 | 4.77184000 | 0.94670000 |
| H | -1.18203500 | 5.39390600 | -0.71104900 |
| H | -2.65108400 | 4.98260200 | 0.19135700 |
| H | -2.26805800 | 2.14904200 | -2.28275200 |
| H | -3.31080800 | 3.50717300 | -1.82976900 |
| H | -1.76907300 | 3.81996500 | -2.63174300 |
| H | -0.39191200 | -0.66775900 | -2.59492400 |
| C | -4.21000800 | -0.02536600 | -1.88281200 |
| C | -5.25248000 | -0.78542900 | -1.39205200 |
| C | -3.48718000 | -1.36753500 | -0.37079500 |
| N | -3.07663800 | -0.40454400 | -1.21896200 |
| H | -4.19936800 | 0.74260200 | -2.64532100 |
| H | -6.29684400 | -0.76245300 | -1.67932800 |
| H | -2.79819600 | -1.86403800 | 0.30503700 |
| N | -4.78957200 | -1.64242100 | -0.42777800 |

Frequencies

| | | |
|---|---|---|
| -1368.6989 | 14.7829 | 28.3606 |
| 34.5123 | 38.7171 | 46.3289 |
| 50.3917 | 53.5308 | 56.2153 |
| 60.7405 | 65.2993 | 68.5272 |
| 71.3448 | 76.9100 | 86.6966 |
| 93.2778 | 98.8622 | 112.2622 |
| 114.7239 | 123.5542 | 126.1548 |
| 129.0133 | 133.3907 | 143.3619 |
| 148.2095 | 156.7528 | 168.1342 |
| 172.3574 | 182.8304 | 197.6199 |
| 218.0701 | 225.0868 | 227.7886 |
| 237.0060 | 241.3350 | 241.8766 |
| 244.5464 | 256.2520 | 262.2390 |
| 266.2123 | 270.2014 | 273.2939 |
| 275.5662 | 285.0536 | 290.7908 |
| 293.4818 | 297.5003 | 309.3679 |
| 319.4763 | 323.1601 | 330.6903 |
| 337.7436 | 358.2060 | 388.1733 |
| 420.1081 | 427.5294 | 440.0258 |
| 445.6016 | 448.5389 | 451.6834 |
| 461.9876 | 477.8328 | 498.8241 |
| 532.5759 | 545.3076 | 555.8471 |
| 561.5421 | 587.6222 | 592.2655 |
| 600.3144 | 625.7506 | 636.1816 |
| 648.3653 | 649.9416 | 669.0724 |
| 681.5051 | 686.9075 | 692.8462 |
| 713.0915 | 743.3474 | 748.0761 |
| 764.1296 | 765.8563 | 770.7752 |

| | | |
|---|---|---|
| 777.7027 | 791.0150 | 797.6175 |
| 810.8747 | 823.1392 | 827.4340 |
| 833.8322 | 835.2796 | 835.9114 |
| 842.5266 | 859.4241 | 885.1903 |
| 899.0575 | 901.7155 | 914.4981 |
| 916.1927 | 923.3763 | 931.8154 |
| 934.0136 | 934.9844 | 937.7518 |
| 940.1264 | 941.9052 | 947.1640 |
| 965.9024 | 969.0717 | 969.8145 |
| 974.6091 | 975.5936 | 976.9796 |
| 978.3562 | 988.1880 | 1000.0027 |
| 1007.1236 | 1018.2586 | 1022.9664 |
| 1070.2336 | 1071.4481 | 1075.4064 |
| 1082.6428 | 1086.5671 | 1108.8969 |
| 1112.4619 | 1121.0611 | 1126.5985 |
| 1137.2847 | 1142.8640 | 1144.9034 |
| 1145.7985 | 1146.5727 | 1148.8527 |
| 1153.0271 | 1163.8321 | 1169.9734 |
| 1183.6943 | 1185.9010 | 1189.1277 |
| 1194.5052 | 1200.4394 | 1210.0517 |
| 1216.5691 | 1232.5870 | 1247.4618 |
| 1250.2405 | 1267.3222 | 1282.3253 |
| 1295.7129 | 1300.2629 | 1306.0268 |
| 1309.7323 | 1326.5931 | 1329.8414 |
| 1330.9607 | 1333.7491 | 1338.5835 |
| 1339.4795 | 1342.3169 | 1350.0817 |
| 1359.4093 | 1370.9583 | 1380.3481 |
| 1385.9040 | 1390.2709 | 1394.9538 |
| 1397.3649 | 1402.5043 | 1408.2507 |
| 1408.6933 | 1408.8504 | 1410.5517 |
| 1412.8751 | 1418.9402 | 1426.2280 |
| 1428.9790 | 1429.3154 | 1430.0963 |
| 1449.6592 | 1476.7807 | 1487.7465 |
| 1491.1412 | 1492.0133 | 1492.4178 |
| 1493.2355 | 1495.6946 | 1497.9204 |
| 1498.1588 | 1499.8222 | 1503.7854 |
| 1505.4936 | 1506.8350 | 1507.8363 |
| 1509.7360 | 1510.4440 | 1511.1701 |
| 1511.9895 | 1516.2100 | 1520.4314 |
| 1524.7550 | 1528.6089 | 1530.6930 |
| 1534.7041 | 1538.8480 | 1546.8081 |
| 1556.3563 | 1568.9141 | 1576.8859 |
| 1635.3225 | 1680.8331 | 1681.8630 |
| 1687.6857 | 1689.5924 | 1691.4308 |

| | | |
|---|---|---|
| 1798.2442 | 3058.5828 | 3062.9541 |
| 3064.3907 | 3065.0230 | 3067.7680 |
| 3067.9255 | 3068.7605 | 3069.0518 |
| 3075.0271 | 3075.7632 | 3076.8394 |
| 3086.2572 | 3087.4253 | 3095.6777 |
| 3117.6628 | 3139.6772 | 3140.2605 |
| 3142.9312 | 3143.5820 | 3143.7089 |
| 3145.6658 | 3145.9088 | 3146.9106 |
| 3148.8125 | 3149.9137 | 3150.7503 |
| 3153.7782 | 3154.5708 | 3156.9391 |
| 3158.4496 | 3160.6954 | 3164.7997 |
| 3170.7950 | 3173.7794 | 3201.4592 |
| 3211.8045 | 3214.0164 | 3216.1191 |
| 3226.7050 | 3228.9219 | 3229.0451 |
| 3234.6579 | 3241.9621 | 3242.2655 |
| 3252.7449 | 3302.8629 | 3323.0987 |

**II**

| | |
|---|---|
| Zero-point correction= | 0.782734 (Hartree/Particle) |
| Thermal correction to Energy= | 0.827113 |
| Thermal correction to Enthalpy= | 0.828057 |
| Thermal correction to Gibbs Free Energy= | 0.703732 |
| Sum of electronic and zero-point Energies= | -1768.686696 |
| Sum of electronic and thermal Energies= | -1768.642317 |
| Sum of electronic and thermal Enthalpies= | -1768.641373 |
| Sum of electronic and thermal Free Energies= | -1768.765698 |

| | | | |
|---|---|---|---|
| C | 0.24893600 | 0.33354700 | -0.57598100 |
| C | -0.87756000 | 1.27226800 | -0.23712800 |
| C | 0.82477000 | 0.10572200 | -1.76534400 |
| H | -1.84534900 | 0.91590700 | -0.61906400 |
| H | -0.95818400 | 1.39843700 | 0.84546000 |
| H | 1.63023700 | -0.61718400 | -1.85517900 |
| C | 0.44379000 | 0.70971200 | -3.06819700 |
| O | 1.03260900 | 0.45005200 | -4.09581800 |
| O | -0.60681500 | 1.51678300 | -2.98129600 |
| C | -1.11167900 | 2.07112600 | -4.21212100 |
| C | -2.28627900 | 2.94687700 | -3.83747300 |
| H | -1.40270400 | 1.24264200 | -4.86415900 |
| H | -0.30694500 | 2.62535000 | -4.70300600 |
| H | -2.76414000 | 3.33146600 | -4.74135700 |
| H | -3.01490000 | 2.37520200 | -3.25555300 |
| H | -1.95340700 | 3.79599800 | -3.23485700 |
| C | 0.78311200 | -0.46957300 | 0.54592600 |
| C | 0.91433300 | -1.96369400 | 2.18109400 |

| | | | |
|---|---|---|---|
| C | 2.09650000 | -1.29537400 | 2.13264200 |
| N | 1.99710900 | -0.37462600 | 1.10599100 |
| H | 0.57378700 | -2.77005200 | 2.81061200 |
| H | 2.99056500 | -1.37593500 | 2.73001600 |
| N | 0.11090100 | -1.42918000 | 1.19362500 |
| C | 3.00027700 | 0.61036800 | 0.76777000 |
| C | 2.89691400 | 1.87352300 | 1.36543100 |
| C | 4.02168900 | 0.24752900 | -0.11943100 |
| C | 3.89152000 | 2.80175000 | 1.05427500 |
| C | 4.99053100 | 1.21433400 | -0.39379900 |
| C | 4.92805000 | 2.47549400 | 0.18772900 |
| H | 3.85353900 | 3.79085300 | 1.49992800 |
| H | 5.80459600 | 0.97547300 | -1.07076000 |
| H | 5.69283900 | 3.21133200 | -0.03791800 |
| C | -1.19527900 | -1.91072000 | 0.79754900 |
| C | -1.25069300 | -2.83623800 | -0.25418300 |
| C | -2.32033400 | -1.42062400 | 1.47106100 |
| C | -2.51689800 | -3.29066000 | -0.62415300 |
| C | -3.56173300 | -1.90533100 | 1.05518200 |
| C | -3.65823600 | -2.82975500 | 0.02219700 |
| H | -2.61034500 | -4.01319800 | -1.42877900 |
| H | -4.46264300 | -1.53709600 | 1.53444700 |
| H | -4.63413800 | -3.18890300 | -0.28820000 |
| C | 4.11965800 | -1.13730200 | -0.73645400 |
| C | 5.21416900 | -1.95433700 | -0.03667800 |
| C | 4.37159000 | -1.08329900 | -2.24810800 |
| H | 3.16811800 | -1.65839100 | -0.57313100 |
| H | 5.02106400 | -2.04876900 | 1.03554700 |
| H | 5.27139700 | -2.95805600 | -0.46662500 |
| H | 6.18828700 | -1.47173300 | -0.16402000 |
| H | 3.63983500 | -0.45720400 | -2.76738800 |
| H | 5.36754600 | -0.68766300 | -2.46747800 |
| H | 4.31983600 | -2.09206500 | -2.66665900 |
| C | 1.79115600 | 2.23537300 | 2.34227600 |
| C | 1.10870500 | 3.55632500 | 1.97266300 |
| C | 2.34306400 | 2.28456400 | 3.77293600 |
| H | 1.02456700 | 1.45248600 | 2.31282200 |
| H | 0.76383600 | 3.55112500 | 0.93550500 |
| H | 0.24510200 | 3.72148900 | 2.62260600 |
| H | 1.78808900 | 4.40411800 | 2.10174800 |
| H | 2.78966600 | 1.32881000 | 4.06130500 |
| H | 3.11262700 | 3.05821100 | 3.85908900 |
| H | 1.54236700 | 2.51963200 | 4.47953000 |
| C | -0.00921600 | -3.37861800 | -0.94217200 |

| | | | |
|---|---|---|---|
| C | -0.11578500 | -3.31448600 | -2.46900500 |
| C | 0.26767800 | -4.81259200 | -0.47157500 |
| H | 0.85262200 | -2.76748800 | -0.64924300 |
| H | -0.36135100 | -2.30577500 | -2.81228600 |
| H | 0.83614800 | -3.61055800 | -2.91915800 |
| H | -0.88458600 | -3.99682500 | -2.84305100 |
| H | 0.39505700 | -4.85629300 | 0.61395200 |
| H | -0.56556400 | -5.46908800 | -0.74140500 |
| H | 1.17517800 | -5.20013000 | -0.94309500 |
| C | -2.22860600 | -0.44000800 | 2.62582700 |
| C | -2.41313900 | -1.17870300 | 3.95866300 |
| C | -3.23913800 | 0.70302700 | 2.48821800 |
| H | -1.22183200 | -0.00374600 | 2.62961600 |
| H | -1.66440000 | -1.96482400 | 4.09514000 |
| H | -2.33295000 | -0.47713000 | 4.79387700 |
| H | -3.40310800 | -1.64440200 | 3.99897900 |
| H | -3.20754200 | 1.16975500 | 1.49919400 |
| H | -4.26411800 | 0.35194700 | 2.63685800 |
| H | -3.03697900 | 1.46269800 | 3.24987400 |
| H | -0.70688400 | 2.24771800 | -0.69548200 |
| C | -4.09307800 | 2.63988900 | -0.47298200 |
| C | -5.16583000 | 2.71977000 | 0.40013000 |
| C | -5.10010200 | 0.77538800 | -0.43115000 |
| N | -4.04933300 | 1.38233100 | -1.01219200 |
| H | -3.36572800 | 3.39926900 | -0.74283200 |
| H | -5.49779300 | 3.56299500 | 0.99657800 |
| H | -5.35178100 | -0.25951100 | -0.64900200 |
| N | -5.81767900 | 1.51758700 | 0.42687600 |

Frequencies

| | | |
|---|---|---|
| 13.2432 | 21.4880 | 26.7806 |
| 35.3937 | 37.8347 | 42.3385 |
| 49.1565 | 53.2372 | 60.0596 |
| 67.4429 | 70.7010 | 71.8936 |
| 75.2925 | 79.8607 | 83.8567 |
| 85.2767 | 94.3806 | 98.3573 |
| 102.0851 | 112.2034 | 115.6829 |
| 124.8487 | 128.4896 | 134.6515 |
| 142.8378 | 148.4160 | 152.3001 |
| 169.5862 | 175.2670 | 190.9839 |
| 216.2886 | 221.0540 | 226.0284 |
| 227.3896 | 235.2599 | 242.5135 |
| 245.6646 | 254.7003 | 258.9419 |
| 262.4105 | 263.5932 | 268.8152 |
| 277.5911 | 283.1009 | 286.8064 |

290.4449 298.0157 306.2094
313.7705 317.4025 328.4590
332.3547 338.0922 360.5446
389.7229 418.0704 424.6606
436.6842 445.8760 446.9902
458.6423 472.5064 490.8749
531.0634 539.6551 549.0564
560.5913 587.4748 594.1567
613.1814 623.9035 649.6053
650.0882 661.1446 682.7322
683.3717 689.8455 720.0479
735.5577 744.4113 762.7485
765.0884 772.2422 778.2597
784.2451 789.5089 803.8699
828.3398 829.9704 831.4371
833.5033 833.7082 834.8564
863.0772 896.2032 906.7459
911.5298 913.2570 917.9504
928.7618 932.5810 933.7271
935.8114 936.7046 938.0424
944.3636 950.7348 965.0668
966.7159 967.3203 970.1817
975.0941 976.0362 976.2945
976.5989 1015.5487 1020.6093
1022.5877 1035.1061 1050.4546
1071.3559 1074.0527 1081.7036
1084.2885 1100.0382 1109.1174
1112.6345 1123.5787 1128.1084
1128.3460 1143.1973 1144.4056
1147.3728 1148.0488 1155.4897
1158.6417 1168.6982 1180.4172
1183.1891 1188.8403 1193.3950
1194.0274 1210.4830 1211.4348
1223.9812 1243.9935 1248.3341
1268.8976 1279.8950 1293.6461
1296.8801 1304.1138 1304.4312
1315.3167 1327.5993 1329.2842
1336.4024 1337.2057 1340.9464
1342.3330 1350.6215 1357.9681
1367.6512 1369.1250 1374.1505
1389.3577 1392.2475 1402.9556
1405.6594 1406.2338 1407.3776
1412.2943 1414.1939 1414.6599
1417.9597 1425.9816 1426.4755

| | | |
|---|---|---|
| 1427.6002 | 1433.1340 | 1449.7311 |
| 1478.3231 | 1484.9284 | 1489.8188 |
| 1490.9196 | 1491.0558 | 1492.8982 |
| 1495.1691 | 1496.5668 | 1497.7658 |
| 1498.3256 | 1501.4379 | 1504.0514 |
| 1504.7657 | 1505.4276 | 1506.6618 |
| 1507.0146 | 1510.2773 | 1511.4594 |
| 1514.5625 | 1514.8101 | 1516.6641 |
| 1519.6941 | 1526.2918 | 1532.8683 |
| 1534.3674 | 1534.4808 | 1537.2542 |
| 1555.1533 | 1565.0645 | 1638.1733 |
| 1678.1532 | 1678.5967 | 1688.3815 |
| 1689.6762 | 1748.8865 | 1841.4498 |
| 3041.7471 | 3060.4285 | 3061.4662 |
| 3063.2132 | 3064.9367 | 3066.0592 |
| 3067.3988 | 3067.7756 | 3068.2752 |
| 3068.6560 | 3069.2589 | 3073.8273 |
| 3084.4814 | 3085.1125 | 3098.6140 |
| 3136.8138 | 3142.0823 | 3145.0801 |
| 3145.0997 | 3145.1413 | 3146.1892 |
| 3146.7608 | 3147.5660 | 3148.0553 |
| 3148.4178 | 3149.3068 | 3149.8258 |
| 3150.4988 | 3151.1015 | 3153.1406 |
| 3153.1883 | 3159.4978 | 3162.4893 |
| 3163.2082 | 3173.1120 | 3180.0462 |
| 3190.0412 | 3203.3302 | 3208.2369 |
| 3212.1683 | 3214.9160 | 3222.6710 |
| 3224.1297 | 3227.9092 | 3228.7200 |
| 3231.7007 | 3302.6557 | 3321.0980 |

**$TS_{III}$**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.783788 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.826441 |
| Thermal correction to Enthalpy= | | | 0.827385 |
| Thermal correction to Gibbs Free Energy= | | | 0.708441 |
| Sum of electronic and zero-point Energies= | | | -1768.676671 |
| Sum of electronic and thermal Energies= | | | -1768.634018 |
| Sum of electronic and thermal Enthalpies= | | | -1768.633074 |
| Sum of electronic and thermal Free Energies= | | | -1768.752018 |
| C | -0.22050400 | 0.46960700 | 0.74391100 |
| C | -1.43799700 | 0.22321100 | 1.62431300 |
| C | 0.19648800 | 1.76077800 | 0.42348700 |
| H | -1.24262500 | 0.65373500 | 2.60332000 |
| H | -2.33094500 | 0.69789400 | 1.21217200 |

| | | | |
|---|---|---|---|
| H | 0.95038600 | 1.88785900 | -0.33404900 |
| C | -0.12213900 | 3.00435700 | 1.07507700 |
| O | 0.37964500 | 4.08128300 | 0.77069800 |
| O | -1.07200800 | 2.93032100 | 2.04276900 |
| C | -1.43120000 | 4.17121200 | 2.65613700 |
| C | -2.49438500 | 3.86617600 | 3.68924700 |
| H | -1.79583500 | 4.85978200 | 1.88723500 |
| H | -0.54217500 | 4.62181900 | 3.10761900 |
| H | -2.80266400 | 4.78518600 | 4.19314800 |
| H | -3.37206700 | 3.41754300 | 3.21710700 |
| H | -2.11103000 | 3.17028900 | 4.43934200 |
| C | -0.04932500 | -0.45015400 | -0.42789500 |
| C | -0.56196800 | -1.72923200 | -2.19227600 |
| C | 0.76912400 | -1.50062900 | -2.22313400 |
| N | 1.07615900 | -0.71039800 | -1.13018600 |
| H | -1.21409800 | -2.27599600 | -2.85377400 |
| H | 1.53210800 | -1.81789400 | -2.91469100 |
| N | -1.05362800 | -1.07614800 | -1.07745800 |
| C | 2.42930600 | -0.22974100 | -0.92089500 |
| C | 3.31071000 | -1.02400400 | -0.17535100 |
| C | 2.81926700 | 0.94312200 | -1.58766900 |
| C | 4.61329800 | -0.54558000 | -0.01880700 |
| C | 4.13272200 | 1.37454100 | -1.39576400 |
| C | 5.01502300 | 0.64834100 | -0.60505500 |
| H | 5.32259400 | -1.12166200 | 0.56554600 |
| H | 4.47126700 | 2.28298700 | -1.88349100 |
| H | 6.03056600 | 1.00429600 | -0.46456800 |
| C | -2.47652200 | -1.01744800 | -0.82231600 |
| C | -3.18327400 | 0.10087500 | -1.28031500 |
| C | -3.07418000 | -2.10618400 | -0.17472100 |
| C | -4.56602900 | 0.09703200 | -1.08286300 |
| C | -4.45877300 | -2.06139700 | -0.00863600 |
| C | -5.19775700 | -0.97353000 | -0.46120100 |
| H | -5.15230100 | 0.94605300 | -1.42124500 |
| H | -4.96361000 | -2.88478500 | 0.48647000 |
| H | -6.27354300 | -0.95719200 | -0.32054500 |
| C | 1.91612700 | 1.67646700 | -2.57088900 |
| C | 2.31222500 | 1.29620100 | -4.00539900 |
| C | 1.94381700 | 3.20030500 | -2.40387900 |
| H | 0.88345600 | 1.34504300 | -2.41273400 |
| H | 2.26030500 | 0.21606600 | -4.16833000 |
| H | 1.64732600 | 1.78462900 | -4.72358400 |
| H | 3.33748200 | 1.61832700 | -4.21359500 |
| H | 1.68853900 | 3.51613200 | -1.38823800 |

| | | | |
|---|---|---|---|
| H | 2.92768200 | 3.60664900 | -2.65727600 |
| H | 1.22064900 | 3.64952100 | -3.09099600 |
| C | 2.92300900 | -2.39467500 | 0.35022800 |
| C | 3.57937000 | -2.71759400 | 1.69333100 |
| C | 3.29300400 | -3.46866900 | -0.68431000 |
| H | 1.83893000 | -2.40696900 | 0.49904500 |
| H | 3.44710900 | -1.90123600 | 2.40590400 |
| H | 3.12734300 | -3.61933600 | 2.11576200 |
| H | 4.64956600 | -2.91653700 | 1.57079800 |
| H | 2.78814300 | -3.31564500 | -1.64174000 |
| H | 4.37237400 | -3.46024300 | -0.86840000 |
| H | 3.01878500 | -4.45991600 | -0.31126000 |
| C | -2.51152000 | 1.28265600 | -1.95873300 |
| C | -2.84877900 | 2.60193800 | -1.25448600 |
| C | -2.88311300 | 1.33298600 | -3.44526500 |
| H | -1.42722300 | 1.15791200 | -1.88649900 |
| H | -2.60600800 | 2.55623900 | -0.18850400 |
| H | -2.26658100 | 3.41541700 | -1.69769900 |
| H | -3.90946300 | 2.85065100 | -1.36046900 |
| H | -2.59921600 | 0.40788000 | -3.95560800 |
| H | -3.96158600 | 1.47383200 | -3.57136500 |
| H | -2.37225000 | 2.16755800 | -3.93418400 |
| C | -2.26754200 | -3.28826500 | 0.33709400 |
| C | -2.41302700 | -4.49045600 | -0.60494800 |
| C | -2.65994000 | -3.67818700 | 1.76664800 |
| H | -1.20969900 | -2.99876700 | 0.35487700 |
| H | -2.08153400 | -4.25183700 | -1.61911500 |
| H | -1.81958300 | -5.33328100 | -0.23992700 |
| H | -3.45991400 | -4.80642300 | -0.65728400 |
| H | -2.62509300 | -2.82111800 | 2.44551900 |
| H | -3.66965100 | -4.09772300 | 1.80312000 |
| H | -1.97286500 | -4.44138100 | 2.14203400 |
| C | 2.23652500 | -0.14346100 | 3.80643200 |
| C | 1.92220600 | 0.42830300 | 2.59218700 |
| C | 0.80889200 | -1.39820800 | 2.86032100 |
| N | 1.52599800 | -1.30713400 | 3.97557500 |
| H | 2.92834000 | 0.21334800 | 4.55887500 |
| H | 2.24872800 | 1.34767700 | 2.12134600 |
| H | 0.11604700 | -2.20837400 | 2.65414700 |
| N | 1.01625900 | -0.38759300 | 1.98442900 |
| H | -1.61961500 | -0.84608900 | 1.73989400 |

Frequencies

| | | |
|---|---|---|
| -263.0786 | 16.1698 | 20.2700 |
| 25.7037 | 30.8062 | 44.7929 |

| | | |
|---|---|---|
| 48.9666 | 53.3308 | 55.9210 |
| 67.3434 | 72.0039 | 73.0882 |
| 84.1071 | 85.7867 | 92.8676 |
| 101.1841 | 103.4902 | 108.5514 |
| 114.2381 | 125.1667 | 128.1967 |
| 135.9500 | 142.2927 | 147.0044 |
| 154.8549 | 169.6768 | 179.3510 |
| 190.6512 | 205.8396 | 218.7552 |
| 224.3350 | 228.9964 | 232.8724 |
| 237.7364 | 243.7647 | 250.5282 |
| 256.5353 | 264.4073 | 266.6637 |
| 269.9315 | 281.4554 | 284.6169 |
| 286.9304 | 295.6432 | 301.6870 |
| 305.2520 | 310.9431 | 317.0011 |
| 327.9977 | 334.9958 | 343.4320 |
| 354.2614 | 363.6352 | 392.7061 |
| 421.2494 | 422.7718 | 428.6679 |
| 442.1403 | 447.6729 | 451.8313 |
| 468.8589 | 470.7967 | 497.2925 |
| 509.1063 | 531.1526 | 543.6547 |
| 567.4101 | 586.5473 | 593.6252 |
| 613.3278 | 624.4636 | 650.0321 |
| 653.8985 | 658.5198 | 666.4860 |
| 687.4491 | 692.1754 | 701.0778 |
| 709.9000 | 741.7051 | 761.9517 |
| 765.3719 | 766.5951 | 785.5691 |
| 792.2344 | 795.6214 | 800.5715 |
| 802.8831 | 818.4254 | 828.1889 |
| 833.0337 | 834.2431 | 836.6473 |
| 843.4257 | 873.8367 | 895.2862 |
| 902.6921 | 914.1856 | 914.6897 |
| 926.0848 | 928.1762 | 934.3361 |
| 936.1196 | 938.7367 | 941.2439 |
| 949.2006 | 951.7590 | 957.7088 |
| 966.0147 | 966.4813 | 967.5291 |
| 974.5636 | 975.1689 | 975.5302 |
| 977.8442 | 1012.3255 | 1016.0357 |
| 1023.0723 | 1031.9242 | 1056.8255 |
| 1073.9618 | 1076.3149 | 1084.9241 |
| 1087.4999 | 1092.0263 | 1108.1838 |
| 1117.2804 | 1122.2386 | 1132.1870 |
| 1135.5353 | 1141.9070 | 1144.3481 |
| 1145.2207 | 1146.3142 | 1155.6414 |
| 1160.3111 | 1165.7931 | 1181.9755 |

| | | |
|---|---|---|
| 1183.2016 | 1188.6537 | 1190.8706 |
| 1193.7502 | 1204.0243 | 1209.2076 |
| 1211.4935 | 1241.1373 | 1246.0003 |
| 1274.3751 | 1282.6775 | 1289.1613 |
| 1293.4076 | 1293.8986 | 1303.0700 |
| 1317.4173 | 1318.6613 | 1327.0406 |
| 1327.9379 | 1329.5056 | 1338.9787 |
| 1345.7456 | 1347.5428 | 1358.5176 |
| 1362.0865 | 1372.6465 | 1381.8063 |
| 1388.6846 | 1393.5312 | 1398.2695 |
| 1403.3033 | 1405.5448 | 1408.0621 |
| 1408.5874 | 1409.4443 | 1413.2193 |
| 1421.5957 | 1428.6733 | 1429.5204 |
| 1431.6851 | 1438.7165 | 1441.4530 |
| 1480.7651 | 1487.2200 | 1487.9552 |
| 1490.1877 | 1490.6688 | 1491.7876 |
| 1492.4510 | 1494.3397 | 1497.3096 |
| 1497.5580 | 1498.2077 | 1500.8962 |
| 1504.1354 | 1505.6994 | 1506.7951 |
| 1507.8810 | 1508.4883 | 1509.7119 |
| 1513.7917 | 1517.5741 | 1520.3778 |
| 1522.1002 | 1525.2375 | 1530.4532 |
| 1533.5176 | 1535.1036 | 1539.3759 |
| 1541.3943 | 1546.7295 | 1581.5463 |
| 1645.3713 | 1677.1756 | 1679.5564 |
| 1683.7286 | 1688.7718 | 1748.0624 |
| 3060.3914 | 3060.9644 | 3061.2846 |
| 3062.2592 | 3064.0618 | 3064.7571 |
| 3065.7177 | 3067.9447 | 3076.5689 |
| 3083.6164 | 3088.6754 | 3089.0083 |
| 3096.9335 | 3097.9299 | 3111.2653 |
| 3127.2599 | 3135.7531 | 3141.0046 |
| 3141.7317 | 3143.0475 | 3145.1634 |
| 3145.6118 | 3146.2991 | 3148.8045 |
| 3148.8339 | 3150.0374 | 3152.0258 |
| 3152.1467 | 3153.2865 | 3153.8344 |
| 3156.7529 | 3160.1257 | 3166.8896 |
| 3179.6608 | 3181.1800 | 3207.0757 |
| 3207.7535 | 3211.6685 | 3214.1056 |
| 3219.8100 | 3224.5733 | 3229.2906 |
| 3234.3570 | 3239.9355 | 3256.7313 |
| 3305.5500 | 3324.9533 | 3353.0715 |

**III**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.787246 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.828804 |
| Thermal correction to Enthalpy= | | | 0.829748 |
| Thermal correction to Gibbs Free Energy= | | | 0.717431 |
| Sum of electronic and zero-point Energies= | | | -1768.689267 |
| Sum of electronic and thermal Energies= | | | -1768.647708 |
| Sum of electronic and thermal Enthalpies= | | | -1768.646764 |
| Sum of electronic and thermal Free Energies= | | | -1768.759082 |
| C | -0.08361500 | -0.00535800 | 1.24831200 |
| C | -0.80138000 | -1.24872000 | 1.80188600 |
| C | -0.84993000 | 1.26847700 | 1.35326600 |
| H | -0.93582000 | -1.10962100 | 2.87542900 |
| H | -1.78275900 | -1.34957900 | 1.35423900 |
| H | -0.32480600 | 2.17029200 | 1.06155700 |
| C | -2.17072700 | 1.50899000 | 1.74726600 |
| O | -2.70129500 | 2.63178800 | 1.84189200 |
| O | -2.94492700 | 0.39815000 | 2.03720500 |
| C | -4.27569700 | 0.66849300 | 2.45116100 |
| C | -4.91887800 | -0.66399700 | 2.77759500 |
| H | -4.81632000 | 1.18592400 | 1.65066400 |
| H | -4.27074800 | 1.33328900 | 3.32200600 |
| H | -5.94876100 | -0.51969200 | 3.11498200 |
| H | -4.92759600 | -1.30633700 | 1.89242700 |
| H | -4.36318600 | -1.17507900 | 3.56901300 |
| C | 0.25147500 | -0.29604300 | -0.23488400 |
| C | -0.10873800 | -0.83282000 | -2.38077200 |
| C | 1.22110300 | -0.68387900 | -2.21613000 |
| N | 1.43825400 | -0.34879600 | -0.88609100 |
| H | -0.69950600 | -1.07247200 | -3.24963700 |
| H | 2.04151100 | -0.74842700 | -2.91160600 |
| N | -0.69883500 | -0.57854400 | -1.15821500 |
| C | 2.80237200 | -0.02311800 | -0.49197400 |
| C | 3.71843900 | -1.07415000 | -0.35294400 |
| C | 3.17250200 | 1.33022800 | -0.45837500 |
| C | 5.06175900 | -0.73130300 | -0.18692800 |
| C | 4.52735700 | 1.61597200 | -0.28589400 |
| C | 5.46437700 | 0.59714300 | -0.16030500 |
| H | 5.80001400 | -1.51860100 | -0.07249500 |
| H | 4.85282100 | 2.65011300 | -0.25384300 |
| H | 6.51423600 | 0.84096200 | -0.03394200 |
| C | -2.13124800 | -0.36818900 | -1.06431000 |
| C | -2.59795600 | 0.92809700 | -1.33971000 |
| C | -2.97056500 | -1.45948300 | -0.82347400 |
| C | -3.97449000 | 1.12989300 | -1.26562100 |

| | | | |
|---|---|---|---|
| C | -4.34535000 | -1.20671300 | -0.78823600 |
| C | -4.83954500 | 0.07574100 | -0.98338600 |
| H | -4.37605400 | 2.12212000 | -1.44438400 |
| H | -5.03458800 | -2.02664100 | -0.61069400 |
| H | -5.90925400 | 0.25475200 | -0.93516100 |
| C | 2.15880800 | 2.44477700 | -0.65605400 |
| C | 1.95076400 | 2.74038200 | -2.14923300 |
| C | 2.53199000 | 3.73138200 | 0.08373600 |
| H | 1.20326600 | 2.10352200 | -0.24496100 |
| H | 1.59751200 | 1.86289900 | -2.69898900 |
| H | 1.20973600 | 3.53692400 | -2.27458400 |
| H | 2.89056200 | 3.07243500 | -2.60239600 |
| H | 2.81882900 | 3.52899900 | 1.11892600 |
| H | 3.36186100 | 4.24898000 | -0.40759000 |
| H | 1.67591500 | 4.41199100 | 0.08508900 |
| C | 3.30839500 | -2.53785100 | -0.37640300 |
| C | 3.97225100 | -3.32921700 | 0.76015900 |
| C | 3.64860800 | -3.19162000 | -1.72313100 |
| H | 2.22101500 | -2.59029600 | -0.23975000 |
| H | 3.91321600 | -2.79914100 | 1.71417000 |
| H | 3.49229200 | -4.30649200 | 0.86249200 |
| H | 5.02957800 | -3.50825500 | 0.54211700 |
| H | 3.12875400 | -2.71618800 | -2.55807300 |
| H | 4.72480800 | -3.12504800 | -1.91209500 |
| H | 3.37088300 | -4.24950300 | -1.70858400 |
| C | -1.67406400 | 2.04243200 | -1.80446600 |
| C | -2.02354100 | 3.41083000 | -1.21619800 |
| C | -1.68100700 | 2.10955000 | -3.33984000 |
| H | -0.65658200 | 1.80176400 | -1.47860600 |
| H | -2.14235600 | 3.35978300 | -0.13099600 |
| H | -1.22821900 | 4.12232400 | -1.46376600 |
| H | -2.94895400 | 3.80282400 | -1.65287800 |
| H | -1.38373000 | 1.16154300 | -3.79712300 |
| H | -2.68351300 | 2.35862100 | -3.70335000 |
| H | -0.99091900 | 2.88564100 | -3.68580500 |
| C | -2.44342000 | -2.87835600 | -0.68613900 |
| C | -2.62011300 | -3.62947100 | -2.01345900 |
| C | -3.11348000 | -3.65367100 | 0.45280800 |
| H | -1.37049900 | -2.82492200 | -0.47170000 |
| H | -2.10339200 | -3.12431900 | -2.83432200 |
| H | -2.22426900 | -4.64588600 | -1.93222500 |
| H | -3.68133700 | -3.69500700 | -2.27421300 |
| H | -3.06198900 | -3.11197700 | 1.40136400 |
| H | -4.16718400 | -3.85036400 | 0.23263000 |

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|---|---|---|---|
| H | -2.62108300 | -4.62149100 | 0.58184200 |
| C | 2.96603200 | 0.80662000 | 3.07899700 |
| C | 1.79417900 | 1.21960100 | 2.50299200 |
| C | 2.04909100 | -0.94441400 | 2.29000000 |
| N | 3.11845800 | -0.55247300 | 2.94413900 |
| H | 3.69859200 | 1.41253600 | 3.59306700 |
| H | 1.31071600 | 2.17968000 | 2.44488900 |
| H | 1.83506600 | -1.96583200 | 2.00995900 |
| N | 1.21300900 | 0.08660900 | 1.98629800 |
| H | -0.21875700 | -2.15523200 | 1.61933000 |

Frequencies

| | | |
|---|---|---|
| 30.9851 | 36.7110 | 40.3268 |
| 51.8539 | 57.7136 | 72.0370 |
| 75.6002 | 83.9230 | 85.9088 |
| 94.4121 | 99.2216 | 101.3470 |
| 105.0422 | 109.4706 | 117.4201 |
| 124.7440 | 127.0594 | 131.1037 |
| 136.1225 | 139.7783 | 143.5507 |
| 158.6190 | 162.3145 | 170.5083 |
| 183.7123 | 209.2233 | 211.8667 |
| 219.1429 | 224.2918 | 231.2346 |
| 237.4033 | 245.5349 | 250.9339 |
| 261.5129 | 268.1096 | 271.3035 |
| 277.1744 | 281.8535 | 287.5633 |
| 290.3831 | 290.9969 | 299.0433 |
| 305.1871 | 306.6418 | 311.6839 |
| 315.6053 | 316.8902 | 329.2735 |
| 338.6238 | 354.3734 | 366.7549 |
| 370.0569 | 389.5490 | 406.9086 |
| 420.4181 | 432.6191 | 441.7510 |
| 449.6726 | 451.9791 | 468.4881 |
| 477.5154 | 487.2732 | 508.9878 |
| 530.8734 | 545.4015 | 566.7452 |
| 587.3861 | 595.9284 | 606.4163 |
| 622.8048 | 647.9780 | 648.8476 |
| 651.3755 | 652.3360 | 655.4988 |
| 689.7970 | 692.2185 | 699.1659 |
| 721.8826 | 742.0353 | 753.6825 |
| 755.0513 | 769.0530 | 773.2688 |
| 780.2360 | 789.7096 | 802.4382 |
| 807.6516 | 818.6170 | 823.1312 |
| 827.4319 | 832.4176 | 834.8215 |
| 854.1928 | 865.2196 | 889.5942 |
| 912.5744 | 917.5751 | 921.0571 |

| | | |
|---|---|---|
| 923.1325 | 929.2230 | 934.6769 |
| 937.1544 | 938.2488 | 940.2331 |
| 942.0122 | 944.9448 | 964.7045 |
| 967.3092 | 971.0449 | 977.1532 |
| 977.4977 | 977.8309 | 982.0989 |
| 1003.1301 | 1004.9220 | 1008.8707 |
| 1012.8032 | 1033.1972 | 1074.3712 |
| 1075.8201 | 1084.7940 | 1090.1351 |
| 1105.0538 | 1111.7541 | 1117.5655 |
| 1118.8074 | 1128.9300 | 1131.7237 |
| 1139.9577 | 1144.7192 | 1147.9035 |
| 1148.9866 | 1159.6468 | 1161.2148 |
| 1169.2656 | 1177.7815 | 1181.1055 |
| 1183.1635 | 1192.1284 | 1193.7702 |
| 1194.0036 | 1209.6474 | 1212.9454 |
| 1213.9411 | 1235.2526 | 1242.2764 |
| 1255.1454 | 1280.9002 | 1289.8203 |
| 1293.7704 | 1295.1955 | 1299.9216 |
| 1306.1734 | 1315.6738 | 1319.6694 |
| 1323.0701 | 1327.8317 | 1335.8188 |
| 1342.1807 | 1345.7065 | 1354.8616 |
| 1370.0641 | 1374.1001 | 1382.3595 |
| 1391.1995 | 1393.5908 | 1395.6902 |
| 1400.7319 | 1409.2821 | 1410.2843 |
| 1411.2348 | 1411.9133 | 1416.1344 |
| 1423.6860 | 1429.0998 | 1431.1107 |
| 1433.4839 | 1434.9645 | 1435.7198 |
| 1464.0276 | 1476.6193 | 1488.5126 |
| 1489.5937 | 1491.7561 | 1492.6530 |
| 1493.6196 | 1494.2313 | 1494.8865 |
| 1498.0064 | 1499.2394 | 1499.9680 |
| 1503.9884 | 1505.1847 | 1509.2271 |
| 1509.6533 | 1511.1933 | 1512.2576 |
| 1513.0961 | 1519.0341 | 1520.8418 |
| 1522.0639 | 1523.7154 | 1526.8225 |
| 1529.4721 | 1533.9671 | 1535.2304 |
| 1538.7315 | 1553.2872 | 1591.5180 |
| 1651.7136 | 1677.2674 | 1679.8298 |
| 1685.1668 | 1686.2601 | 1698.9257 |
| 3051.5851 | 3058.5621 | 3061.2148 |
| 3066.1478 | 3069.4951 | 3070.2067 |
| 3070.3301 | 3071.2591 | 3072.5299 |
| 3073.0437 | 3076.0312 | 3092.0188 |
| 3094.3867 | 3110.5408 | 3112.3354 |

| | | |
|---|---|---|
| 3120.1550 | 3125.1929 | 3140.3799 |
| 3142.7353 | 3144.9790 | 3146.1893 |
| 3148.0912 | 3148.7518 | 3149.7016 |
| 3150.3821 | 3152.3447 | 3153.8058 |
| 3155.2253 | 3157.0870 | 3161.8211 |
| 3161.9607 | 3163.9819 | 3167.1175 |
| 3168.4587 | 3181.0950 | 3201.0349 |
| 3209.3838 | 3214.8890 | 3227.4232 |
| 3227.6775 | 3230.3484 | 3236.8774 |
| 3263.5125 | 3275.0365 | 3287.0047 |
| 3318.0343 | 3327.0165 | 3343.0873 |

**E-TS$_{IV}$**

Zero-point correction= 0.784205 (Hartree/Particle)
Thermal correction to Energy= 0.826029
Thermal correction to Enthalpy= 0.826974
Thermal correction to Gibbs Free Energy= 0.713406
Sum of electronic and zero-point Energies= -1768.672403
Sum of electronic and thermal Energies= -1768.630579
Sum of electronic and thermal Enthalpies= -1768.629635
Sum of electronic and thermal Free Energies= -1768.743203

| | | | |
|---|---|---|---|
| C | 0.22924900 | -0.52920600 | 1.51206500 |
| C | 0.83218000 | 0.70467200 | 2.15170700 |
| C | 1.00086100 | -1.67265800 | 1.27962300 |
| H | 1.08274000 | 0.46833900 | 3.19045700 |
| H | 1.74788000 | 0.97745900 | 1.63839300 |
| H | 0.50042500 | -2.57926100 | 0.95954500 |
| C | 2.41479100 | -1.84936300 | 1.43397200 |
| O | 2.99356900 | -2.92415700 | 1.27651600 |
| O | 3.11868700 | -0.75448800 | 1.83432000 |
| C | 4.49802800 | -0.97751000 | 2.12441200 |
| C | 5.04176400 | 0.30299900 | 2.72159200 |
| H | 5.02315100 | -1.24827100 | 1.20245400 |
| H | 4.59096500 | -1.81816500 | 2.81871400 |
| H | 6.09724800 | 0.18122100 | 2.97780100 |
| H | 4.94810600 | 1.12631900 | 2.00863300 |
| H | 4.49166800 | 0.56615400 | 3.62907500 |
| C | -0.32260000 | 0.36987800 | -0.27710000 |
| C | 0.02732300 | 1.38050700 | -2.28023700 |
| C | -1.30567700 | 1.22624200 | -2.13672300 |
| N | -1.50126200 | 0.59758400 | -0.91178500 |
| H | 0.61691100 | 1.79921400 | -3.08007300 |
| H | -2.12927800 | 1.46504200 | -2.79019500 |
| N | 0.61006000 | 0.84110300 | -1.14193700 |

| | | | |
|---|---|---|---|
| C | -2.82725600 | 0.17321600 | -0.52529200 |
| C | -3.75998900 | 1.15450100 | -0.16545500 |
| C | -3.15185000 | -1.19085100 | -0.62444900 |
| C | -5.07780500 | 0.74617200 | 0.04793500 |
| C | -4.47866500 | -1.54742600 | -0.38023200 |
| C | -5.43595400 | -0.58942400 | -0.06395900 |
| H | -5.82705900 | 1.48267500 | 0.32275000 |
| H | -4.77139700 | -2.58982700 | -0.44053100 |
| H | -6.46388300 | -0.89110100 | 0.11049200 |
| C | 2.03768300 | 0.64751500 | -1.05197000 |
| C | 2.55923000 | -0.56613500 | -1.53420900 |
| C | 2.83920700 | 1.69242300 | -0.57825600 |
| C | 3.94441100 | -0.72432700 | -1.49577200 |
| C | 4.22247600 | 1.49373500 | -0.58578000 |
| C | 4.76828100 | 0.29654800 | -1.03056500 |
| H | 4.38484600 | -1.65390000 | -1.84183900 |
| H | 4.87909700 | 2.28679600 | -0.24079300 |
| H | 5.84514600 | 0.15717800 | -1.01877800 |
| C | -2.11794100 | -2.23335200 | -1.02712600 |
| C | -1.86802000 | -2.20390700 | -2.54306900 |
| C | -2.49597600 | -3.65313400 | -0.60110100 |
| H | -1.17780400 | -1.98097400 | -0.52158600 |
| H | -1.48930800 | -1.23646800 | -2.88494900 |
| H | -1.13274900 | -2.96854300 | -2.81688500 |
| H | -2.79788700 | -2.41841300 | -3.08020300 |
| H | -2.79394500 | -3.68995100 | 0.44972300 |
| H | -3.31804900 | -4.04639300 | -1.20845600 |
| H | -1.63745700 | -4.31591200 | -0.74381300 |
| C | -3.37737500 | 2.61109200 | 0.04149700 |
| C | -3.91796500 | 3.14326600 | 1.37662600 |
| C | -3.87678900 | 3.49436300 | -1.10920600 |
| H | -2.28272300 | 2.67435500 | 0.07225900 |
| H | -3.70588500 | 2.45909900 | 2.20293500 |
| H | -3.47234000 | 4.11697000 | 1.59867800 |
| H | -5.00254500 | 3.28129700 | 1.33233300 |
| H | -3.45420200 | 3.19352900 | -2.07100000 |
| H | -4.96728300 | 3.43201500 | -1.18650200 |
| H | -3.60859600 | 4.53981400 | -0.93066500 |
| C | 1.66486000 | -1.62967300 | -2.15220700 |
| C | 2.14118300 | -3.06171200 | -1.90031000 |
| C | 1.53677800 | -1.39165000 | -3.66513700 |
| H | 0.67179300 | -1.53041000 | -1.70041200 |
| H | 2.34550600 | -3.24272600 | -0.84334800 |
| H | 1.36853900 | -3.76032400 | -2.23841800 |

| | | | |
|---|---|---|---|
| H | 3.04674900 | -3.28545200 | -2.47499500 |
| H | 1.12267500 | -0.40730800 | -3.89689100 |
| H | 2.52066900 | -1.46836500 | -4.14036300 |
| H | 0.88323300 | -2.14776800 | -4.11155300 |
| C | 2.24861600 | 3.01689400 | -0.12286100 |
| C | 2.33805100 | 4.05353100 | -1.25142100 |
| C | 2.91931100 | 3.55985800 | 1.14331200 |
| H | 1.18921700 | 2.85213100 | 0.10429800 |
| H | 1.81117300 | 3.71909900 | -2.14902600 |
| H | 1.90125500 | 5.00438300 | -0.93210400 |
| H | 3.38446000 | 4.23171400 | -1.52040700 |
| H | 2.92838700 | 2.82016000 | 1.94896700 |
| H | 3.95313600 | 3.86217000 | 0.94913900 |
| H | 2.38166700 | 4.44479200 | 1.49509300 |
| C | -2.90526100 | -1.71945900 | 2.84554500 |
| C | -1.66472000 | -2.00152300 | 2.34614500 |
| C | -2.03988400 | 0.15798000 | 2.34265700 |
| N | -3.13267500 | -0.36190700 | 2.84420700 |
| H | -3.64033000 | -2.41922300 | 3.21721800 |
| H | -1.12681100 | -2.92786800 | 2.24087900 |
| H | -1.87421900 | 1.21167800 | 2.17008000 |
| N | -1.10830400 | -0.78378100 | 2.01175000 |
| H | 0.14099400 | 1.54669500 | 2.13363500 |

Frequencies

| | | |
|---|---|---|
| -257.0535 | 23.9769 | 35.7049 |
| 43.5567 | 49.1128 | 57.3951 |
| 62.0186 | 73.9440 | 77.1891 |
| 83.4487 | 88.2614 | 94.5247 |
| 100.1328 | 102.0649 | 112.2791 |
| 114.6516 | 121.5338 | 125.6458 |
| 127.3277 | 135.1775 | 137.6576 |
| 141.9437 | 154.6220 | 165.5248 |
| 169.0499 | 177.5066 | 191.7782 |
| 202.5910 | 205.5721 | 219.1805 |
| 226.6509 | 234.2604 | 238.5211 |
| 242.1477 | 251.5126 | 256.8988 |
| 259.5198 | 262.8244 | 267.0314 |
| 273.5744 | 281.4024 | 289.3055 |
| 296.6720 | 303.7244 | 307.2250 |
| 312.8622 | 315.5221 | 319.1948 |
| 322.9195 | 336.2544 | 346.7492 |
| 353.4798 | 384.5329 | 395.2126 |
| 417.2993 | 424.7537 | 427.0138 |
| 443.2698 | 448.2127 | 449.9448 |

| | | |
|---|---|---|
| 469.2095 | 481.9935 | 483.8836 |
| 525.6729 | 533.2247 | 534.3980 |
| 567.6169 | 581.7642 | 587.5592 |
| 598.5567 | 622.8165 | 646.6246 |
| 650.8938 | 651.3621 | 652.7242 |
| 687.6502 | 694.0352 | 698.2743 |
| 712.1666 | 735.8785 | 744.1203 |
| 751.5233 | 761.4682 | 764.1649 |
| 777.5297 | 784.7944 | 789.9211 |
| 798.2435 | 813.1089 | 826.2670 |
| 827.4756 | 832.4599 | 832.6140 |
| 876.4192 | 885.3498 | 888.4036 |
| 897.7702 | 913.1030 | 915.9899 |
| 920.5495 | 929.6925 | 930.0771 |
| 935.6530 | 937.3151 | 940.2560 |
| 941.1650 | 945.2117 | 962.3482 |
| 964.2020 | 966.7883 | 973.5021 |
| 973.9027 | 978.0380 | 980.3449 |
| 981.0578 | 1007.0952 | 1007.6893 |
| 1018.3492 | 1041.6589 | 1056.7150 |
| 1072.9173 | 1075.9415 | 1084.4584 |
| 1089.8103 | 1100.9621 | 1103.1968 |
| 1109.3810 | 1119.7452 | 1131.6051 |
| 1138.6985 | 1141.5229 | 1144.9893 |
| 1145.9634 | 1148.8216 | 1151.9449 |
| 1159.9532 | 1162.8105 | 1175.2521 |
| 1178.1331 | 1179.9889 | 1184.8263 |
| 1190.4748 | 1190.6881 | 1210.1965 |
| 1210.7191 | 1238.9256 | 1269.7003 |
| 1276.6338 | 1290.7331 | 1293.3582 |
| 1296.9180 | 1298.5756 | 1302.8113 |
| 1315.6984 | 1321.3610 | 1322.8186 |
| 1325.0465 | 1334.9915 | 1336.1198 |
| 1337.3875 | 1342.9389 | 1347.7205 |
| 1352.2660 | 1366.5996 | 1372.8509 |
| 1382.1177 | 1390.0052 | 1391.5633 |
| 1401.5320 | 1406.0541 | 1408.4169 |
| 1409.0394 | 1410.8007 | 1419.1639 |
| 1421.2141 | 1426.8721 | 1428.4241 |
| 1429.4300 | 1432.5752 | 1439.2225 |
| 1447.3710 | 1459.7664 | 1479.9124 |
| 1487.9856 | 1489.9129 | 1491.6187 |
| 1492.9809 | 1495.6585 | 1496.2764 |
| 1497.3572 | 1497.9366 | 1499.0564 |

| | | |
|---|---|---|
| 1502.5532 | 1505.6569 | 1507.1763 |
| 1507.9237 | 1509.9794 | 1511.7429 |
| 1517.2971 | 1517.7575 | 1518.8733 |
| 1519.5551 | 1525.9028 | 1526.7307 |
| 1529.5437 | 1531.9545 | 1534.7848 |
| 1540.2670 | 1556.6907 | 1604.3731 |
| 1645.2099 | 1679.6676 | 1682.5927 |
| 1683.6525 | 1687.0069 | 1730.9144 |
| 3056.3754 | 3059.2379 | 3061.2480 |
| 3061.2919 | 3063.2473 | 3064.3161 |
| 3065.2415 | 3066.1900 | 3074.9740 |
| 3077.0613 | 3079.5663 | 3084.0314 |
| 3090.5691 | 3099.0317 | 3112.8405 |
| 3124.5133 | 3129.0603 | 3131.0559 |
| 3135.5010 | 3141.5412 | 3142.3971 |
| 3143.6720 | 3145.5830 | 3146.8365 |
| 3149.5750 | 3153.2414 | 3154.2880 |
| 3154.7617 | 3157.0080 | 3157.1060 |
| 3158.4984 | 3163.7760 | 3167.1631 |
| 3176.1301 | 3180.1720 | 3198.5071 |
| 3200.5190 | 3214.2316 | 3214.2906 |
| 3218.0781 | 3228.3487 | 3233.9988 |
| 3255.5765 | 3281.3119 | 3288.1927 |
| 3296.6426 | 3319.8422 | 3322.5575 |

**Z-TS$_{IV}$**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.784235 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.826025 |
| Thermal correction to Enthalpy= | | | 0.826970 |
| Thermal correction to Gibbs Free Energy= | | | 0.713068 |
| Sum of electronic and zero-point Energies= | | | -1768.668284 |
| Sum of electronic and thermal Energies= | | | -1768.626493 |
| Sum of electronic and thermal Enthalpies= | | | -1768.625549 |
| Sum of electronic and thermal Free Energies= | | | -1768.739450 |
| C | 0.22234200 | 0.56027400 | -1.70956200 |
| C | 0.85421000 | -0.50297500 | -2.59101500 |
| C | 0.96777600 | 1.73501600 | -1.60511100 |
| H | 0.69774700 | -0.21519500 | -3.63531800 |
| H | 1.92621000 | -0.55852200 | -2.39648200 |
| H | 1.96816200 | 1.70994200 | -2.02088100 |
| C | 0.63681000 | 2.96626400 | -0.95191700 |
| O | 1.19310400 | 4.04225400 | -1.13888500 |
| O | -0.35988500 | 2.84806500 | -0.02123000 |
| C | -0.78730300 | 4.06627700 | 0.59669100 |

| | | | |
|---|---|---|---|
| C | -1.67973200 | 4.87643500 | -0.32709500 |
| H | 0.09078200 | 4.64268300 | 0.89786400 |
| H | -1.32896900 | 3.74892700 | 1.49211200 |
| H | -2.04696400 | 5.76793400 | 0.18866900 |
| H | -1.11792500 | 5.19148400 | -1.20922000 |
| H | -2.54031900 | 4.28124700 | -0.64452900 |
| C | 0.22281400 | -0.40983300 | 0.13733500 |
| C | 1.17781500 | -0.77716500 | 2.16741800 |
| C | -0.15599300 | -0.90356600 | 2.32549600 |
| N | -0.72658800 | -0.66504100 | 1.08081500 |
| H | 1.99307500 | -0.90951300 | 2.85987900 |
| H | -0.75108600 | -1.17117800 | 3.18413400 |
| N | 1.39074600 | -0.46688000 | 0.83074600 |
| C | -2.08785600 | -1.07355200 | 0.81556300 |
| C | -2.29062500 | -2.42926900 | 0.51632100 |
| C | -3.13740200 | -0.14681400 | 0.90464600 |
| C | -3.59592800 | -2.84157700 | 0.23730400 |
| C | -4.42230200 | -0.61146200 | 0.62302900 |
| C | -4.64972400 | -1.93956200 | 0.27888900 |
| H | -3.78624800 | -3.88186900 | -0.01176500 |
| H | -5.25922500 | 0.07660000 | 0.65878600 |
| H | -5.65709700 | -2.27283800 | 0.05076900 |
| C | 2.72684800 | -0.40562700 | 0.28673200 |
| C | 3.50430600 | 0.73778400 | 0.51989200 |
| C | 3.22290900 | -1.54040400 | -0.38062800 |
| C | 4.82176900 | 0.72466400 | 0.05270200 |
| C | 4.54255200 | -1.49748000 | -0.83292400 |
| C | 5.33655000 | -0.37710200 | -0.61647100 |
| H | 5.45019100 | 1.59441500 | 0.21250000 |
| H | 4.95691900 | -2.35232500 | -1.35655400 |
| H | 6.36155500 | -0.36364100 | -0.97302200 |
| C | -2.88468800 | 1.29058600 | 1.32259700 |
| C | -2.73478400 | 1.38782600 | 2.84940900 |
| C | -3.98207200 | 2.25358200 | 0.86804100 |
| H | -1.94357700 | 1.59697400 | 0.85457200 |
| H | -1.88531900 | 0.81133600 | 3.22076500 |
| H | -2.58746000 | 2.43011000 | 3.15097400 |
| H | -3.64128500 | 1.01994300 | 3.34214300 |
| H | -4.15579000 | 2.18392900 | -0.20892600 |
| H | -4.92536200 | 2.06150400 | 1.39055000 |
| H | -3.68970100 | 3.28070900 | 1.10690100 |
| C | -1.16482800 | -3.45409500 | 0.51495300 |
| C | -0.98793900 | -4.11611500 | -0.85549500 |
| C | -1.40051500 | -4.51229800 | 1.60024500 |

| | | | |
|---|---|---|---|
| H | -0.22673300 | -2.94826400 | 0.76174800 |
| H | -0.72678500 | -3.38620100 | -1.62937000 |
| H | -0.18448400 | -4.85910300 | -0.81324900 |
| H | -1.90153100 | -4.62895300 | -1.17144400 |
| H | -1.51707700 | -4.04677500 | 2.58290200 |
| H | -2.30202700 | -5.09707800 | 1.39196200 |
| H | -0.55287900 | -5.20305800 | 1.64350000 |
| C | 2.97505300 | 1.94829300 | 1.27161600 |
| C | 3.50289100 | 3.26493200 | 0.69038000 |
| C | 3.35184100 | 1.87620800 | 2.75966000 |
| H | 1.88159500 | 1.94599500 | 1.18322400 |
| H | 3.37788800 | 3.30973100 | -0.39244900 |
| H | 2.94898400 | 4.10433500 | 1.11961200 |
| H | 4.56015700 | 3.40628800 | 0.93742800 |
| H | 2.92656300 | 1.00423000 | 3.25994500 |
| H | 4.44066300 | 1.83098000 | 2.86840900 |
| H | 2.99570900 | 2.77028400 | 3.28002800 |
| C | 2.38188200 | -2.79396200 | -0.57149300 |
| C | 2.51207300 | -3.71723400 | 0.64818800 |
| C | 2.71825100 | -3.55740100 | -1.85428400 |
| H | 1.33613000 | -2.48226600 | -0.64629200 |
| H | 2.19869400 | -3.21682700 | 1.56924900 |
| H | 1.89103500 | -4.61024100 | 0.51715600 |
| H | 3.55123900 | -4.04023300 | 0.77007300 |
| H | 2.72479300 | -2.89823500 | -2.72737200 |
| H | 3.69408100 | -4.04840900 | -1.78849500 |
| H | 1.97138500 | -4.33904300 | -2.02034400 |
| C | -3.17868400 | 1.28997800 | -2.62324800 |
| C | -1.94766300 | 1.75005900 | -2.25349200 |
| C | -2.03257700 | -0.43986600 | -2.14749000 |
| N | -3.22465800 | -0.08654300 | -2.55506300 |
| H | -4.03068800 | 1.87271800 | -2.94432100 |
| H | -1.52934400 | 2.74085900 | -2.22920800 |
| H | -1.71294800 | -1.45493000 | -1.96583600 |
| N | -1.20733300 | 0.63049000 | -1.92723300 |
| H | 0.41789600 | -1.49012500 | -2.43601900 |

Frequencies

| | | |
|---|---|---|
| -280.3849 | 23.0588 | 32.8599 |
| 45.4456 | 49.1411 | 56.3845 |
| 59.5104 | 63.6469 | 67.7021 |
| 72.3667 | 77.1142 | 81.4174 |
| 88.7201 | 100.2808 | 103.5198 |
| 109.8306 | 121.1280 | 127.3314 |
| 137.2946 | 140.9329 | 153.3383 |

157.2153 160.3043 171.4400
174.7240 187.3998 193.7730
209.0299 213.9412 221.2352
225.0029 233.9868 242.9001
245.6071 252.2375 257.1037
269.4239 270.5013 281.0413
283.8168 287.4119 293.0076
295.4153 306.7283 307.2279
310.6293 314.8787 323.2360
334.4823 345.9008 349.1100
355.4250 366.4128 400.0638
416.8493 422.7204 438.5890
444.6850 446.4305 450.5415
463.9105 477.3424 479.3012
533.1606 538.6673 552.9171
570.4240 582.3121 584.8747
600.2558 621.6945 637.0844
646.3042 649.4651 650.9222
656.1020 684.8076 689.7227
693.8374 719.9530 726.4703
745.2822 746.3648 762.4624
781.3241 782.7104 790.0793
797.7617 810.6319 826.1559
827.1583 833.1012 833.7946
854.9634 877.4233 885.8816
898.9726 911.5410 914.9783
916.5233 925.7940 929.0208
932.2008 936.2076 942.4408
943.5153 950.6244 960.8825
963.2682 964.3863 972.8563
974.8247 975.6605 978.7433
980.8917 1010.3948 1012.5219
1023.7893 1048.7449 1053.7792
1073.8387 1077.1260 1085.6612
1090.0653 1097.9401 1101.5533
1108.0933 1113.9541 1120.7578
1134.6667 1139.0113 1140.9204
1147.0848 1148.2076 1150.6696
1153.2733 1161.5224 1167.9935
1177.5107 1179.5660 1188.9861
1192.0101 1202.0737 1209.3295
1209.8771 1241.8031 1245.4318
1279.6052 1284.0375 1289.3437
1289.6261 1298.4967 1304.5194

| | | |
|---|---|---|
| 1316.7816 | 1320.7593 | 1326.9235 |
| 1335.6063 | 1336.7880 | 1337.6126 |
| 1345.2433 | 1351.2729 | 1352.5546 |
| 1357.9689 | 1369.6592 | 1372.1686 |
| 1377.8235 | 1389.3040 | 1397.0238 |
| 1397.8310 | 1404.1224 | 1405.0127 |
| 1406.4791 | 1409.3585 | 1414.9887 |
| 1420.1074 | 1423.2778 | 1426.4302 |
| 1427.2020 | 1430.0097 | 1432.6323 |
| 1446.0725 | 1454.9228 | 1482.1696 |
| 1484.2495 | 1487.5802 | 1490.8034 |
| 1492.3514 | 1493.1268 | 1493.8459 |
| 1494.5488 | 1497.0174 | 1498.6513 |
| 1502.9879 | 1504.3067 | 1506.2050 |
| 1507.9878 | 1508.8873 | 1510.5559 |
| 1514.8055 | 1515.3422 | 1523.0616 |
| 1523.5522 | 1524.1070 | 1525.0624 |
| 1528.8707 | 1529.8982 | 1532.4383 |
| 1547.0977 | 1560.3376 | 1605.3258 |
| 1646.2569 | 1678.6420 | 1679.5560 |
| 1683.2082 | 1685.3740 | 1762.0194 |
| 3052.5073 | 3057.0292 | 3058.4236 |
| 3061.5116 | 3064.4866 | 3064.7442 |
| 3065.9562 | 3069.6674 | 3077.3461 |
| 3084.4174 | 3087.1375 | 3107.7145 |
| 3111.5758 | 3118.5028 | 3124.5645 |
| 3130.8933 | 3133.0810 | 3134.3987 |
| 3138.1073 | 3143.0477 | 3143.1971 |
| 3144.6224 | 3146.3710 | 3147.0767 |
| 3149.8827 | 3154.7278 | 3155.7511 |
| 3155.7994 | 3160.3351 | 3162.5511 |
| 3165.9568 | 3166.5551 | 3168.9945 |
| 3180.0608 | 3180.2799 | 3196.4043 |
| 3205.3086 | 3208.3160 | 3218.4984 |
| 3218.8409 | 3221.0532 | 3228.8723 |
| 3232.6986 | 3273.9802 | 3288.9322 |
| 3304.1807 | 3323.8393 | 3331.6531 |

**E-P**

Zero-point correction= 0.206281 (Hartree/Particle)
Thermal correction to Energy= 0.219190
Thermal correction to Enthalpy= 0.220134
Thermal correction to Gibbs Free Energy= 0.165249
Sum of electronic and zero-point Energies= -609.685152

| | | | |
|---|---|---|---|
| Sum of electronic and thermal Energies= | | | -609.672242 |
| Sum of electronic and thermal Enthalpies= | | | -609.671298 |
| Sum of electronic and thermal Free Energies= | | | -609.726184 |
| C | 0.85242000 | 0.64253400 | -0.03261700 |
| C | 0.96464200 | 2.12954400 | -0.17273000 |
| C | -0.27979100 | -0.07534700 | 0.06813600 |
| H | -0.00637500 | 2.56350800 | -0.39098700 |
| H | 1.33498500 | 2.56358200 | 0.76210600 |
| H | -0.23315400 | -1.14489700 | 0.23226900 |
| C | -1.64498500 | 0.47844500 | -0.01984100 |
| O | -1.97082600 | 1.64070900 | -0.15269100 |
| O | -2.54093800 | -0.51683400 | 0.07485200 |
| C | -3.92124900 | -0.12237400 | 0.00826900 |
| C | -4.75367700 | -1.37677900 | 0.14839700 |
| H | -4.09627200 | 0.38277600 | -0.94606300 |
| H | -4.12039500 | 0.59624700 | 0.80839300 |
| H | -5.81475900 | -1.12200600 | 0.10357500 |
| H | -4.53097000 | -2.07925400 | -0.65771800 |
| H | -4.55481700 | -1.86661000 | 1.10420200 |
| H | 1.67838800 | 2.37526900 | -0.96298500 |
| C | 4.20891500 | -0.53512500 | 0.25865500 |
| C | 3.31223900 | 0.48331000 | 0.39181200 |
| C | 2.33306500 | -1.34180200 | -0.36643200 |
| N | 3.58962100 | -1.66899000 | -0.22483300 |
| H | 5.26590600 | -0.51736700 | 0.48000900 |
| H | 3.41791500 | 1.49648300 | 0.74263200 |
| H | 1.55394400 | -1.97501700 | -0.76543200 |
| N | 2.09184300 | -0.03931600 | -0.00219300 |

Frequencies

| | | |
|---|---|---|
| 32.9350 | 64.0562 | 69.0315 |
| 77.4281 | 89.8152 | 142.9653 |
| 150.9581 | 190.9391 | 252.8185 |
| 273.5836 | 292.8217 | 336.2494 |
| 345.0974 | 421.0646 | 487.5241 |
| 534.3758 | 645.1527 | 678.3287 |
| 688.6152 | 757.4478 | 765.4132 |
| 801.0616 | 814.4902 | 856.6738 |
| 892.5066 | 901.0526 | 916.7163 |
| 920.1870 | 944.2114 | 1036.7139 |
| 1047.4126 | 1069.3579 | 1109.6014 |
| 1111.1980 | 1140.9802 | 1153.4452 |
| 1172.2487 | 1187.8569 | 1247.0993 |
| 1293.2790 | 1303.3160 | 1334.1592 |
| 1358.3745 | 1391.4171 | 1407.1512 |

| | | |
|---|---|---|
| 1433.0115 | 1451.9805 | 1468.5649 |
| 1482.8140 | 1493.5115 | 1497.6922 |
| 1504.1610 | 1531.6178 | 1554.7250 |
| 1610.1675 | 1745.2612 | 1826.0055 |
| 3079.9142 | 3081.5517 | 3096.8494 |
| 3141.9173 | 3148.0240 | 3169.3616 |
| 3170.8478 | 3231.4031 | 3239.0889 |
| 3279.2313 | 3282.6618 | 3319.3009 |

**Z-P**

| | |
|---|---|
| Zero-point correction= | 0.206130 (Hartree/Particle) |
| Thermal correction to Energy= | 0.219032 |
| Thermal correction to Enthalpy= | 0.219977 |
| Thermal correction to Gibbs Free Energy= | 0.164850 |
| Sum of electronic and zero-point Energies= | -609.679946 |
| Sum of electronic and thermal Energies= | -609.667044 |
| Sum of electronic and thermal Enthalpies= | -609.666099 |
| Sum of electronic and thermal Free Energies= | -609.721226 |

| | | | |
|---|---|---|---|
| C | 1.28103500 | -1.24176400 | -0.16562200 |
| C | 2.61198400 | -1.85170600 | -0.48571800 |
| C | 0.14876500 | -1.95097800 | -0.07708500 |
| H | 3.32692400 | -1.64705400 | 0.31563600 |
| H | 2.51589000 | -2.92826500 | -0.62505100 |
| H | 0.20325700 | -3.03116500 | -0.15098100 |
| C | -1.21514200 | -1.40956900 | 0.15341600 |
| O | -2.05916400 | -1.98174400 | 0.80804200 |
| O | -1.41957100 | -0.24471600 | -0.46644000 |
| C | -2.65313500 | 0.42814200 | -0.16236600 |
| C | -2.58335200 | 1.78619400 | -0.82297100 |
| H | -2.74698300 | 0.50558100 | 0.92532200 |
| H | -3.48750500 | -0.17540200 | -0.53120100 |
| H | -3.48789200 | 2.35591500 | -0.59924800 |
| H | -1.71598300 | 2.33784100 | -0.45108100 |
| H | -2.49467900 | 1.68413900 | -1.90686600 |
| C | 1.01135300 | 2.12553300 | 0.99789100 |
| C | 0.70171900 | 0.80577500 | 1.15652700 |
| C | 1.95907900 | 1.11187700 | -0.62604700 |
| N | 1.79104900 | 2.30889900 | -0.12498800 |
| H | 0.72763900 | 2.95285000 | 1.63187600 |
| H | 0.14344600 | 0.26903500 | 1.90828300 |
| H | 2.51432600 | 0.87003000 | -1.52132900 |
| N | 1.31458500 | 0.15132200 | 0.10663900 |
| H | 3.01817200 | -1.42440400 | -1.40788700 |

Frequencies

| | | |
|---|---|---|
| 21.6994 | 33.4606 | 75.9873 |
| 87.2522 | 108.1524 | 133.6996 |
| 188.3269 | 210.2988 | 238.9018 |
| 249.3183 | 281.5231 | 319.9247 |
| 375.0171 | 421.3982 | 520.6773 |
| 566.4114 | 623.8736 | 668.2496 |
| 682.2236 | 714.8321 | 767.2331 |
| 784.1000 | 812.0608 | 853.5664 |
| 866.0457 | 902.0797 | 910.3370 |
| 918.8065 | 994.0121 | 1026.1050 |
| 1047.1146 | 1069.3003 | 1102.4700 |
| 1116.3355 | 1141.1977 | 1154.8280 |
| 1173.9516 | 1185.1589 | 1262.4464 |
| 1293.3555 | 1303.9352 | 1330.0212 |
| 1369.9996 | 1374.6616 | 1407.2588 |
| 1424.6287 | 1443.4275 | 1470.5279 |
| 1481.2212 | 1492.2134 | 1493.2904 |
| 1503.1877 | 1528.9677 | 1557.0156 |
| 1599.8390 | 1762.5097 | 1839.3619 |
| 3077.7692 | 3080.1659 | 3097.9256 |
| 3143.7462 | 3147.0973 | 3168.7225 |
| 3173.6149 | 3190.3648 | 3241.5735 |
| 3280.3178 | 3292.5476 | 3303.1492 |

**TS'II**

Zero-point correction= 0.779623 (Hartree/Particle)
Thermal correction to Energy= 0.822306
Thermal correction to Enthalpy= 0.823250
Thermal correction to Gibbs Free Energy= 0.705485
Sum of electronic and zero-point Energies= -1768.689262
Sum of electronic and thermal Energies= -1768.646579
Sum of electronic and thermal Enthalpies= -1768.645635
Sum of electronic and thermal Free Energies= -1768.763400

| | | | |
|---|---|---|---|
| C | -0.70424600 | -0.15828900 | 0.23991000 |
| C | -0.56959200 | -0.60048600 | 2.41426700 |
| C | -1.85347800 | -0.26513000 | 2.14338100 |
| N | -1.92806000 | -0.01680700 | 0.78529100 |
| H | -0.08628700 | -0.89601400 | 3.33175400 |
| H | -2.72280900 | -0.19034800 | 2.77611900 |
| N | 0.12591400 | -0.55068600 | 1.22080500 |
| C | -3.18734900 | 0.11389800 | 0.08133300 |
| C | -3.68118400 | 1.38338200 | -0.23086200 |
| C | -3.87096400 | -1.07804200 | -0.21512900 |
| C | -4.91506300 | 1.44152700 | -0.88528100 |

| | | | |
|---|---|---|---|
| C | -5.10437600 | -0.96175900 | -0.85531800 |
| C | -5.62090500 | 0.28565300 | -1.19069400 |
| H | -5.32531300 | 2.40989900 | -1.15587700 |
| H | -5.66629200 | -1.85798300 | -1.09806400 |
| H | -6.57984500 | 0.35497800 | -1.69397800 |
| C | 1.48566400 | -1.03138200 | 1.07570900 |
| C | 1.67806700 | -2.27122900 | 0.43985900 |
| C | 2.52505300 | -0.29947900 | 1.66309900 |
| C | 2.98661400 | -2.74514200 | 0.35991800 |
| C | 3.80836400 | -0.84148800 | 1.58166400 |
| C | 4.04260600 | -2.03812700 | 0.92103600 |
| H | 3.18443800 | -3.68111700 | -0.14894300 |
| H | 4.63985200 | -0.30197700 | 2.02575700 |
| H | 5.05321200 | -2.42328900 | 0.83728700 |
| C | -3.32685300 | -2.44898100 | 0.15821900 |
| C | -3.42951800 | -3.45931300 | -0.98987600 |
| C | -4.04005700 | -2.99258900 | 1.40363700 |
| H | -2.26448600 | -2.34589000 | 0.40652800 |
| H | -2.96487700 | -3.09021500 | -1.90855400 |
| H | -2.92907100 | -4.38996300 | -0.70584000 |
| H | -4.47167400 | -3.70456300 | -1.21453900 |
| H | -3.94732200 | -2.31041100 | 2.25269000 |
| H | -5.10613100 | -3.13497500 | 1.19902200 |
| H | -3.61462400 | -3.95878800 | 1.69117400 |
| C | -2.91603800 | 2.65307500 | 0.08210800 |
| C | -3.77398400 | 3.65842000 | 0.85638600 |
| C | -2.37638500 | 3.27303900 | -1.21265500 |
| H | -2.05381400 | 2.39455600 | 0.70022400 |
| H | -4.16434600 | 3.22078200 | 1.77932800 |
| H | -3.17293400 | 4.53344100 | 1.11919500 |
| H | -4.62287100 | 4.00654200 | 0.25962500 |
| H | -1.77400000 | 2.55101500 | -1.77277900 |
| H | -3.19782200 | 3.60254700 | -1.85828800 |
| H | -1.75186400 | 4.14196900 | -0.98320200 |
| C | 2.32107400 | 1.02006800 | 2.38601700 |
| C | 3.20805000 | 2.11616000 | 1.78450200 |
| C | 2.60332100 | 0.86635300 | 3.88599600 |
| H | 1.28461200 | 1.33837500 | 2.25484400 |
| H | 3.03671200 | 2.22637800 | 0.70892300 |
| H | 2.99835600 | 3.07402500 | 2.27066800 |
| H | 4.26962900 | 1.89517500 | 1.93466900 |
| H | 1.96311000 | 0.10529700 | 4.34219100 |
| H | 3.64376100 | 0.57255200 | 4.05937700 |
| H | 2.42969000 | 1.81429200 | 4.40363200 |

| | | | |
|---|---|---|---|
| C | 0.51992600 | -3.12565300 | -0.05743500 |
| C | -0.11157700 | -3.89039000 | 1.11613600 |
| C | 0.91822800 | -4.10244700 | -1.16552700 |
| H | -0.23912900 | -2.46566300 | -0.48593000 |
| H | -0.48459300 | -3.21870200 | 1.89565100 |
| H | -0.95053600 | -4.50184400 | 0.76587800 |
| H | 0.62870000 | -4.55763000 | 1.56930700 |
| H | 1.48750200 | -3.59883900 | -1.95112500 |
| H | 1.52368600 | -4.92626100 | -0.77426800 |
| H | 0.01716800 | -4.53930600 | -1.60550800 |
| C | -0.35104100 | 0.13092100 | -1.16852600 |
| C | -1.01030400 | -0.52522700 | -2.13416000 |
| H | -0.80861700 | -0.30917600 | -3.17835100 |
| H | -1.74526500 | -1.29146600 | -1.91487400 |
| C | 0.71747800 | 1.12858100 | -1.42549700 |
| H | 0.71134600 | 1.43235400 | -2.47529700 |
| C | 0.72008700 | 2.30915000 | -0.55473900 |
| O | 0.19145000 | 2.41354700 | 0.54444400 |
| O | 1.44508700 | 3.31464300 | -1.08706500 |
| C | 1.50720700 | 4.52769300 | -0.32495200 |
| C | 2.55107700 | 5.41007200 | -0.97281700 |
| H | 1.76025100 | 4.29083800 | 0.71099300 |
| H | 0.51733000 | 4.99746400 | -0.32749400 |
| H | 2.62503300 | 6.35736700 | -0.43387000 |
| H | 3.52784100 | 4.92046800 | -0.95221500 |
| H | 2.29022600 | 5.62080000 | -2.01239200 |
| C | 2.88009000 | -1.23583800 | -2.66128600 |
| C | 4.12204700 | -1.79450100 | -2.88202500 |
| C | 4.37047200 | -0.14254000 | -1.57266700 |
| N | 3.04682000 | -0.17439200 | -1.81450800 |
| H | 1.90181600 | 0.55221300 | -1.43132900 |
| H | 1.90367100 | -1.50589800 | -3.04387100 |
| H | 4.37941000 | -2.64737400 | -3.49864800 |
| H | 4.81348200 | 0.59907000 | -0.91679200 |
| N | 5.07337200 | -1.09382600 | -2.18790600 |

Frequencies

| | | |
|---|---|---|
| -1275.1537 | 18.8266 | 28.2765 |
| 31.7727 | 40.8167 | 45.2817 |
| 51.0948 | 58.5028 | 64.2471 |
| 76.1903 | 78.1623 | 81.3794 |
| 85.6438 | 93.4916 | 98.3124 |
| 101.4606 | 107.6000 | 115.2567 |
| 121.5211 | 128.6903 | 132.3844 |
| 132.9100 | 140.0765 | 147.7517 |

| | | |
|---|---|---|
| 153.7652 | 158.4393 | 161.5880 |
| 177.3651 | 183.5438 | 193.3044 |
| 196.8832 | 212.7899 | 227.7518 |
| 238.3121 | 244.4347 | 255.5838 |
| 261.6979 | 265.2410 | 268.4207 |
| 270.4836 | 283.1011 | 288.6813 |
| 292.9547 | 301.4859 | 305.8531 |
| 311.4215 | 318.6177 | 326.0893 |
| 331.3288 | 332.7805 | 340.3760 |
| 342.9343 | 350.2251 | 389.1650 |
| 393.6574 | 420.4254 | 422.8549 |
| 446.4299 | 448.5231 | 451.1856 |
| 461.8944 | 475.1575 | 506.4167 |
| 532.5280 | 547.1024 | 552.9555 |
| 564.3646 | 588.3005 | 599.9524 |
| 620.5792 | 626.3379 | 644.7857 |
| 651.2602 | 655.4437 | 667.5652 |
| 672.6120 | 686.0746 | 702.2768 |
| 708.0126 | 727.8321 | 748.9381 |
| 763.5453 | 766.3753 | 779.6292 |
| 783.3539 | 783.9798 | 793.0774 |
| 808.0100 | 815.2883 | 822.3050 |
| 833.5517 | 834.4980 | 835.5910 |
| 849.4879 | 867.2806 | 892.2187 |
| 911.1195 | 915.1528 | 915.6693 |
| 925.6375 | 927.8984 | 929.4437 |
| 934.4889 | 938.9802 | 942.9311 |
| 943.3611 | 944.4852 | 946.7989 |
| 965.4383 | 966.7833 | 968.7223 |
| 971.5500 | 974.8589 | 977.7734 |
| 980.4131 | 981.0390 | 1001.4547 |
| 1005.6326 | 1011.3801 | 1018.5570 |
| 1039.7907 | 1074.0212 | 1077.3168 |
| 1086.1332 | 1090.4846 | 1106.2241 |
| 1108.3451 | 1110.6148 | 1123.6302 |
| 1136.5867 | 1144.4697 | 1146.7320 |
| 1147.5737 | 1148.8283 | 1151.0252 |
| 1155.6321 | 1165.7803 | 1177.9765 |
| 1182.4904 | 1184.9673 | 1187.2762 |
| 1194.2136 | 1196.4517 | 1211.0729 |
| 1213.6035 | 1224.5322 | 1228.4780 |
| 1244.9756 | 1266.1316 | 1284.7104 |
| 1292.9708 | 1296.6187 | 1302.2712 |
| 1307.3259 | 1307.7333 | 1326.1796 |

| | | |
|---|---|---|
| 1328.5660 | 1330.3422 | 1337.0914 |
| 1349.2762 | 1351.1829 | 1354.5724 |
| 1362.4219 | 1363.2519 | 1376.5869 |
| 1380.8427 | 1388.6906 | 1396.3953 |
| 1399.8913 | 1402.6468 | 1403.6653 |
| 1407.1823 | 1407.9578 | 1412.3698 |
| 1413.9938 | 1417.3131 | 1425.5852 |
| 1427.3470 | 1431.2942 | 1433.2189 |
| 1443.3301 | 1459.5088 | 1483.9541 |
| 1491.4218 | 1493.9011 | 1494.6795 |
| 1495.3873 | 1496.2680 | 1498.1955 |
| 1499.3836 | 1500.7618 | 1502.3139 |
| 1503.3898 | 1507.5557 | 1510.1404 |
| 1510.7162 | 1512.2232 | 1514.8157 |
| 1517.4639 | 1520.5936 | 1522.3888 |
| 1525.9014 | 1526.7316 | 1532.8259 |
| 1535.6932 | 1537.4283 | 1546.0420 |
| 1548.0625 | 1556.8212 | 1576.8652 |
| 1639.6707 | 1678.9643 | 1681.4469 |
| 1688.6868 | 1689.5873 | 1718.6177 |
| 1783.1770 | 3058.0878 | 3058.1310 |
| 3058.4021 | 3059.8804 | 3060.9442 |
| 3063.7478 | 3067.9155 | 3068.7368 |
| 3077.4352 | 3091.2837 | 3099.2498 |
| 3121.9863 | 3128.0677 | 3134.1835 |
| 3136.1939 | 3136.3012 | 3136.8134 |
| 3141.3277 | 3142.4596 | 3143.8376 |
| 3143.9214 | 3146.7725 | 3147.8917 |
| 3149.6179 | 3149.6697 | 3150.8631 |
| 3152.3987 | 3154.0423 | 3155.6746 |
| 3155.8732 | 3163.7017 | 3166.4038 |
| 3166.9223 | 3174.9691 | 3191.4741 |
| 3202.1818 | 3206.5297 | 3218.4908 |
| 3223.6336 | 3224.5922 | 3230.8743 |
| 3233.4449 | 3242.8881 | 3255.3359 |
| 3284.7893 | 3305.2278 | 3326.5491 |

**II’**

| | |
|---|---|
| Zero-point correction= | 0.783457 (Hartree/Particle) |
| Thermal correction to Energy= | 0.827211 |
| Thermal correction to Enthalpy= | 0.828155 |
| Thermal correction to Gibbs Free Energy= | 0.706744 |
| Sum of electronic and zero-point Energies= | -1768.692598 |
| Sum of electronic and thermal Energies= | -1768.648844 |

Sum of electronic and thermal Enthalpies= -1768.647900

Sum of electronic and thermal Free Energies= -1768.769311

| | | | |
|---|---|---|---|
| C | -0.84409700 | -0.18981200 | 0.22475500 |
| C | -0.78383900 | -0.89523700 | 2.33120200 |
| C | -2.02490200 | -0.40170000 | 2.09725400 |
| N | -2.05526800 | 0.01338600 | 0.77892200 |
| H | -0.34495900 | -1.34149200 | 3.20913400 |
| H | -2.89387400 | -0.31998200 | 2.72998200 |
| N | -0.07076800 | -0.76986000 | 1.15551600 |
| C | -3.28304100 | 0.34103800 | 0.08405900 |
| C | -3.62008100 | 1.67886900 | -0.13958200 |
| C | -4.09166500 | -0.73957500 | -0.30932400 |
| C | -4.81855000 | 1.92682000 | -0.81419200 |
| C | -5.28358900 | -0.43398200 | -0.96620900 |
| C | -5.64149200 | 0.88559600 | -1.22284100 |
| H | -5.10794700 | 2.95354100 | -1.01699000 |
| H | -5.93945500 | -1.24035400 | -1.28036300 |
| H | -6.56973600 | 1.10140000 | -1.74154800 |
| C | 1.22268300 | -1.37431600 | 0.91067000 |
| C | 1.25022700 | -2.54977400 | 0.13366400 |
| C | 2.35936000 | -0.79342400 | 1.47852100 |
| C | 2.49936900 | -3.12451900 | -0.08296100 |
| C | 3.58354800 | -1.42128700 | 1.23225000 |
| C | 3.65613200 | -2.56340500 | 0.45210600 |
| H | 2.57524300 | -4.02232200 | -0.68700700 |
| H | 4.49435000 | -0.98669900 | 1.63017200 |
| H | 4.62296900 | -3.00411100 | 0.23793100 |
| C | -3.73256100 | -2.19117000 | -0.02281100 |
| C | -3.77443400 | -3.06319500 | -1.28313500 |
| C | -4.65792200 | -2.76545900 | 1.05787600 |
| H | -2.71049100 | -2.23365000 | 0.36898600 |
| H | -3.10583800 | -2.68985800 | -2.06449300 |
| H | -3.46692000 | -4.08391700 | -1.03616300 |
| H | -4.78447200 | -3.11516000 | -1.69995800 |
| H | -4.61836000 | -2.17196100 | 1.97539300 |
| H | -5.69499900 | -2.77704800 | 0.70800300 |
| H | -4.36646600 | -3.79208500 | 1.29766400 |
| C | -2.73593600 | 2.82852800 | 0.29906600 |
| C | -3.50366800 | 3.82645300 | 1.17276500 |
| C | -2.12565000 | 3.52741900 | -0.92153100 |
| H | -1.91343100 | 2.42468200 | 0.89345500 |
| H | -3.95424100 | 3.33209200 | 2.03760600 |
| H | -2.82258200 | 4.60100900 | 1.53619400 |
| H | -4.30150900 | 4.32206900 | 0.61066800 |

| | | | |
|---|---|---|---|
| H | -1.58418500 | 2.81812000 | -1.55548100 |
| H | -2.90474000 | 3.99652600 | -1.53164700 |
| H | -1.42841100 | 4.30675700 | -0.60015300 |
| C | 2.30830900 | 0.45749200 | 2.33606800 |
| C | 3.29578900 | 1.51877900 | 1.83669400 |
| C | 2.58836700 | 0.11264900 | 3.80449900 |
| H | 1.30557900 | 0.88723700 | 2.26656700 |
| H | 3.20831000 | 1.67639200 | 0.75660100 |
| H | 3.12022800 | 2.46115900 | 2.36534600 |
| H | 4.32937000 | 1.21548900 | 2.03332200 |
| H | 1.86362300 | -0.60567600 | 4.19936600 |
| H | 3.58557300 | -0.32638200 | 3.91216900 |
| H | 2.54723000 | 1.01529300 | 4.42127000 |
| C | -0.01331000 | -3.22819900 | -0.37829800 |
| C | -0.55643700 | -4.19781300 | 0.68074400 |
| C | 0.18709000 | -3.93831500 | -1.71841500 |
| H | -0.77887100 | -2.46648300 | -0.55172200 |
| H | -0.76668500 | -3.68588700 | 1.62541200 |
| H | -1.48306300 | -4.66656700 | 0.33264600 |
| H | 0.17471300 | -4.98794800 | 0.87899600 |
| H | 0.63646000 | -3.26690000 | -2.45565700 |
| H | 0.82648000 | -4.82031800 | -1.61970600 |
| H | -0.77966100 | -4.27829600 | -2.10100800 |
| C | -0.41851600 | 0.17519300 | -1.14205000 |
| C | -1.16779900 | -0.18263600 | -2.18779700 |
| H | -0.87860700 | 0.10409900 | -3.19351100 |
| H | -2.07602700 | -0.76467900 | -2.07737600 |
| C | 0.85539000 | 0.96785100 | -1.30071400 |
| H | 0.97685900 | 1.26205300 | -2.34532100 |
| C | 0.89995100 | 2.19700100 | -0.42755600 |
| O | 0.34448000 | 2.30311400 | 0.64849700 |
| O | 1.66368600 | 3.14559300 | -0.95718700 |
| C | 1.86461500 | 4.32611700 | -0.15662800 |
| C | 2.88294900 | 5.18037800 | -0.87590900 |
| H | 2.20918500 | 4.01876400 | 0.83386900 |
| H | 0.90312100 | 4.83516600 | -0.03921200 |
| H | 3.06915700 | 6.09268200 | -0.30502100 |
| H | 3.82443200 | 4.63750200 | -0.98512200 |
| H | 2.52220500 | 5.45861000 | -1.86848500 |
| C | 3.86407700 | -0.66374900 | -2.27388300 |
| C | 5.03610300 | -1.39867500 | -2.21054500 |
| C | 5.18234300 | 0.24768800 | -0.89101600 |
| N | 3.95689900 | 0.40327700 | -1.42444000 |
| H | 1.76718600 | 0.39816200 | -1.04991300 |

| | | | |
|---|---|---|---|
| H | 2.97257300 | -0.84582000 | -2.86741300 |
| H | 5.30458600 | -2.30145400 | -2.74935900 |
| H | 5.57885200 | 0.94820600 | -0.15961800 |
| N | 5.88900000 | -0.81128700 | -1.31711000 |

Frequencies

| | | |
|---|---|---|
| 21.3860 | 25.9357 | 29.9049 |
| 32.3389 | 46.2521 | 53.2783 |
| 54.1828 | 59.1076 | 62.6027 |
| 69.0301 | 72.7489 | 75.8651 |
| 83.6689 | 87.1633 | 88.3166 |
| 92.4838 | 100.5062 | 104.4184 |
| 111.0271 | 114.2218 | 118.7302 |
| 122.1163 | 136.6139 | 143.1029 |
| 145.3705 | 148.6301 | 162.8668 |
| 173.3891 | 177.4689 | 186.4272 |
| 203.4020 | 227.3270 | 234.0652 |
| 243.2073 | 248.1417 | 252.4489 |
| 257.1355 | 261.9876 | 264.8307 |
| 268.4149 | 275.5355 | 277.6354 |
| 283.4285 | 290.4949 | 295.7172 |
| 301.8344 | 306.2321 | 319.6065 |
| 322.2875 | 325.6450 | 332.0713 |
| 344.6232 | 367.6611 | 384.6484 |
| 403.7888 | 421.6189 | 431.1332 |
| 444.9994 | 450.1258 | 457.0487 |
| 459.7115 | 500.6747 | 523.0419 |
| 531.9528 | 543.5033 | 556.1269 |
| 585.3473 | 592.1344 | 607.1153 |
| 617.8297 | 623.5180 | 642.1552 |
| 652.8350 | 656.5007 | 662.5560 |
| 675.8127 | 686.1227 | 706.1195 |
| 716.2426 | 748.6097 | 755.3119 |
| 763.7354 | 775.9846 | 780.6770 |
| 782.6404 | 793.9287 | 807.9641 |
| 809.8740 | 816.3368 | 822.0337 |
| 831.9494 | 834.3984 | 837.9621 |
| 861.4204 | 891.5044 | 907.6375 |
| 913.0469 | 914.0716 | 918.9698 |
| 925.8327 | 935.1899 | 935.9872 |
| 937.3660 | 942.5416 | 948.9290 |
| 954.0139 | 954.1238 | 962.9664 |
| 965.8677 | 967.5259 | 969.3902 |
| 975.1984 | 976.2510 | 977.8469 |
| 979.1972 | 979.5421 | 997.8188 |

| | | |
|---|---|---|
| 1003.0634 | 1013.6897 | 1023.2800 |
| 1073.2386 | 1076.0709 | 1083.7308 |
| 1087.1171 | 1092.0035 | 1108.5115 |
| 1113.6334 | 1123.2905 | 1131.3345 |
| 1144.1614 | 1145.8838 | 1146.8924 |
| 1148.4317 | 1151.8224 | 1154.8482 |
| 1162.0542 | 1174.2760 | 1181.9751 |
| 1183.3119 | 1183.9582 | 1192.8123 |
| 1199.4330 | 1211.0064 | 1214.1652 |
| 1216.1281 | 1227.2317 | 1247.4704 |
| 1265.1194 | 1271.6047 | 1283.9201 |
| 1292.5214 | 1295.5598 | 1301.9018 |
| 1309.6117 | 1310.6634 | 1313.7440 |
| 1325.8287 | 1334.2348 | 1335.3996 |
| 1343.3304 | 1349.4676 | 1350.4784 |
| 1362.2720 | 1370.8406 | 1378.5579 |
| 1386.9578 | 1395.8644 | 1398.6504 |
| 1402.7816 | 1403.9235 | 1405.8693 |
| 1409.3118 | 1411.4461 | 1414.8495 |
| 1419.6026 | 1424.3235 | 1425.2728 |
| 1428.0261 | 1433.3598 | 1441.7678 |
| 1452.7780 | 1463.0772 | 1485.8952 |
| 1488.5517 | 1491.5536 | 1491.6577 |
| 1493.0305 | 1495.6572 | 1496.5636 |
| 1498.5794 | 1500.2380 | 1502.4163 |
| 1503.3946 | 1506.1568 | 1506.9367 |
| 1509.4374 | 1509.5353 | 1510.5202 |
| 1513.1317 | 1516.5431 | 1518.8712 |
| 1521.3954 | 1525.3191 | 1525.6743 |
| 1533.2201 | 1534.8859 | 1539.0238 |
| 1549.6985 | 1556.6480 | 1638.0470 |
| 1676.5913 | 1680.2735 | 1686.9378 |
| 1688.0712 | 1745.6442 | 1825.5343 |
| 3018.6672 | 3055.7923 | 3056.1508 |
| 3057.9499 | 3066.2303 | 3066.6090 |
| 3066.9218 | 3067.7072 | 3068.0581 |
| 3078.8403 | 3096.1782 | 3097.9157 |
| 3118.4418 | 3123.7185 | 3128.1629 |
| 3136.5678 | 3136.9869 | 3140.1366 |
| 3141.1916 | 3143.4102 | 3146.2647 |
| 3146.7066 | 3147.4758 | 3148.3858 |
| 3149.4872 | 3150.0485 | 3150.4933 |
| 3151.5737 | 3152.2513 | 3152.6851 |
| 3153.3855 | 3154.9620 | 3155.6755 |

| | | |
|---|---|---|
| 3166.1242 | 3170.1832 | 3184.1218 |
| 3189.5049 | 3202.6410 | 3207.2243 |
| 3216.6065 | 3221.5262 | 3222.5431 |
| 3228.3844 | 3229.1065 | 3244.2562 |
| 3284.0507 | 3302.3528 | 3321.7824 |

**TS'$_{III}$**

Zero-point correction= 0.784810 (Hartree/Particle)
Thermal correction to Energy= 0.826960
Thermal correction to Enthalpy= 0.827904
Thermal correction to Gibbs Free Energy= 0.712079
Sum of electronic and zero-point Energies= -1768.684394
Sum of electronic and thermal Energies= -1768.642245
Sum of electronic and thermal Enthalpies= -1768.641300
Sum of electronic and thermal Free Energies= -1768.757125

| | | | |
|---|---|---|---|
| C | 0.10514200 | 0.24559900 | -0.47393200 |
| C | -0.32118300 | -0.02255800 | -2.66276900 |
| C | 0.71361100 | 0.83858000 | -2.55271900 |
| N | 0.97894100 | 0.98819800 | -1.20109800 |
| H | -0.82057000 | -0.42805300 | -3.52767300 |
| H | 1.29786700 | 1.35425200 | -3.29759300 |
| N | -0.66735700 | -0.41071700 | -1.37601700 |
| C | 2.14272700 | 1.67607100 | -0.69902400 |
| C | 2.01241600 | 2.96454500 | -0.16953900 |
| C | 3.37026800 | 0.99722100 | -0.77828800 |
| C | 3.17468900 | 3.58308100 | 0.29808700 |
| C | 4.50007300 | 1.66088500 | -0.29802800 |
| C | 4.40500700 | 2.94124100 | 0.23638400 |
| H | 3.10994800 | 4.58306400 | 0.71711800 |
| H | 5.46561100 | 1.16522900 | -0.34044200 |
| H | 5.29513600 | 3.43948600 | 0.60677400 |
| C | -1.49433800 | -1.55867900 | -1.07944800 |
| C | -0.85160700 | -2.75718100 | -0.70271000 |
| C | -2.88352600 | -1.44085900 | -1.21019500 |
| C | -1.67524700 | -3.84095700 | -0.39687100 |
| C | -3.65620400 | -2.56849200 | -0.91525200 |
| C | -3.06061000 | -3.74893400 | -0.49674300 |
| H | -1.22639100 | -4.77514000 | -0.07959700 |
| H | -4.73645700 | -2.51345100 | -1.00802900 |
| H | -3.67533300 | -4.60949600 | -0.25331200 |
| C | 3.50212100 | -0.41201200 | -1.33505100 |
| C | 3.93993500 | -1.40058300 | -0.24708700 |
| C | 4.46150400 | -0.44656100 | -2.53025300 |
| H | 2.52307200 | -0.73994500 | -1.69668600 |

| | | | |
|---|---|---|---|
| H | 3.20171300 | -1.46990000 | 0.55903600 |
| H | 4.05976400 | -2.40041800 | -0.67811800 |
| H | 4.90187300 | -1.10722600 | 0.18671000 |
| H | 4.15639900 | 0.26190000 | -3.30567800 |
| H | 5.48279700 | -0.19695800 | -2.22582500 |
| H | 4.47927300 | -1.44965600 | -2.96670600 |
| C | 0.68029300 | 3.68188900 | -0.08626800 |
| C | 0.69953400 | 4.96999900 | -0.91740700 |
| C | 0.31255000 | 3.97260000 | 1.37222100 |
| H | -0.09347600 | 3.02581800 | -0.49034200 |
| H | 0.94976400 | 4.76299700 | -1.96176500 |
| H | -0.28317500 | 5.44952300 | -0.88741500 |
| H | 1.43290400 | 5.68327300 | -0.52749100 |
| H | 0.24438100 | 3.04392300 | 1.94685800 |
| H | 1.05631000 | 4.62005000 | 1.84862000 |
| H | -0.65388700 | 4.48104900 | 1.42122800 |
| C | -3.55447400 | -0.16306100 | -1.68213800 |
| C | -4.74404600 | 0.22110400 | -0.79561400 |
| C | -4.01398000 | -0.31018800 | -3.13916900 |
| H | -2.82446300 | 0.64937800 | -1.62569300 |
| H | -4.47447500 | 0.23791800 | 0.26480700 |
| H | -5.10995600 | 1.21242100 | -1.07859800 |
| H | -5.57504400 | -0.48068200 | -0.91623500 |
| H | -3.18193100 | -0.54752700 | -3.80756500 |
| H | -4.75141200 | -1.11474600 | -3.22698000 |
| H | -4.47797900 | 0.61741400 | -3.48666500 |
| C | 0.66492900 | -2.91511800 | -0.71883800 |
| C | 1.16001800 | -3.04493900 | -2.17006300 |
| C | 1.17181900 | -4.11763500 | 0.07855800 |
| H | 1.10727500 | -2.02372600 | -0.25891100 |
| H | 0.89774900 | -2.18574900 | -2.79156400 |
| H | 2.25019000 | -3.15225800 | -2.18478900 |
| H | 0.72739000 | -3.94041700 | -2.62872600 |
| H | 0.77203700 | -4.13925900 | 1.09430000 |
| H | 0.92424200 | -5.05755800 | -0.42805400 |
| H | 2.26149500 | -4.05846200 | 0.15092300 |
| C | -0.05172500 | 0.24241700 | 0.96189400 |
| C | 1.03307200 | 0.18328300 | 1.79848100 |
| H | 0.90006200 | 0.42657600 | 2.84573900 |
| H | 2.04470700 | 0.27729500 | 1.42339600 |
| C | -1.44676800 | 0.25486100 | 1.54229700 |
| H | -1.38017700 | 0.22856900 | 2.63312100 |
| C | -2.28151000 | 1.45814100 | 1.15316600 |
| O | -2.12720400 | 2.13460900 | 0.15860300 |

| | | | |
|---|---|---|---|
| O | -3.27084600 | 1.65195700 | 2.03326800 |
| C | -4.21131300 | 2.70531400 | 1.74441500 |
| C | -3.66941600 | 4.05672900 | 2.16353600 |
| H | -5.10221400 | 2.43462500 | 2.31261800 |
| H | -4.44316200 | 2.68601000 | 0.67740500 |
| H | -4.44478900 | 4.81755000 | 2.04529400 |
| H | -3.35707500 | 4.03823800 | 3.21020900 |
| H | -2.81727500 | 4.33114000 | 1.53998600 |
| C | 2.42498600 | -2.53018400 | 2.97661100 |
| C | 1.88569500 | -3.63329200 | 3.61164900 |
| C | 0.28975900 | -2.48723600 | 2.81368700 |
| N | 1.39071200 | -1.80290100 | 2.45628400 |
| H | -2.04805500 | -0.62445100 | 1.26627900 |
| H | 3.45724100 | -2.22369800 | 2.86221900 |
| H | 2.40192000 | -4.43541000 | 4.12614200 |
| H | -0.70511600 | -2.15844400 | 2.53057800 |
| N | 0.52063000 | -3.60574400 | 3.50863600 |

Frequencies

| | | |
|---|---|---|
| -197.2712 | 23.0082 | 30.9056 |
| 42.2218 | 46.9468 | 53.2563 |
| 53.8276 | 62.0531 | 70.8169 |
| 71.5667 | 79.4627 | 85.3247 |
| 88.1400 | 92.4260 | 96.5013 |
| 104.1551 | 110.5979 | 113.2306 |
| 113.9163 | 122.1048 | 135.6460 |
| 141.6624 | 148.8865 | 153.0940 |
| 157.2829 | 160.6465 | 176.0110 |
| 188.3261 | 197.9667 | 211.3724 |
| 221.4083 | 225.8962 | 232.9680 |
| 235.4071 | 240.3369 | 249.7227 |
| 252.3697 | 255.4498 | 261.1469 |
| 270.6617 | 284.1806 | 289.7947 |
| 293.4346 | 298.8609 | 306.4421 |
| 315.9072 | 320.7315 | 322.6555 |
| 328.4597 | 332.3776 | 346.4531 |
| 354.9598 | 384.7095 | 387.9693 |
| 422.1592 | 426.3360 | 444.1856 |
| 449.5907 | 452.3805 | 458.4935 |
| 468.0189 | 509.0954 | 529.9475 |
| 534.3471 | 552.7630 | 561.9682 |
| 584.9748 | 594.4663 | 597.8491 |
| 617.6514 | 621.1250 | 650.1525 |
| 654.3444 | 657.8109 | 666.2097 |
| 669.8758 | 685.3517 | 705.7061 |

| | | |
|---|---|---|
| 721.8653 | 749.3606 | 752.0785 |
| 765.6257 | 783.0254 | 784.3001 |
| 787.8049 | 795.1730 | 820.0179 |
| 830.6714 | 831.9532 | 833.3712 |
| 834.7126 | 847.7473 | 855.8631 |
| 878.2204 | 880.9726 | 906.2294 |
| 913.8670 | 915.7801 | 930.3274 |
| 932.7063 | 933.6284 | 938.0114 |
| 939.5536 | 942.3152 | 946.3316 |
| 946.8943 | 957.3028 | 959.4194 |
| 962.5997 | 965.1370 | 970.1146 |
| 975.7763 | 976.1260 | 977.2257 |
| 981.1499 | 995.2070 | 1015.1699 |
| 1022.2424 | 1025.9555 | 1052.7569 |
| 1073.9231 | 1075.9944 | 1084.8344 |
| 1088.3110 | 1090.8919 | 1104.2852 |
| 1110.4710 | 1118.1505 | 1130.2754 |
| 1135.2844 | 1138.0481 | 1143.4446 |
| 1146.6462 | 1149.2834 | 1150.4075 |
| 1153.2790 | 1168.3452 | 1179.5287 |
| 1183.6203 | 1189.2143 | 1193.4674 |
| 1201.2371 | 1210.0964 | 1211.2871 |
| 1214.1334 | 1224.4001 | 1247.2695 |
| 1253.7729 | 1268.8062 | 1283.2682 |
| 1289.7672 | 1291.2932 | 1301.1068 |
| 1314.0402 | 1319.5788 | 1320.4150 |
| 1325.9424 | 1335.9397 | 1343.5304 |
| 1351.0851 | 1353.6242 | 1355.8514 |
| 1359.9050 | 1362.5881 | 1375.4283 |
| 1379.6466 | 1383.6179 | 1391.0952 |
| 1402.3362 | 1403.7713 | 1405.6346 |
| 1407.8128 | 1408.3671 | 1410.4915 |
| 1416.5562 | 1423.4998 | 1424.6664 |
| 1426.4418 | 1428.3783 | 1429.9285 |
| 1444.3300 | 1456.0296 | 1487.1855 |
| 1491.8187 | 1491.9457 | 1492.7533 |
| 1493.2195 | 1494.8214 | 1496.6135 |
| 1497.1273 | 1497.6462 | 1499.2844 |
| 1503.2833 | 1504.7011 | 1507.4728 |
| 1508.7227 | 1510.3312 | 1511.2464 |
| 1512.6526 | 1515.8811 | 1518.3760 |
| 1520.5276 | 1521.0175 | 1523.5115 |
| 1528.7868 | 1531.0089 | 1532.4118 |
| 1535.6745 | 1554.3967 | 1601.6145 |

| | | |
|---|---|---|
| 1638.6111 | 1675.2165 | 1679.8750 |
| 1680.3857 | 1685.4249 | 1830.9474 |
| 3053.3873 | 3057.7442 | 3058.6566 |
| 3060.3917 | 3061.3457 | 3061.7133 |
| 3062.0315 | 3065.3525 | 3066.2479 |
| 3091.9285 | 3104.8335 | 3121.9544 |
| 3122.1223 | 3123.7384 | 3132.5847 |
| 3132.7438 | 3137.6563 | 3138.3521 |
| 3139.3975 | 3139.7475 | 3141.9602 |
| 3143.1454 | 3147.2277 | 3147.4374 |
| 3149.7838 | 3150.1377 | 3150.2930 |
| 3154.7578 | 3156.7066 | 3158.6916 |
| 3171.4802 | 3171.9552 | 3175.3565 |
| 3178.7089 | 3196.4417 | 3197.5167 |
| 3199.4573 | 3208.6241 | 3217.1700 |
| 3221.9457 | 3224.7334 | 3227.9256 |
| 3230.6320 | 3242.6056 | 3255.1404 |
| 3289.2240 | 3299.3741 | 3319.3485 |

**III'**

Zero-point correction= 0.786962 (Hartree/Particle)
Thermal correction to Energy= 0.829461
Thermal correction to Enthalpy= 0.830405
Thermal correction to Gibbs Free Energy= 0.712161
Sum of electronic and zero-point Energies= -1768.717739
Sum of electronic and thermal Energies= -1768.675240
Sum of electronic and thermal Enthalpies= -1768.674296
Sum of electronic and thermal Free Energies= -1768.792540

| | | | |
|---|---|---|---|
| C | 0.06198700 | 0.03289600 | -0.49684000 |
| C | -0.32314300 | -0.77639500 | -2.60756000 |
| C | 0.84911900 | -0.13078600 | -2.64176300 |
| N | 1.11118400 | 0.34679600 | -1.35425200 |
| H | -0.86600700 | -1.30355300 | -3.37524800 |
| H | 1.53809000 | 0.06039700 | -3.44911400 |
| N | -0.80634400 | -0.72112800 | -1.29031000 |
| C | 2.29158200 | 1.08142200 | -1.03757300 |
| C | 2.22617400 | 2.48285000 | -0.98266900 |
| C | 3.47260700 | 0.36549500 | -0.78580300 |
| C | 3.38955900 | 3.17052000 | -0.63399100 |
| C | 4.60887600 | 1.09741500 | -0.42948500 |
| C | 4.56695400 | 2.48477900 | -0.34812900 |
| H | 3.37297400 | 4.25558800 | -0.57993700 |
| H | 5.53654000 | 0.57362300 | -0.21551600 |
| H | 5.45882100 | 3.03693800 | -0.06887300 |
| C | -1.72454000 | -1.71918000 | -0.82036400 |

| | | | |
|---|---|---|---|
| C | -1.22713200 | -2.90108200 | -0.23429400 |
| C | -3.09796100 | -1.49916000 | -1.01031800 |
| C | -2.15769300 | -3.86548600 | 0.15737700 |
| C | -3.98662100 | -2.50483200 | -0.62077900 |
| C | -3.52226400 | -3.67662000 | -0.03962600 |
| H | -1.80931400 | -4.78540500 | 0.61501400 |
| H | -5.05334100 | -2.36117400 | -0.76588500 |
| H | -4.22348400 | -4.44658500 | 0.26652400 |
| C | 3.54089100 | -1.14846300 | -0.91055500 |
| C | 3.81619300 | -1.82537500 | 0.43581700 |
| C | 4.58494400 | -1.56146400 | -1.95475800 |
| H | 2.56768300 | -1.50250900 | -1.26350400 |
| H | 3.01902900 | -1.62473200 | 1.15763300 |
| H | 3.89197900 | -2.90986800 | 0.29960100 |
| H | 4.76014400 | -1.47499400 | 0.86735200 |
| H | 4.39375700 | -1.08127500 | -2.91872700 |
| H | 5.59570500 | -1.28800600 | -1.63493600 |
| H | 4.56267800 | -2.64585300 | -2.09950200 |
| C | 0.93924400 | 3.23382300 | -1.27662700 |
| C | 1.06357300 | 3.99368800 | -2.60277500 |
| C | 0.55560700 | 4.17966300 | -0.13523700 |
| H | 0.12766400 | 2.50690200 | -1.36735400 |
| H | 1.29302400 | 3.31259500 | -3.42761600 |
| H | 0.12877300 | 4.51271900 | -2.83408200 |
| H | 1.86277400 | 4.74099900 | -2.54848300 |
| H | 0.44890900 | 3.63290600 | 0.80609900 |
| H | 1.30079800 | 4.97006400 | 0.00322600 |
| H | -0.40602500 | 4.65166600 | -0.35417100 |
| C | -3.61748400 | -0.20787400 | -1.61747900 |
| C | -4.78614600 | 0.37774300 | -0.81717700 |
| C | -4.03318400 | -0.42531000 | -3.07798500 |
| H | -2.80252100 | 0.52207900 | -1.59304600 |
| H | -4.54546200 | 0.46739600 | 0.24731600 |
| H | -5.03108200 | 1.37318300 | -1.20021000 |
| H | -5.68581500 | -0.23965000 | -0.90608100 |
| H | -3.19795900 | -0.78417100 | -3.68556400 |
| H | -4.83751200 | -1.16632700 | -3.13989900 |
| H | -4.39662400 | 0.50933000 | -3.51535500 |
| C | 0.26475200 | -3.16712500 | -0.07776600 |
| C | 0.84743800 | -3.76351600 | -1.36898800 |
| C | 0.59363500 | -4.09762000 | 1.09509400 |
| H | 0.76243500 | -2.20957900 | 0.11330800 |
| H | 0.71706000 | -3.09731400 | -2.22517400 |
| H | 1.91965000 | -3.95223700 | -1.24276600 |

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|---|---|---|---|
| H | 0.35897300 | -4.71779000 | -1.59385300 |
| H | 0.06133900 | -3.82307700 | 2.00949300 |
| H | 0.34512500 | -5.13745800 | 0.85775200 |
| H | 1.66542700 | -4.05159000 | 1.30757100 |
| C | -0.14310200 | 0.40363400 | 0.81289200 |
| C | 0.91562300 | 0.97616600 | 1.70520500 |
| H | 0.46204100 | 1.70949100 | 2.38379300 |
| H | 1.72439200 | 1.48612800 | 1.18661500 |
| C | -1.52672800 | 0.42064800 | 1.40907300 |
| H | -1.48160700 | 0.37253900 | 2.50232000 |
| C | -2.30646200 | 1.67813700 | 1.04649800 |
| O | -2.12736400 | 2.37151400 | 0.07072400 |
| O | -3.27383200 | 1.92322700 | 1.94536300 |
| C | -4.10551000 | 3.06499500 | 1.67756700 |
| C | -5.15400300 | 3.12317500 | 2.76522100 |
| H | -4.55035700 | 2.95028100 | 0.68488600 |
| H | -3.47690300 | 3.96015000 | 1.66170300 |
| H | -5.81008100 | 3.98102900 | 2.60168300 |
| H | -5.76214100 | 2.21550800 | 2.76065500 |
| H | -4.68701800 | 3.22546800 | 3.74730500 |
| C | 2.76711400 | 0.10742700 | 3.21194900 |
| C | 2.96087800 | -1.06377800 | 3.90139700 |
| C | 1.10218300 | -1.27244700 | 2.87573500 |
| N | 1.57403100 | -0.04349600 | 2.55520700 |
| H | -2.16767500 | -0.41927500 | 1.11717700 |
| H | 3.35865900 | 1.00510600 | 3.11142300 |
| H | 3.80044100 | -1.33341900 | 4.52679900 |
| H | 0.16566800 | -1.63694100 | 2.47722000 |
| N | 1.91515800 | -1.92574500 | 3.68535900 |

Frequencies

| | | |
|---|---|---|
| 19.8984 | 23.9904 | 30.9963 |
| 34.0942 | 41.9404 | 45.6642 |
| 47.9160 | 51.8133 | 65.2661 |
| 67.2887 | 68.2864 | 77.7285 |
| 90.0579 | 98.9872 | 105.3238 |
| 109.1366 | 112.6574 | 121.9118 |
| 125.3937 | 136.7743 | 140.9813 |
| 144.4152 | 152.8299 | 160.5001 |
| 172.9360 | 176.1293 | 180.1080 |
| 201.9289 | 221.2298 | 224.0170 |
| 234.7512 | 236.7074 | 243.2953 |
| 249.8931 | 256.9478 | 260.6161 |
| 266.8807 | 271.9741 | 277.3256 |
| 284.0564 | 284.1810 | 292.4158 |

| | | |
|---|---|---|
| 296.7924 | 299.9215 | 304.2750 |
| 310.4545 | 318.7757 | 319.1916 |
| 323.1683 | 348.9019 | 352.0206 |
| 374.6937 | 396.3352 | 407.4531 |
| 420.5645 | 432.4217 | 446.3157 |
| 448.6051 | 458.6995 | 472.3503 |
| 501.8353 | 524.4918 | 529.7848 |
| 548.4525 | 559.5332 | 574.7897 |
| 581.2629 | 592.5473 | 615.6899 |
| 621.7255 | 627.1010 | 642.5516 |
| 655.0183 | 657.2560 | 673.6745 |
| 683.7137 | 692.1548 | 697.0309 |
| 722.6995 | 729.5827 | 748.9149 |
| 767.3120 | 769.4625 | 778.9661 |
| 793.6736 | 801.9118 | 810.9992 |
| 829.7854 | 831.0105 | 831.6931 |
| 839.5759 | 845.0463 | 875.8160 |
| 891.4517 | 904.3225 | 913.8595 |
| 914.4193 | 924.3243 | 926.3814 |
| 931.0776 | 934.0624 | 937.7644 |
| 937.8987 | 939.1956 | 945.0636 |
| 947.2673 | 951.9984 | 964.3083 |
| 965.1191 | 973.3780 | 975.4257 |
| 975.4373 | 978.1749 | 979.4332 |
| 995.1682 | 1008.8287 | 1017.0371 |
| 1062.3750 | 1072.7004 | 1076.2113 |
| 1085.8833 | 1088.8793 | 1090.2043 |
| 1100.6091 | 1101.6230 | 1108.3367 |
| 1119.1364 | 1139.5327 | 1144.3136 |
| 1146.6918 | 1147.2169 | 1149.3849 |
| 1152.3578 | 1155.2268 | 1159.9417 |
| 1178.1833 | 1181.2156 | 1190.1256 |
| 1190.5022 | 1190.8291 | 1205.8608 |
| 1209.8074 | 1210.2695 | 1236.9093 |
| 1243.6189 | 1259.0871 | 1260.3912 |
| 1278.4066 | 1280.6097 | 1290.1718 |
| 1292.1930 | 1295.6660 | 1306.1515 |
| 1307.0525 | 1310.7354 | 1315.8307 |
| 1320.4345 | 1339.5856 | 1344.1435 |
| 1347.6004 | 1350.2649 | 1353.9089 |
| 1358.5656 | 1358.8825 | 1375.3081 |
| 1378.9271 | 1393.9881 | 1401.6534 |
| 1403.7046 | 1404.5932 | 1406.0178 |
| 1406.5774 | 1407.1638 | 1415.8570 |

| | | |
|---|---|---|
| 1417.8458 | 1423.1862 | 1423.6666 |
| 1426.4676 | 1428.0867 | 1442.6793 |
| 1453.7917 | 1459.2920 | 1465.9182 |
| 1489.2775 | 1491.5246 | 1491.9109 |
| 1493.6422 | 1493.7299 | 1494.1649 |
| 1495.9921 | 1497.3035 | 1498.6015 |
| 1505.1866 | 1505.6086 | 1506.3428 |
| 1508.4216 | 1508.8411 | 1509.2352 |
| 1511.2063 | 1511.4325 | 1516.1060 |
| 1520.9726 | 1524.6717 | 1529.2148 |
| 1530.6684 | 1534.3339 | 1536.9163 |
| 1577.2035 | 1580.8418 | 1656.6268 |
| 1675.7847 | 1678.0558 | 1678.4926 |
| 1682.7786 | 1702.8547 | 1839.4931 |
| 3053.3558 | 3056.6956 | 3056.7070 |
| 3059.8746 | 3060.4684 | 3062.8490 |
| 3065.2411 | 3066.4875 | 3068.7077 |
| 3081.0020 | 3083.2473 | 3102.4044 |
| 3106.7349 | 3106.9764 | 3114.7745 |
| 3121.6641 | 3125.4425 | 3130.8604 |
| 3136.0711 | 3136.4537 | 3140.0204 |
| 3140.4960 | 3142.8099 | 3142.9809 |
| 3143.0493 | 3145.7017 | 3146.4623 |
| 3147.9997 | 3150.8553 | 3150.8803 |
| 3151.7807 | 3156.0308 | 3158.3486 |
| 3166.8429 | 3169.7377 | 3175.8491 |
| 3198.5874 | 3201.4255 | 3202.6767 |
| 3207.0978 | 3216.4165 | 3227.6615 |
| 3229.0411 | 3268.9165 | 3289.1616 |
| 3297.4284 | 3300.9075 | 3324.7767 |

**TS'IV**

| | | | |
|---|---|---|---|
| Zero-point correction= | | | 0.857468 (Hartree/Particle) |
| Thermal correction to Energy= | | | 0.903928 |
| Thermal correction to Enthalpy= | | | 0.904872 |
| Thermal correction to Gibbs Free Energy= | | | 0.779209 |
| Sum of electronic and zero-point Energies= | | | -1994.780128 |
| Sum of electronic and thermal Energies= | | | -1994.733668 |
| Sum of electronic and thermal Enthalpies= | | | -1994.732723 |
| Sum of electronic and thermal Free Energies= | | | -1994.858387 |
| C | 0.04589600 | 0.23011400 | -0.59360500 |
| C | -0.55632300 | 0.31920200 | -2.77059800 |
| C | 0.73655000 | 0.67593100 | -2.69886800 |
| N | 1.11096000 | 0.60069000 | -1.36135300 |

| | | | |
|---|---|---|---|
| H | -1.22639100 | 0.21455200 | -3.60812300 |
| H | 1.45143900 | 0.94764600 | -3.45839400 |
| N | -0.97069100 | 0.01305700 | -1.48203500 |
| C | 2.52827500 | 0.68321600 | -1.07501200 |
| C | 3.10247000 | 1.94672000 | -0.87805900 |
| C | 3.28240400 | -0.49348400 | -1.21575100 |
| C | 4.49451700 | 2.00977200 | -0.77849400 |
| C | 4.66897300 | -0.37625900 | -1.09491200 |
| C | 5.26991200 | 0.85989800 | -0.88309600 |
| H | 4.97426900 | 2.97192600 | -0.62705100 |
| H | 5.28814600 | -1.26297000 | -1.17942600 |
| H | 6.35010600 | 0.92769200 | -0.80359200 |
| C | -2.26709800 | -0.60476200 | -1.29177700 |
| C | -2.33888800 | -2.00828000 | -1.25132500 |
| C | -3.40210700 | 0.22184300 | -1.29513800 |
| C | -3.61380100 | -2.57241500 | -1.15982300 |
| C | -4.65033300 | -0.39695600 | -1.20909000 |
| C | -4.75511600 | -1.77987500 | -1.13454300 |
| H | -3.71457100 | -3.65008000 | -1.10294400 |
| H | -5.54867800 | 0.21234700 | -1.20482100 |
| H | -5.73274900 | -2.24512100 | -1.06079600 |
| C | 2.63241100 | -1.84397200 | -1.47471800 |
| C | 2.33928700 | -2.56735300 | -0.15336600 |
| C | 3.46967900 | -2.73230100 | -2.39870300 |
| H | 1.67451500 | -1.66619100 | -1.97951600 |
| H | 1.64932300 | -1.99602000 | 0.47403000 |
| H | 1.88817300 | -3.54644500 | -0.34977000 |
| H | 3.26191400 | -2.71391600 | 0.41915100 |
| H | 3.75889100 | -2.20478500 | -3.31174500 |
| H | 4.37820300 | -3.08548300 | -1.90179000 |
| H | 2.88992100 | -3.61604100 | -2.67899200 |
| C | 2.26237200 | 3.20988000 | -0.81274600 |
| C | 2.40578200 | 4.00895800 | -2.11480900 |
| C | 2.62168000 | 4.08188400 | 0.39540900 |
| H | 1.21403900 | 2.91904900 | -0.70322600 |
| H | 2.09861900 | 3.41836200 | -2.98268300 |
| H | 1.78553900 | 4.90897100 | -2.07727200 |
| H | 3.44566900 | 4.31716400 | -2.26646700 |
| H | 2.58262000 | 3.51636800 | 1.33152000 |
| H | 3.62527400 | 4.50781300 | 0.29984300 |
| H | 1.91314500 | 4.91121100 | 0.47163600 |
| C | -3.30814900 | 1.73387500 | -1.41576000 |
| C | -4.18788400 | 2.45398200 | -0.38652700 |
| C | -3.69346100 | 2.18057900 | -2.83333300 |

| | | | |
|---|---|---|---|
| H | -2.26975400 | 2.03141300 | -1.23603100 |
| H | -3.98919800 | 2.11626800 | 0.63475500 |
| H | -4.00320400 | 3.53166800 | -0.43536900 |
| H | -5.25082500 | 2.29669500 | -0.59256700 |
| H | -3.05060500 | 1.72760300 | -3.59254400 |
| H | -4.72730900 | 1.89579900 | -3.05427500 |
| H | -3.61205100 | 3.26761800 | -2.92280900 |
| C | -1.10661700 | -2.89480500 | -1.36134700 |
| C | -0.66979300 | -3.05335200 | -2.82670200 |
| C | -1.31807000 | -4.28502600 | -0.75801200 |
| H | -0.29686000 | -2.41377700 | -0.80074300 |
| H | -0.42233400 | -2.10328600 | -3.30457800 |
| H | 0.21552700 | -3.69659300 | -2.87803700 |
| H | -1.46777300 | -3.52964500 | -3.40597400 |
| H | -1.76745900 | -4.23689400 | 0.23555400 |
| H | -1.95319800 | -4.89826800 | -1.40712200 |
| H | -0.35357200 | -4.79369600 | -0.67324700 |
| C | -0.06045400 | 0.11155000 | 0.86619700 |
| C | 1.09386600 | 0.73309300 | 1.67980800 |
| H | 0.65141500 | 1.22420700 | 2.55284300 |
| H | 1.61761600 | 1.51812300 | 1.13460400 |
| C | -1.35767200 | 0.72885400 | 1.40932400 |
| H | -1.48705400 | 0.41998400 | 2.45183100 |
| C | -1.37124200 | 2.24249500 | 1.34974900 |
| O | -0.72108500 | 2.91083000 | 0.57203200 |
| O | -2.19928200 | 2.77040600 | 2.25260000 |
| C | -2.32462900 | 4.20628600 | 2.23835900 |
| C | -3.46988000 | 4.56519300 | 3.15685100 |
| H | -2.50281600 | 4.53190600 | 1.21008000 |
| H | -1.37536100 | 4.63741200 | 2.56963300 |
| H | -3.58896700 | 5.65026400 | 3.19079400 |
| H | -4.40218400 | 4.12451700 | 2.79533600 |
| H | -3.28157100 | 4.20399700 | 4.17011800 |
| C | 3.47389600 | -0.08125700 | 2.01290400 |
| C | 4.01999300 | -1.08309200 | 2.77021600 |
| C | 1.91078600 | -1.19411800 | 3.07250900 |
| N | 2.11628800 | -0.17324400 | 2.19896200 |
| H | -2.25418800 | 0.37606700 | 0.89159900 |
| H | 3.91022900 | 0.67421700 | 1.37858000 |
| H | 5.06489300 | -1.33822000 | 2.87631300 |
| H | 0.91807200 | -1.46231600 | 3.40490200 |
| N | 3.03410900 | -1.77875500 | 3.42965500 |
| C | -0.21322300 | -3.45501800 | 2.27147300 |
| C | -1.19792300 | -4.27085800 | 2.78188300 |

| | | | |
|---|---|---|---|
| C | -2.13709200 | -2.50454300 | 2.07026900 |
| N | -0.82251200 | -2.31309200 | 1.81549400 |
| H | -0.31819200 | -1.18035000 | 1.26285000 |
| H | 0.85740700 | -3.59627300 | 2.21036400 |
| H | -1.09223400 | -5.25195200 | 3.22724800 |
| H | -2.88798600 | -1.76727300 | 1.80659600 |
| N | -2.42228400 | -3.66704700 | 2.64922800 |

Frequencies

| | | |
|---|---|---|
| -1337.5420 | 17.7529 | 26.7877 |
| 33.7480 | 40.0983 | 44.3277 |
| 54.6299 | 55.2478 | 56.4770 |
| 58.1742 | 67.3164 | 73.0490 |
| 84.1151 | 86.2594 | 93.2093 |
| 95.9283 | 100.5479 | 107.8000 |
| 113.4458 | 117.9347 | 125.5337 |
| 134.6377 | 137.4571 | 143.3761 |
| 147.1502 | 151.4536 | 154.4630 |
| 162.5305 | 163.4487 | 167.2001 |
| 181.6207 | 183.1979 | 190.2078 |
| 198.5336 | 203.3834 | 212.3671 |
| 216.7073 | 226.8544 | 239.5637 |
| 247.1868 | 252.3795 | 259.9388 |
| 265.5206 | 272.9878 | 275.0507 |
| 281.6130 | 293.0095 | 297.3376 |
| 304.4381 | 314.2446 | 317.3914 |
| 321.7169 | 324.3426 | 327.2011 |
| 335.9240 | 346.5821 | 353.7372 |
| 360.5841 | 396.4226 | 405.4713 |
| 418.0496 | 434.3894 | 442.6506 |
| 445.1289 | 453.5486 | 470.4931 |
| 477.3863 | 516.3686 | 532.1551 |
| 535.9621 | 552.1385 | 567.1159 |
| 583.0934 | 591.7816 | 599.2454 |
| 616.8749 | 625.0424 | 646.5640 |
| 652.0943 | 655.2968 | 661.0076 |
| 669.7085 | 679.7676 | 691.1069 |
| 701.5724 | 702.5073 | 728.0253 |
| 743.6031 | 749.2134 | 768.2390 |
| 770.3099 | 792.5763 | 796.9938 |
| 800.4856 | 801.6630 | 815.1770 |
| 829.9896 | 830.7858 | 832.2147 |
| 837.7105 | 839.3462 | 840.1492 |
| 866.7473 | 876.2815 | 881.7947 |
| 894.9825 | 907.3548 | 914.4193 |

| | | |
|---|---|---|
| 915.9451 | 924.0305 | 928.5986 |
| 931.9413 | 933.7192 | 935.8346 |
| 937.0634 | 937.7726 | 942.2001 |
| 945.6081 | 945.6897 | 959.4362 |
| 965.3181 | 967.3420 | 976.1695 |
| 976.7302 | 977.4503 | 980.1533 |
| 980.9185 | 994.0918 | 1007.3543 |
| 1019.7095 | 1019.9868 | 1065.5002 |
| 1071.3751 | 1073.5073 | 1077.8782 |
| 1086.6559 | 1088.9637 | 1092.0848 |
| 1107.7563 | 1112.9950 | 1120.7741 |
| 1121.9917 | 1134.7534 | 1141.6582 |
| 1143.7799 | 1145.1196 | 1147.1910 |
| 1150.1295 | 1152.2123 | 1157.6143 |
| 1159.7270 | 1177.0873 | 1180.4701 |
| 1181.3571 | 1186.1895 | 1192.5379 |
| 1195.6537 | 1207.0085 | 1211.4137 |
| 1212.7899 | 1224.2478 | 1239.4538 |
| 1255.4761 | 1264.8689 | 1272.7312 |
| 1278.6616 | 1283.0156 | 1286.3938 |
| 1290.9923 | 1294.3682 | 1299.7974 |
| 1310.8002 | 1318.4492 | 1318.9139 |
| 1321.7692 | 1323.4034 | 1335.5562 |
| 1341.4063 | 1344.6648 | 1351.6661 |
| 1360.2458 | 1361.2610 | 1376.7176 |
| 1383.4614 | 1388.8788 | 1390.0079 |
| 1400.5892 | 1404.5368 | 1406.7838 |
| 1407.5850 | 1408.6374 | 1410.1944 |
| 1411.4323 | 1416.7057 | 1425.6395 |
| 1429.5086 | 1430.4903 | 1431.6262 |
| 1434.8975 | 1440.6396 | 1448.5361 |
| 1460.9118 | 1473.4363 | 1484.1386 |
| 1487.6030 | 1488.0039 | 1489.5884 |
| 1490.2518 | 1493.2042 | 1493.8038 |
| 1495.1624 | 1496.6485 | 1498.9464 |
| 1501.2662 | 1502.4405 | 1505.8185 |
| 1507.2141 | 1507.9018 | 1509.7188 |
| 1511.8569 | 1513.8497 | 1520.4980 |
| 1521.1235 | 1526.2194 | 1526.7746 |
| 1530.0140 | 1530.2746 | 1530.4274 |
| 1532.7844 | 1544.6677 | 1552.2413 |
| 1577.7811 | 1591.2294 | 1608.6222 |
| 1665.3400 | 1673.7408 | 1678.0247 |
| 1680.1444 | 1681.3090 | 1826.8870 |

| | | |
|---|---|---|
| 3059.7438 | 3061.8169 | 3064.2205 |
| 3064.4838 | 3066.8474 | 3067.0493 |
| 3068.6101 | 3069.0404 | 3081.6071 |
| 3083.3819 | 3085.6282 | 3102.7169 |
| 3106.3940 | 3106.8497 | 3107.9805 |
| 3125.1272 | 3137.1099 | 3137.3956 |
| 3141.0704 | 3142.4556 | 3142.7980 |
| 3146.8734 | 3147.9726 | 3148.8198 |
| 3151.9601 | 3152.6641 | 3153.3586 |
| 3153.8651 | 3154.0221 | 3155.6580 |
| 3158.5688 | 3165.7761 | 3168.2101 |
| 3170.2455 | 3174.3690 | 3187.1094 |
| 3195.6248 | 3216.4688 | 3218.2614 |
| 3218.4013 | 3225.6253 | 3235.6187 |
| 3236.1112 | 3244.2851 | 3249.3041 |
| 3258.7498 | 3272.1181 | 3286.2492 |
| 3294.6200 | 3310.5368 | 3318.2376 |

**IV'**

| | |
|---|---|
| Zero-point correction= | 0.862627 (Hartree/Particle) |
| Thermal correction to Energy= | 0.909533 |
| Thermal correction to Enthalpy= | 0.910477 |
| Thermal correction to Gibbs Free Energy= | 0.783368 |
| Sum of electronic and zero-point Energies= | -1994.787286 |
| Sum of electronic and thermal Energies= | -1994.740380 |
| Sum of electronic and thermal Enthalpies= | -1994.739435 |
| Sum of electronic and thermal Free Energies= | -1994.866544 |

| | | | |
|---|---|---|---|
| C | 0.18750000 | 0.27616200 | -0.61651600 |
| C | -0.23749800 | 0.60023100 | -2.79033600 |
| C | 1.08108500 | 0.80920700 | -2.59679900 |
| N | 1.33645300 | 0.59149500 | -1.25357800 |
| H | -0.84734700 | 0.62963500 | -3.67849500 |
| H | 1.87749400 | 1.05679700 | -3.27961500 |
| N | -0.77494900 | 0.24980000 | -1.56513500 |
| C | 2.72324500 | 0.41896200 | -0.85421300 |
| C | 3.47052400 | 1.54405100 | -0.48143400 |
| C | 3.27883000 | -0.85397300 | -1.04935700 |
| C | 4.83704400 | 1.35400200 | -0.26557500 |
| C | 4.65092400 | -0.98665900 | -0.82290300 |
| C | 5.42270800 | 0.10290500 | -0.43762400 |
| H | 5.45082500 | 2.20169200 | 0.02377200 |
| H | 5.11837100 | -1.95753700 | -0.95706700 |
| H | 6.48798200 | -0.02159400 | -0.27287400 |
| C | -2.17143600 | -0.13617900 | -1.46757800 |

| | | | |
|---|---|---|---|
| C | -2.49081400 | -1.50364800 | -1.42733400 |
| C | -3.13007800 | 0.88765600 | -1.52285400 |
| C | -3.85043000 | -1.82404500 | -1.43488800 |
| C | -4.47161400 | 0.50407900 | -1.53475100 |
| C | -4.82730500 | -0.83785900 | -1.49180800 |
| H | -4.15011500 | -2.86340000 | -1.37743000 |
| H | -5.24393100 | 1.26575900 | -1.57751200 |
| H | -5.87514500 | -1.11944000 | -1.49508300 |
| C | 2.46923500 | -2.04496600 | -1.53463500 |
| C | 2.52058200 | -3.21506400 | -0.54824900 |
| C | 2.93944100 | -2.47262300 | -2.93050200 |
| H | 1.41920800 | -1.74697300 | -1.62379200 |
| H | 2.15391600 | -2.92439200 | 0.43955000 |
| H | 1.89716000 | -4.03489200 | -0.91985300 |
| H | 3.54063900 | -3.59558800 | -0.43445100 |
| H | 2.86349400 | -1.64883400 | -3.64658900 |
| H | 3.98153500 | -2.80621800 | -2.90473600 |
| H | 2.32854300 | -3.30322100 | -3.29553200 |
| C | 2.85100500 | 2.92442200 | -0.36282700 |
| C | 3.32135100 | 3.81485200 | -1.52074200 |
| C | 3.16337800 | 3.58500500 | 0.98438200 |
| H | 1.76524500 | 2.82008200 | -0.42732800 |
| H | 3.06788700 | 3.37818500 | -2.49110300 |
| H | 2.85036200 | 4.79955800 | -1.45430400 |
| H | 4.40687100 | 3.95335100 | -1.48634500 |
| H | 2.85437800 | 2.95976100 | 1.82730700 |
| H | 4.23281100 | 3.79196600 | 1.09130700 |
| H | 2.62913500 | 4.53608600 | 1.05828100 |
| C | -2.75979700 | 2.36208000 | -1.57111200 |
| C | -3.54774200 | 3.18483600 | -0.54358300 |
| C | -2.98843000 | 2.93044100 | -2.97839700 |
| H | -1.69639000 | 2.46607600 | -1.32809900 |
| H | -3.46409600 | 2.77336500 | 0.46650600 |
| H | -3.17245900 | 4.21263400 | -0.53138200 |
| H | -4.61029600 | 3.22855200 | -0.79978200 |
| H | -2.40151600 | 2.40202600 | -3.73394700 |
| H | -4.04447600 | 2.84467700 | -3.25388300 |
| H | -2.71208000 | 3.98805400 | -3.00912800 |
| C | -1.43339800 | -2.60054900 | -1.42138800 |
| C | -0.82229300 | -2.78297300 | -2.82027600 |
| C | -1.97461100 | -3.94582500 | -0.93385500 |
| H | -0.64219000 | -2.30586900 | -0.71994100 |
| H | -0.32940600 | -1.88390200 | -3.19937500 |
| H | -0.07903000 | -3.58700500 | -2.79461900 |

| | | | |
|---|---|---|---|
| H | -1.60313800 | -3.06785500 | -3.53297000 |
| H | -2.52487200 | -3.84848400 | 0.00397600 |
| H | -2.62348500 | -4.40024100 | -1.69126100 |
| H | -1.13612900 | -4.62817600 | -0.76882600 |
| C | -0.06348200 | 0.02293900 | 0.85080600 |
| C | 1.12773500 | 0.31451600 | 1.79099400 |
| H | 0.71879200 | 0.72625100 | 2.71907000 |
| H | 1.79337400 | 1.07292600 | 1.38328700 |
| C | -1.26940500 | 0.81990600 | 1.38106100 |
| H | -1.50946800 | 0.43095500 | 2.37423700 |
| C | -1.00149400 | 2.30259000 | 1.44597300 |
| O | -0.17522300 | 2.87766900 | 0.76543300 |
| O | -1.79158800 | 2.91640200 | 2.32087100 |
| C | -1.65419500 | 4.35051500 | 2.40607400 |
| C | -2.76053100 | 4.85163700 | 3.30484800 |
| H | -1.71961500 | 4.76593500 | 1.39695000 |
| H | -0.66041100 | 4.57629900 | 2.80318300 |
| H | -2.68347100 | 5.93574600 | 3.41179300 |
| H | -3.73795900 | 4.61249700 | 2.87923700 |
| H | -2.68856200 | 4.39838000 | 4.29568700 |
| C | 3.29271200 | -0.93136600 | 2.18031600 |
| C | 3.57126200 | -2.14817800 | 2.74165300 |
| C | 1.43875600 | -1.99630400 | 2.70132900 |
| N | 1.92159000 | -0.85174400 | 2.13710600 |
| H | -2.17031800 | 0.66293900 | 0.78244900 |
| H | 3.91831300 | -0.13531100 | 1.80525700 |
| H | 4.54260400 | -2.58612100 | 2.92216100 |
| H | 0.37202200 | -2.15820900 | 2.80746800 |
| N | 2.40778600 | -2.80806100 | 3.06465700 |
| C | -1.62116100 | -3.64005900 | 2.43191800 |
| C | -2.89207400 | -4.17467500 | 2.53479800 |
| C | -3.04895900 | -2.17784400 | 1.84796000 |
| N | -1.71967300 | -2.34732000 | 1.98833700 |
| H | -0.37695900 | -1.02836500 | 0.98246000 |
| H | -0.66178200 | -4.10482300 | 2.63458600 |
| H | -3.18842900 | -5.16816900 | 2.85167600 |
| H | -3.47504200 | -1.24057700 | 1.49745300 |
| N | -3.81288900 | -3.23513700 | 2.15458000 |

Frequencies

| | | |
|---|---|---|
| 21.2547 | 24.8243 | 29.1964 |
| 36.8529 | 39.6758 | 55.2002 |
| 60.3639 | 61.4012 | 66.2176 |
| 70.2468 | 78.0360 | 81.2081 |
| 83.9451 | 86.7227 | 93.2525 |

| | | |
|---|---|---|
| 94.7143 | 102.4508 | 103.2388 |
| 108.1148 | 116.1630 | 117.7384 |
| 125.6927 | 132.9709 | 136.0195 |
| 141.8900 | 144.7211 | 152.7017 |
| 154.7267 | 157.3795 | 167.1360 |
| 174.5136 | 177.5642 | 190.5282 |
| 198.1192 | 214.8590 | 220.6709 |
| 223.3127 | 233.4969 | 246.7049 |
| 251.8833 | 253.3416 | 259.8063 |
| 269.5294 | 273.6187 | 275.8016 |
| 279.3914 | 292.7244 | 298.4658 |
| 313.7023 | 319.7425 | 320.3416 |
| 321.5441 | 325.7614 | 331.5511 |
| 341.3837 | 351.8523 | 358.9115 |
| 392.2481 | 402.1376 | 420.1578 |
| 422.6139 | 443.9411 | 449.4096 |
| 452.9514 | 466.7119 | 475.7826 |
| 506.7939 | 529.8478 | 531.8326 |
| 545.8369 | 566.6600 | 582.6416 |
| 592.9090 | 601.6455 | 614.4391 |
| 622.6012 | 640.9712 | 649.2648 |
| 654.2080 | 663.1310 | 676.7741 |
| 678.7345 | 690.0793 | 691.7923 |
| 712.9513 | 724.7276 | 747.7515 |
| 749.5844 | 766.6977 | 788.3636 |
| 796.7747 | 798.1786 | 799.5334 |
| 803.0229 | 817.3336 | 828.3963 |
| 831.8767 | 832.7111 | 840.3531 |
| 842.6837 | 843.3970 | 847.8306 |
| 887.5270 | 905.9665 | 908.0411 |
| 913.6777 | 915.1367 | 920.5868 |
| 924.0497 | 928.9765 | 930.0517 |
| 931.8638 | 936.4935 | 937.2766 |
| 938.0800 | 941.8983 | 943.3139 |
| 957.5252 | 958.9272 | 963.1861 |
| 964.7290 | 966.0016 | 974.6576 |
| 976.0183 | 976.5163 | 980.8636 |
| 994.4788 | 1006.7321 | 1022.2345 |
| 1024.6777 | 1059.5272 | 1067.2156 |
| 1073.8539 | 1076.2664 | 1084.7928 |
| 1087.6660 | 1090.0292 | 1105.3176 |
| 1115.0483 | 1117.9152 | 1125.7348 |
| 1129.4685 | 1135.8722 | 1140.4467 |
| 1142.6423 | 1146.3125 | 1148.9031 |

| | | |
|---|---|---|
| 1151.5207 | 1153.3318 | 1156.0187 |
| 1172.3744 | 1180.4023 | 1182.0073 |
| 1186.4244 | 1190.6713 | 1195.0961 |
| 1199.7186 | 1210.3794 | 1212.3960 |
| 1219.1050 | 1231.7032 | 1243.5773 |
| 1246.3653 | 1259.8376 | 1276.3836 |
| 1281.0361 | 1291.3131 | 1293.0461 |
| 1293.5838 | 1299.8063 | 1301.4137 |
| 1311.4560 | 1313.9136 | 1320.4871 |
| 1323.3068 | 1325.8095 | 1335.7178 |
| 1342.6674 | 1345.2078 | 1352.7069 |
| 1356.1096 | 1368.6373 | 1372.4761 |
| 1376.2818 | 1384.9255 | 1390.8692 |
| 1398.2296 | 1404.1774 | 1405.9349 |
| 1407.4261 | 1408.0389 | 1409.3603 |
| 1410.1755 | 1419.7647 | 1424.3821 |
| 1427.0045 | 1428.3478 | 1429.7430 |
| 1430.3941 | 1433.3645 | 1453.5269 |
| 1458.2703 | 1476.2536 | 1485.2544 |
| 1485.6157 | 1490.8894 | 1492.5607 |
| 1493.6143 | 1493.9973 | 1496.4036 |
| 1497.9291 | 1498.9840 | 1501.2696 |
| 1503.1263 | 1503.5888 | 1505.1341 |
| 1506.4648 | 1509.1665 | 1512.5759 |
| 1514.2184 | 1515.2111 | 1518.3670 |
| 1520.3474 | 1521.8824 | 1524.6222 |
| 1528.3659 | 1529.9324 | 1531.7972 |
| 1533.9196 | 1538.6748 | 1544.5428 |
| 1575.1056 | 1595.3421 | 1649.7706 |
| 1673.3754 | 1676.1755 | 1682.1384 |
| 1683.6696 | 1822.0657 | 2986.3475 |
| 3059.1411 | 3060.5354 | 3061.2877 |
| 3062.0205 | 3064.0197 | 3064.8799 |
| 3064.9046 | 3070.4810 | 3078.8167 |
| 3083.9106 | 3096.2741 | 3101.0936 |
| 3104.0271 | 3110.2976 | 3123.6937 |
| 3132.4647 | 3134.3300 | 3137.1198 |
| 3138.2261 | 3141.7558 | 3144.2528 |
| 3145.8479 | 3147.8793 | 3149.7675 |
| 3150.7268 | 3150.8576 | 3152.1691 |
| 3156.8488 | 3156.9811 | 3159.6551 |
| 3160.4850 | 3165.3515 | 3168.1424 |
| 3171.8666 | 3178.1231 | 3197.0339 |
| 3199.7056 | 3205.2680 | 3207.5680 |

| | | |
|---|---|---|
| 3211.0574 | 3216.5452 | 3228.9246 |
| 3232.6002 | 3236.1652 | 3236.5118 |
| 3253.8704 | 3261.3622 | 3274.6474 |
| 3296.7826 | 3309.1455 | 3341.0331 |

**TS'v**

Zero-point correction= 0.856741 (Hartree/Particle)
Thermal correction to Energy= 0.903538
Thermal correction to Enthalpy= 0.904482
Thermal correction to Gibbs Free Energy= 0.776767
Sum of electronic and zero-point Energies= -1994.776701
Sum of electronic and thermal Energies= -1994.729904
Sum of electronic and thermal Enthalpies= -1994.728960
Sum of electronic and thermal Free Energies= -1994.856675

| | | | |
|---|---|---|---|
| C | 0.10636300 | 0.25576100 | -0.74207800 |
| C | -0.22617700 | 0.31148800 | -2.95633600 |
| C | 0.90925000 | 0.99433900 | -2.69333200 |
| N | 1.11833700 | 0.93580700 | -1.32263300 |
| H | -0.72756100 | 0.08562000 | -3.88323100 |
| H | 1.61812500 | 1.48221400 | -3.34271500 |
| N | -0.70482100 | -0.14817000 | -1.74352400 |
| C | 2.45105300 | 1.20180700 | -0.80510200 |
| C | 2.73365600 | 2.44151000 | -0.21730100 |
| C | 3.41940100 | 0.21631900 | -1.04780100 |
| C | 4.05092600 | 2.66277400 | 0.18786000 |
| C | 4.72537100 | 0.49794500 | -0.63811300 |
| C | 5.03730600 | 1.70200800 | -0.02122900 |
| H | 4.31136900 | 3.60490300 | 0.65823300 |
| H | 5.50341200 | -0.24140500 | -0.80283000 |
| H | 6.05669300 | 1.89920500 | 0.29446900 |
| C | -1.83424600 | -1.04603600 | -1.62825000 |
| C | -1.56677100 | -2.40739800 | -1.40359400 |
| C | -3.12569600 | -0.52595100 | -1.79486000 |
| C | -2.66658800 | -3.26555300 | -1.34753900 |
| C | -4.18624400 | -1.43263600 | -1.73782200 |
| C | -3.96103900 | -2.78521400 | -1.51525500 |
| H | -2.50757000 | -4.32390000 | -1.17207800 |
| H | -5.20155800 | -1.07200600 | -1.86499400 |
| H | -4.80007700 | -3.47168500 | -1.47025200 |
| C | 3.12389400 | -1.09227200 | -1.76629300 |
| C | 3.47152700 | -2.31313300 | -0.91028200 |
| C | 3.85825700 | -1.13609500 | -3.11283500 |
| H | 2.05231700 | -1.14564600 | -1.98290000 |
| H | 2.84606400 | -2.36603500 | -0.01571500 |

| | | | |
|---|---|---|---|
| H | 3.32251700 | -3.22868500 | -1.49174300 |
| H | 4.51715800 | -2.29216800 | -0.58856900 |
| H | 3.61097400 | -0.26981800 | -3.73331300 |
| H | 4.94282700 | -1.14733100 | -2.96588200 |
| H | 3.58210600 | -2.04231300 | -3.66000400 |
| C | 1.67362700 | 3.51954500 | -0.09569600 |
| C | 1.69580700 | 4.40641000 | -1.34905600 |
| C | 1.82494700 | 4.36487600 | 1.16865800 |
| H | 0.69685200 | 3.03213600 | -0.03137200 |
| H | 1.51061500 | 3.82755800 | -2.25899900 |
| H | 0.92643200 | 5.18046400 | -1.27609600 |
| H | 2.66902000 | 4.89745800 | -1.45236000 |
| H | 1.88031300 | 3.73479900 | 2.05976700 |
| H | 2.71311500 | 5.00346600 | 1.12654600 |
| H | 0.94989500 | 5.01019300 | 1.27630600 |
| C | -3.38833600 | 0.94978400 | -2.05067400 |
| C | -4.54700800 | 1.49235900 | -1.20651700 |
| C | -3.67295300 | 1.18807200 | -3.54060900 |
| H | -2.48930400 | 1.51107600 | -1.76981200 |
| H | -4.39274100 | 1.31583800 | -0.13983800 |
| H | -4.62707700 | 2.57266600 | -1.35752400 |
| H | -5.50042800 | 1.04802400 | -1.50733900 |
| H | -2.85228600 | 0.85029100 | -4.17852400 |
| H | -4.57436500 | 0.64504300 | -3.84280900 |
| H | -3.83724600 | 2.25252800 | -3.72921600 |
| C | -0.15113300 | -2.95917100 | -1.30372000 |
| C | 0.38069900 | -3.26710400 | -2.71151200 |
| C | -0.04503900 | -4.19129200 | -0.40190600 |
| H | 0.49881400 | -2.19576500 | -0.85999300 |
| H | 0.39233000 | -2.37623800 | -3.34787700 |
| H | 1.40018200 | -3.66078700 | -2.65590500 |
| H | -0.25080100 | -4.02030600 | -3.19332900 |
| H | -0.54533000 | -4.02652700 | 0.55761200 |
| H | -0.48101200 | -5.07640200 | -0.87545300 |
| H | 1.00927500 | -4.40658500 | -0.20436300 |
| C | -0.25765000 | -0.00267000 | 0.70472800 |
| C | 0.81647800 | 0.28438700 | 1.76331100 |
| H | 0.29243200 | 0.41772000 | 2.71211900 |
| H | 1.35353500 | 1.21095000 | 1.57186600 |
| C | -1.58118900 | 0.66299500 | 1.09029800 |
| H | -1.83785100 | -0.17682900 | 2.20407300 |
| C | -1.57075400 | 2.06530400 | 1.44270700 |
| O | -0.61774300 | 2.73013800 | 1.83870900 |
| O | -2.81421000 | 2.61176000 | 1.37109900 |

| | | | |
|---|---|---|---|
| C | -2.92820700 | 3.96355000 | 1.82204900 |
| C | -4.38321100 | 4.36001700 | 1.69227900 |
| H | -2.27804700 | 4.60356200 | 1.21630700 |
| H | -2.58160900 | 4.03060200 | 2.85796600 |
| H | -4.52407100 | 5.38605900 | 2.04024800 |
| H | -4.70917000 | 4.29905100 | 0.65110200 |
| H | -5.01471900 | 3.70029500 | 2.29194700 |
| C | 3.13629200 | -0.61453000 | 2.12464900 |
| C | 3.62106900 | -1.84664700 | 2.47348100 |
| C | 1.51784200 | -2.10099100 | 2.18218800 |
| N | 1.78960800 | -0.78986300 | 1.91689500 |
| H | -2.41591500 | 0.39898900 | 0.44535900 |
| H | 3.60370900 | 0.35008400 | 1.98874600 |
| H | 4.64422900 | -2.11933300 | 2.68986200 |
| H | 0.50910800 | -2.50152900 | 2.15591700 |
| N | 2.60465400 | -2.77193500 | 2.50213700 |
| C | -2.18530300 | -2.44720500 | 2.32659600 |
| C | -1.76626000 | -3.44592200 | 3.18241300 |
| C | -1.24304200 | -1.58545200 | 4.06847300 |
| N | -1.85552700 | -1.25315300 | 2.91098900 |
| H | -0.46301300 | -1.08117700 | 0.75047400 |
| H | -2.69433800 | -2.49117400 | 1.37107900 |
| H | -1.86837800 | -4.51740000 | 3.06539200 |
| H | -0.85675900 | -0.83663900 | 4.74985200 |
| N | -1.17055100 | -2.89470900 | 4.28605500 |

Frequencies

| | | |
|---|---|---|
| -1152.3395 | 11.9357 | 28.0848 |
| 31.9186 | 38.1037 | 41.7825 |
| 50.5162 | 52.5704 | 55.7113 |
| 59.5910 | 63.2197 | 69.7463 |
| 74.2315 | 75.9627 | 87.2897 |
| 88.4450 | 93.3930 | 96.5837 |
| 99.4424 | 107.8031 | 112.1479 |
| 118.0553 | 123.8806 | 125.6919 |
| 134.0324 | 145.5682 | 149.4413 |
| 156.5031 | 163.3197 | 171.4968 |
| 173.4784 | 189.9733 | 195.2313 |
| 195.8845 | 202.3970 | 210.6142 |
| 218.7611 | 235.4502 | 241.2491 |
| 253.3677 | 255.2449 | 258.9300 |
| 260.5359 | 267.0249 | 269.6134 |
| 273.9003 | 283.8911 | 294.7652 |
| 300.9998 | 304.1381 | 309.0369 |
| 311.8103 | 317.4786 | 320.6789 |

| | | |
|---|---|---|
| 335.2864 | 342.5748 | 349.1668 |
| 376.2495 | 399.4230 | 407.8899 |
| 419.0633 | 430.5631 | 446.0324 |
| 449.6496 | 459.0537 | 473.3397 |
| 486.5067 | 517.1069 | 530.5599 |
| 533.7917 | 559.0627 | 577.8873 |
| 585.0047 | 596.5080 | 616.1668 |
| 619.6548 | 642.4813 | 651.5219 |
| 653.0559 | 659.0221 | 668.5001 |
| 683.2464 | 688.5641 | 692.7528 |
| 698.9931 | 722.1727 | 749.0969 |
| 752.2333 | 756.3219 | 765.6908 |
| 784.7420 | 788.8240 | 793.3970 |
| 795.0955 | 798.5736 | 806.3437 |
| 828.2644 | 829.9023 | 831.9494 |
| 832.2219 | 835.3692 | 862.9830 |
| 868.4618 | 872.8177 | 881.1866 |
| 894.6998 | 896.0779 | 913.1008 |
| 914.1139 | 921.1879 | 925.8620 |
| 931.0629 | 932.1609 | 934.4191 |
| 936.3844 | 939.3642 | 945.0556 |
| 946.0591 | 946.6684 | 961.0910 |
| 963.8016 | 964.2538 | 975.7170 |
| 978.2393 | 979.4765 | 980.3846 |
| 985.1302 | 1011.8505 | 1015.3724 |
| 1022.0126 | 1029.8042 | 1060.4893 |
| 1067.7677 | 1072.9302 | 1077.3710 |
| 1083.7587 | 1089.7416 | 1099.6198 |
| 1105.6624 | 1107.3837 | 1111.3666 |
| 1122.4070 | 1137.5746 | 1141.0785 |
| 1144.9685 | 1147.5991 | 1151.5654 |
| 1151.9842 | 1154.8961 | 1157.1390 |
| 1165.0446 | 1176.7002 | 1181.2470 |
| 1182.4054 | 1187.6638 | 1192.8594 |
| 1193.3582 | 1209.0443 | 1210.4755 |
| 1214.2428 | 1217.9695 | 1228.2779 |
| 1240.9290 | 1250.1994 | 1262.8187 |
| 1279.9620 | 1287.2249 | 1288.4609 |
| 1292.4560 | 1294.7572 | 1297.6044 |
| 1301.3401 | 1322.4604 | 1325.2440 |
| 1325.5619 | 1328.9484 | 1334.5787 |
| 1336.2250 | 1338.2999 | 1355.6777 |
| 1360.0834 | 1372.4212 | 1375.3604 |
| 1380.9968 | 1383.8742 | 1386.2616 |

| | | |
|---|---|---|
| 1392.7939 | 1394.4814 | 1396.8890 |
| 1405.1381 | 1407.5313 | 1409.3454 |
| 1410.7255 | 1412.3537 | 1425.6498 |
| 1427.0847 | 1427.3721 | 1428.9204 |
| 1431.5857 | 1434.0732 | 1445.8104 |
| 1454.5171 | 1471.9691 | 1480.7988 |
| 1482.3514 | 1484.9242 | 1488.1479 |
| 1491.7025 | 1492.9732 | 1493.2213 |
| 1496.1372 | 1498.1679 | 1499.0910 |
| 1502.4901 | 1504.2372 | 1504.9883 |
| 1506.2483 | 1506.9108 | 1509.7370 |
| 1511.8344 | 1513.2641 | 1513.8771 |
| 1517.5186 | 1521.8279 | 1525.6714 |
| 1528.0536 | 1532.0341 | 1533.9194 |
| 1535.0978 | 1543.9913 | 1547.9698 |
| 1571.6920 | 1587.4038 | 1609.4307 |
| 1640.4912 | 1672.1914 | 1676.6027 |
| 1682.7233 | 1687.2435 | 1772.8404 |
| 3060.3492 | 3061.7130 | 3062.5795 |
| 3064.0607 | 3066.2001 | 3069.9095 |
| 3070.6890 | 3070.9503 | 3071.8567 |
| 3079.0371 | 3079.6000 | 3084.7195 |
| 3088.7653 | 3110.9176 | 3121.6265 |
| 3128.2774 | 3132.7131 | 3142.2637 |
| 3142.7969 | 3143.4181 | 3143.9012 |
| 3145.1681 | 3147.4491 | 3147.9851 |
| 3149.2008 | 3150.3327 | 3150.9260 |
| 3152.1198 | 3153.3755 | 3153.9852 |
| 3162.1003 | 3164.1237 | 3170.2821 |
| 3171.2982 | 3185.9970 | 3200.0553 |
| 3209.5630 | 3211.1095 | 3213.6398 |
| 3223.4302 | 3226.6903 | 3231.0785 |
| 3232.3258 | 3235.7492 | 3240.4443 |
| 3249.3328 | 3256.7614 | 3274.2389 |
| 3303.0893 | 3305.2989 | 3323.5241 |

**V'**

| | |
|---|---|
| Zero-point correction= | 0.787608 (Hartree/Particle) |
| Thermal correction to Energy= | 0.829316 |
| Thermal correction to Enthalpy= | 0.830260 |
| Thermal correction to Gibbs Free Energy= | 0.715800 |
| Sum of electronic and zero-point Energies= | -1768.698896 |
| Sum of electronic and thermal Energies= | -1768.657187 |
| Sum of electronic and thermal Enthalpies= | -1768.656243 |

Sum of electronic and thermal Free Energies= -1768.770703

| | | | |
|---|---|---|---|
| C | 0.10375100 | 0.06258800 | -0.15731300 |
| C | 0.77202300 | 0.62192400 | -2.21014700 |
| C | -0.24245500 | -0.26237100 | -2.33160900 |
| N | -0.67766700 | -0.57337800 | -1.05232200 |
| H | 1.36370100 | 1.13742300 | -2.94882500 |
| H | -0.72980900 | -0.67695300 | -3.19907000 |
| N | 0.95513200 | 0.83591200 | -0.85825900 |
| C | -1.98558600 | -1.18121800 | -0.87718000 |
| C | -2.09487500 | -2.54024100 | -0.54649900 |
| C | -3.09269900 | -0.36797200 | -1.16548800 |
| C | -3.38127000 | -3.07904300 | -0.48603000 |
| C | -4.35572800 | -0.96435900 | -1.10936400 |
| C | -4.50108800 | -2.30265700 | -0.77208400 |
| H | -3.50740700 | -4.12459400 | -0.22591800 |
| H | -5.23471700 | -0.36593300 | -1.32990500 |
| H | -5.49076600 | -2.74615700 | -0.72990400 |
| C | 1.81765200 | 1.86116100 | -0.31158100 |
| C | 1.20165100 | 3.02912900 | 0.18106800 |
| C | 3.20582800 | 1.68897000 | -0.35605100 |
| C | 2.03641700 | 4.03088900 | 0.67505300 |
| C | 3.99315400 | 2.73671700 | 0.13312300 |
| C | 3.41995200 | 3.88692800 | 0.65326500 |
| H | 1.60209500 | 4.94329600 | 1.06820600 |
| H | 5.07405000 | 2.64285100 | 0.10429200 |
| H | 4.05151600 | 4.68253100 | 1.03531600 |
| C | -2.97941700 | 1.09773100 | -1.55893000 |
| C | -3.77383900 | 2.00533400 | -0.61558000 |
| C | -3.41944700 | 1.29979900 | -3.01429800 |
| H | -1.93167900 | 1.40382500 | -1.49073700 |
| H | -3.37379500 | 1.97285100 | 0.40087200 |
| H | -3.73249600 | 3.03951100 | -0.97185800 |
| H | -4.82803300 | 1.71451100 | -0.57131500 |
| H | -2.85046300 | 0.66339700 | -3.69800100 |
| H | -4.48125100 | 1.06375300 | -3.13722300 |
| H | -3.26833400 | 2.34270200 | -3.30904600 |
| C | -0.86406200 | -3.39345400 | -0.31724900 |
| C | -0.35384800 | -3.94594400 | -1.65401400 |
| C | -1.09271000 | -4.52484200 | 0.68559900 |
| H | -0.06502300 | -2.75163700 | 0.06117400 |
| H | -0.10123900 | -3.13490600 | -2.34241800 |
| H | 0.55387900 | -4.53221400 | -1.48730300 |
| H | -1.10795700 | -4.58698300 | -2.12412300 |
| H | -1.53169100 | -4.15851900 | 1.61936200 |

| | | | |
|---|---|---|---|
| H | -1.74999300 | -5.30275400 | 0.28333300 |
| H | -0.13493500 | -4.99589800 | 0.92277800 |
| C | 3.87290500 | 0.46696400 | -0.96023000 |
| C | 4.94591000 | -0.10969900 | -0.02952500 |
| C | 4.48928500 | 0.82872200 | -2.31927300 |
| H | 3.11717900 | -0.31110300 | -1.10483900 |
| H | 4.51483300 | -0.39212300 | 0.93366300 |
| H | 5.38022300 | -1.00645700 | -0.48302000 |
| H | 5.76358600 | 0.59969800 | 0.13424400 |
| H | 3.74752700 | 1.23802000 | -3.01177300 |
| H | 5.27880000 | 1.57874200 | -2.19963000 |
| H | 4.93237200 | -0.05871600 | -2.78061900 |
| C | -0.30097300 | 3.26261600 | 0.09120800 |
| C | -0.65003800 | 3.77918000 | -1.31357800 |
| C | -0.83454800 | 4.22897600 | 1.15186300 |
| H | -0.82257600 | 2.30982300 | 0.24571900 |
| H | -0.35416500 | 3.07213900 | -2.09474500 |
| H | -1.72642100 | 3.95559500 | -1.40126500 |
| H | -0.13264400 | 4.72598500 | -1.49909300 |
| H | -0.45351000 | 3.98979700 | 2.14910500 |
| H | -0.56063500 | 5.26417300 | 0.92565700 |
| H | -1.92673300 | 4.17158400 | 1.18027000 |
| C | 0.23743600 | -0.07265300 | 1.33747200 |
| C | -0.94733000 | -0.69507200 | 2.09453900 |
| H | -0.58018800 | -0.89206200 | 3.10480600 |
| H | -1.23014700 | -1.65529900 | 1.66415700 |
| C | 1.50689800 | -0.82705600 | 1.65991600 |
| C | 2.12074800 | -1.72392300 | 0.81090100 |
| O | 1.85342400 | -1.99865700 | -0.38813100 |
| O | 3.19987500 | -2.37602000 | 1.41281700 |
| C | 3.87546000 | -3.31814000 | 0.59870500 |
| C | 5.15125400 | -3.70619700 | 1.31937100 |
| H | 4.08981000 | -2.88487000 | -0.38357700 |
| H | 3.23793200 | -4.19628300 | 0.42593500 |
| H | 5.70539000 | -4.45234100 | 0.74377300 |
| H | 5.78950600 | -2.82881000 | 1.45811400 |
| H | 4.92732700 | -4.12471300 | 2.30410500 |
| C | -3.44454400 | -0.32565400 | 2.09218500 |
| C | -4.23774500 | 0.70380100 | 2.52465000 |
| C | -2.22522500 | 1.38949600 | 2.70500400 |
| N | -2.15238300 | 0.12798400 | 2.19653100 |
| H | 1.88506100 | -0.70497500 | 2.66712200 |
| H | -3.66420700 | -1.31373600 | 1.71369200 |
| H | -5.31699200 | 0.73684700 | 2.56643900 |

| | | | |
|---|---|---|---|
| H | -1.34022000 | 1.96768900 | 2.93386500 |
| N | -3.46695200 | 1.77733500 | 2.90402000 |
| H | 0.34254200 | 0.96114000 | 1.70355700 |

Frequencies

| | | |
|---|---|---|
| 15.2995 | 33.4536 | 41.2870 |
| 43.8005 | 49.1840 | 54.1589 |
| 63.3032 | 70.8894 | 75.0721 |
| 79.7006 | 89.8015 | 94.0007 |
| 105.6740 | 113.0776 | 117.2208 |
| 123.5381 | 130.5465 | 131.8817 |
| 138.5033 | 143.4269 | 150.6039 |
| 153.8378 | 156.5080 | 169.8108 |
| 178.8507 | 188.2398 | 192.2896 |
| 199.2958 | 212.7230 | 230.8002 |
| 237.3814 | 241.1452 | 245.9996 |
| 253.7174 | 258.5539 | 268.1730 |
| 271.6166 | 276.0591 | 277.9703 |
| 292.0180 | 298.2431 | 301.6680 |
| 307.6753 | 308.4876 | 314.1594 |
| 318.6478 | 323.6048 | 328.5486 |
| 332.2815 | 341.1478 | 357.5977 |
| 358.5504 | 397.4442 | 412.8366 |
| 417.9457 | 444.5497 | 446.7462 |
| 450.9871 | 462.3317 | 475.0866 |
| 514.7622 | 530.8140 | 533.9365 |
| 550.8874 | 576.9502 | 583.1977 |
| 592.5372 | 604.4628 | 614.8106 |
| 620.7242 | 641.8620 | 650.4151 |
| 651.7463 | 656.8948 | 664.3165 |
| 686.3277 | 688.2308 | 722.5683 |
| 748.8454 | 754.8393 | 759.5471 |
| 765.6943 | 770.2705 | 785.0514 |
| 791.4994 | 798.0068 | 812.7589 |
| 817.3407 | 828.6206 | 831.4690 |
| 834.1721 | 834.8882 | 849.3103 |
| 874.7646 | 903.9588 | 912.1811 |
| 912.9077 | 914.6312 | 924.1998 |
| 929.1838 | 937.3765 | 938.1093 |
| 942.8961 | 945.0898 | 947.9396 |
| 948.6908 | 962.7345 | 963.1709 |
| 963.5560 | 976.2015 | 977.0167 |
| 978.9865 | 980.9474 | 989.0347 |
| 1015.0558 | 1016.4924 | 1028.8558 |
| 1060.6972 | 1073.6390 | 1075.9031 |

| | | |
|---|---|---|
| 1078.2688 | 1088.7299 | 1091.5450 |
| 1095.4720 | 1104.4536 | 1115.6869 |
| 1123.4657 | 1136.6080 | 1142.6971 |
| 1146.3292 | 1150.6291 | 1151.7374 |
| 1155.5986 | 1160.1668 | 1162.2149 |
| 1170.3341 | 1178.6422 | 1181.8563 |
| 1183.6990 | 1192.2935 | 1192.9367 |
| 1195.1145 | 1210.0882 | 1210.9605 |
| 1218.3897 | 1223.1588 | 1243.5999 |
| 1257.1900 | 1271.7612 | 1279.9802 |
| 1285.8464 | 1291.5926 | 1292.5723 |
| 1304.1558 | 1323.1769 | 1324.9220 |
| 1328.3807 | 1329.0909 | 1334.4404 |
| 1356.2414 | 1359.7692 | 1368.7428 |
| 1374.1777 | 1377.3517 | 1380.9432 |
| 1384.2365 | 1394.1301 | 1401.3988 |
| 1403.0383 | 1407.2414 | 1408.8132 |
| 1409.9511 | 1414.8207 | 1418.7482 |
| 1423.8483 | 1424.7621 | 1425.9009 |
| 1429.2067 | 1429.7211 | 1430.3082 |
| 1444.7437 | 1476.7101 | 1483.0013 |
| 1487.0226 | 1489.3717 | 1490.1242 |
| 1491.0416 | 1491.5248 | 1494.2286 |
| 1494.8098 | 1499.0420 | 1500.6996 |
| 1504.2427 | 1504.6079 | 1505.2774 |
| 1505.8444 | 1508.8933 | 1510.0460 |
| 1515.0230 | 1516.7836 | 1518.4090 |
| 1523.8540 | 1526.4677 | 1530.2567 |
| 1531.1478 | 1540.1493 | 1546.4305 |
| 1551.7026 | 1571.0447 | 1585.2134 |
| 1641.3022 | 1673.8516 | 1679.1536 |
| 1685.1593 | 1686.2587 | 1715.2905 |
| 3025.9349 | 3052.2126 | 3056.4955 |
| 3059.0104 | 3059.2754 | 3060.8504 |
| 3060.9725 | 3062.7057 | 3065.1682 |
| 3065.7132 | 3069.6952 | 3080.8980 |
| 3112.6348 | 3118.9910 | 3119.4214 |
| 3125.9568 | 3126.5087 | 3134.4634 |
| 3137.7966 | 3139.7436 | 3142.6111 |
| 3144.3872 | 3144.6873 | 3145.9853 |
| 3146.0927 | 3147.7445 | 3148.4172 |
| 3149.1008 | 3149.4695 | 3149.6043 |
| 3150.9545 | 3153.4531 | 3153.9575 |
| 3169.8625 | 3173.7062 | 3197.3787 |

| | | |
|---|---|---|
| 3206.6335 | 3206.7200 | 3219.1580 |
| 3223.7705 | 3226.9555 | 3233.5735 |
| 3237.8709 | 3266.6512 | 3282.7092 |
| 3290.1814 | 3302.0415 | 3321.8455 |

**TS'$_{VI}$**

Zero-point correction= 0.784189 (Hartree/Particle)
Thermal correction to Energy= 0.826634
Thermal correction to Enthalpy= 0.827578
Thermal correction to Gibbs Free Energy= 0.708363
Sum of electronic and zero-point Energies= -1768.673984
Sum of electronic and thermal Energies= -1768.631540
Sum of electronic and thermal Enthalpies= -1768.630595
Sum of electronic and thermal Free Energies= -1768.749810

| | | | |
|---|---|---|---|
| C | -0.13096100 | 0.31761800 | -0.39816300 |
| C | 0.45840400 | 1.09925800 | -2.45196300 |
| C | -0.52264200 | 0.18918400 | -2.63574000 |
| N | -0.86398600 | -0.27817900 | -1.37024100 |
| H | 0.99729400 | 1.71775300 | -3.15125200 |
| H | -1.02561400 | -0.15223300 | -3.52707300 |
| N | 0.68658300 | 1.15856300 | -1.08268900 |
| C | -2.05972700 | -1.04507900 | -1.13598600 |
| C | -1.96877900 | -2.43752800 | -0.98484300 |
| C | -3.27419100 | -0.34742800 | -1.10588100 |
| C | -3.16091400 | -3.13696000 | -0.78643100 |
| C | -4.43974100 | -1.09410200 | -0.91081000 |
| C | -4.38501500 | -2.47256200 | -0.75311900 |
| H | -3.13490600 | -4.21374800 | -0.65857000 |
| H | -5.39840800 | -0.58420800 | -0.87423700 |
| H | -5.30001900 | -3.03585000 | -0.59911900 |
| C | 1.62178600 | 2.06377200 | -0.46915300 |
| C | 1.11246300 | 3.09869900 | 0.33796700 |
| C | 2.99299700 | 1.88988400 | -0.70709800 |
| C | 2.03216900 | 3.97366100 | 0.91606100 |
| C | 3.86934700 | 2.80871800 | -0.12046600 |
| C | 3.39760100 | 3.83511300 | 0.68508200 |
| H | 1.67893900 | 4.78020300 | 1.54929600 |
| H | 4.93675300 | 2.70929800 | -0.29157700 |
| H | 4.09542700 | 4.53215400 | 1.13790800 |
| C | -3.35866400 | 1.16159200 | -1.27673800 |
| C | -3.86426800 | 1.83654000 | 0.00127500 |
| C | -4.23200400 | 1.53000400 | -2.48160000 |
| H | -2.35398200 | 1.55033100 | -1.47121800 |
| H | -3.17281000 | 1.67466500 | 0.83352600 |

| | | | |
|---|---|---|---|
| H | -3.97295600 | 2.91402900 | -0.15984400 |
| H | -4.84119500 | 1.44214700 | 0.29959500 |
| H | -3.86704800 | 1.05485100 | -3.39683000 |
| H | -5.27038600 | 1.21892100 | -2.32829900 |
| H | -4.22612500 | 2.61396900 | -2.62988300 |
| C | -0.62969200 | -3.14950000 | -1.08206000 |
| C | -0.27501400 | -3.40684200 | -2.55370700 |
| C | -0.58595100 | -4.45671700 | -0.29147400 |
| H | 0.13543400 | -2.49090200 | -0.65525200 |
| H | -0.21489200 | -2.47653800 | -3.12479600 |
| H | 0.69212500 | -3.91322000 | -2.62580900 |
| H | -1.03220100 | -4.04596800 | -3.02030700 |
| H | -0.91990500 | -4.31265000 | 0.73984200 |
| H | -1.20583600 | -5.22974600 | -0.75814500 |
| H | 0.44294900 | -4.82035600 | -0.25447000 |
| C | 3.54214300 | 0.77104300 | -1.57912600 |
| C | 4.72478800 | 0.04350200 | -0.92925600 |
| C | 3.96956300 | 1.32070400 | -2.94801000 |
| H | 2.74598100 | 0.03306700 | -1.72669200 |
| H | 4.46321800 | -0.36889000 | 0.04712100 |
| H | 5.03434700 | -0.78735400 | -1.57124900 |
| H | 5.58871100 | 0.70566100 | -0.81621500 |
| H | 3.15606800 | 1.83734900 | -3.46343700 |
| H | 4.78911400 | 2.03686900 | -2.82576700 |
| H | 4.32188000 | 0.50896100 | -3.59095600 |
| C | -0.38597800 | 3.30312800 | 0.51903700 |
| C | -0.96416500 | 3.99477200 | -0.72477200 |
| C | -0.75212000 | 4.08507500 | 1.78081800 |
| H | -0.85769300 | 2.31757500 | 0.60691200 |
| H | -0.76844300 | 3.41987100 | -1.63529800 |
| H | -2.04679300 | 4.12009700 | -0.62480100 |
| H | -0.51406900 | 4.98582800 | -0.84580100 |
| H | -0.24771700 | 3.68529500 | 2.66607500 |
| H | -0.49114800 | 5.14478500 | 1.69172300 |
| H | -1.83162100 | 4.02041400 | 1.94640200 |
| C | 0.59219000 | -0.15702700 | 1.52139000 |
| C | -0.51251400 | -1.05593900 | 2.03054100 |
| H | -0.15198400 | -1.56038200 | 2.93284200 |
| H | -0.75630800 | -1.83855100 | 1.31409100 |
| C | 1.90016900 | -0.60835700 | 1.44043100 |
| C | 2.23259300 | -2.00025000 | 1.38782600 |
| O | 1.45743700 | -2.95503900 | 1.40695000 |
| O | 3.58088700 | -2.20294300 | 1.33737300 |
| C | 4.00462200 | -3.56373800 | 1.26391600 |

| | | | |
|---|---|---|---|
| C | 5.51277100 | -3.55678000 | 1.13186800 |
| H | 3.52597100 | -4.04805100 | 0.40630200 |
| H | 3.67981500 | -4.09718500 | 2.16337200 |
| H | 5.89003800 | -4.57998500 | 1.06610000 |
| H | 5.81473800 | -3.01585900 | 0.23137000 |
| H | 5.97252500 | -3.07202700 | 1.99638600 |
| C | -3.00606200 | -0.84885500 | 2.21002100 |
| C | -3.83893500 | 0.03114000 | 2.84953300 |
| C | -1.86472900 | 0.80988900 | 3.07362000 |
| N | -1.74111400 | -0.33600000 | 2.34981200 |
| H | 2.70796400 | 0.10938700 | 1.37766400 |
| H | -3.18357300 | -1.76313000 | 1.66190400 |
| H | -4.91536800 | -0.01712400 | 2.93423300 |
| H | -1.00955800 | 1.40356000 | 3.36651700 |
| N | -3.11803500 | 1.07109200 | 3.38424300 |
| H | 0.48130300 | 0.88865300 | 1.79732100 |

Frequencies

| | | |
|---|---|---|
| -243.6181 | 11.8943 | 13.8738 |
| 26.5116 | 34.0293 | 39.8391 |
| 49.4510 | 54.6893 | 57.1098 |
| 63.3931 | 65.4959 | 71.7445 |
| 84.9585 | 86.5286 | 95.2636 |
| 100.8650 | 107.1037 | 110.8112 |
| 119.5004 | 130.8875 | 133.4098 |
| 141.4721 | 145.9312 | 153.2352 |
| 160.9415 | 164.9105 | 176.6871 |
| 177.6721 | 186.3303 | 198.7223 |
| 213.7593 | 228.9258 | 233.4617 |
| 240.6096 | 245.7208 | 251.9511 |
| 260.9195 | 268.0932 | 269.8309 |
| 276.0622 | 284.0693 | 294.3008 |
| 297.3024 | 301.4762 | 303.4327 |
| 310.5301 | 317.4128 | 320.9288 |
| 323.2934 | 331.1605 | 340.4123 |
| 343.1250 | 385.3239 | 402.0426 |
| 411.9039 | 418.4723 | 441.8320 |
| 447.2991 | 449.2064 | 449.8822 |
| 461.3167 | 478.8140 | 532.8839 |
| 533.3364 | 563.1777 | 573.7787 |
| 580.4935 | 586.6788 | 600.4361 |
| 620.9739 | 641.2941 | 644.1951 |
| 651.8795 | 655.3751 | 679.8709 |
| 686.4652 | 705.7010 | 722.6472 |
| 732.1036 | 744.7439 | 757.5940 |

763.7780 784.4436 788.2169
790.8581 798.6264 811.3657
822.0321 829.6211 830.4439
832.3509 834.9655 846.5751
864.3265 890.5704 912.7256
916.1111 919.7550 925.2549
928.6394 932.9088 934.1766
936.0839 941.8543 942.9441
945.2361 960.2400 962.7303
965.2709 973.7589 974.5297
975.4204 978.0716 978.8534
980.7920 1009.3910 1015.3683
1058.1462 1067.7980 1074.1063
1076.5610 1087.7781 1089.4544
1092.2368 1105.3430 1110.3144
1112.5788 1116.6294 1131.8524
1138.7160 1144.4757 1147.9585
1149.7099 1154.8438 1155.3525
1158.8882 1162.1214 1178.8336
1179.8155 1187.4193 1190.8728
1194.7453 1210.1766 1211.7930
1214.1584 1229.1068 1247.6752
1256.4026 1280.2208 1283.9355
1289.8923 1290.7809 1293.6994
1302.2663 1315.6435 1324.0721
1330.1332 1331.5659 1332.8280
1335.0251 1338.5390 1342.8150
1347.9257 1355.2630 1373.6866
1380.7617 1387.5110 1393.7514
1397.4832 1404.1254 1404.9752
1407.4212 1411.2171 1422.0842
1423.2032 1423.8147 1426.0200
1427.1898 1431.9449 1434.0257
1438.2732 1456.1286 1461.6652
1470.9541 1480.0463 1486.5121
1488.5825 1491.2810 1492.4425
1494.9671 1496.8615 1498.1044
1500.3338 1503.8007 1504.6629
1505.4709 1506.0633 1507.5399
1512.1699 1512.7157 1514.7787
1518.4432 1526.4001 1530.0246
1532.3191 1533.1451 1534.6762
1562.3635 1576.6138 1584.5696
1636.5928 1677.8388 1678.5989

| | | |
|---|---|---|
| 1683.4676 | 1684.5993 | 1747.7618 |
| 3055.5757 | 3057.9431 | 3059.1153 |
| 3059.3909 | 3061.6730 | 3064.1950 |
| 3065.0001 | 3066.3039 | 3075.9021 |
| 3081.3467 | 3090.2922 | 3091.0076 |
| 3095.1875 | 3105.4412 | 3108.1433 |
| 3122.5200 | 3135.0702 | 3135.6431 |
| 3135.6746 | 3138.6271 | 3141.4288 |
| 3141.7763 | 3141.8555 | 3142.7846 |
| 3144.7449 | 3147.5212 | 3151.6136 |
| 3154.4270 | 3157.7954 | 3161.3715 |
| 3162.0634 | 3162.6705 | 3163.0063 |
| 3175.8285 | 3185.6515 | 3196.6977 |
| 3196.8431 | 3211.4805 | 3212.0745 |
| 3219.9652 | 3230.0572 | 3233.7790 |
| 3242.6373 | 3266.3525 | 3284.9066 |
| 3289.4813 | 3291.8142 | 3315.8306 |

**P’**

Zero-point correction= 0.206908 (Hartree/Particle)
Thermal correction to Energy= 0.219598
Thermal correction to Enthalpy= 0.220542
Thermal correction to Gibbs Free Energy= 0.165202
Sum of electronic and zero-point Energies= -609.676331
Sum of electronic and thermal Energies= -609.663641
Sum of electronic and thermal Enthalpies= -609.662697
Sum of electronic and thermal Free Energies= -609.718037

| | | | |
|---|---|---|---|
| C | -0.38612700 | 0.85638900 | 0.40461600 |
| C | -1.07965800 | -0.34284400 | -0.19052200 |
| H | -0.79268900 | -1.25597100 | 0.33734000 |
| H | -0.77736300 | -0.48784400 | -1.23135700 |
| C | 0.93443100 | 1.03427200 | 0.49530400 |
| C | 1.89723900 | 0.02687900 | 0.00183200 |
| O | 1.59776300 | -1.02682800 | -0.52460000 |
| O | 3.16096400 | 0.41440500 | 0.20675400 |
| C | 4.17617700 | -0.50178100 | -0.23987000 |
| C | 5.51599900 | 0.11814500 | 0.08536600 |
| H | 4.04912200 | -0.66795900 | -1.31345700 |
| H | 4.03040200 | -1.45998700 | 0.26689700 |
| H | 6.31840500 | -0.54603000 | -0.24285900 |
| H | 5.62995600 | 1.07800400 | -0.42313400 |
| H | 5.61608800 | 0.27805200 | 1.16116800 |
| C | -3.30578500 | 0.62609700 | -0.88462700 |
| C | -4.58566100 | 0.44641600 | -0.42991400 |

| | | | |
|---|---|---|---|
| C | -3.35702600 | -0.83802700 | 0.74888200 |
| N | -2.52539700 | -0.20897400 | -0.12193400 |
| H | 1.34588500 | 1.93205200 | 0.94185500 |
| H | -2.88397300 | 1.24479800 | -1.66187400 |
| H | -5.48794500 | 0.92251200 | -0.78613000 |
| H | -2.98439500 | -1.55431800 | 1.46895200 |
| N | -4.60989300 | -0.47245900 | 0.59178500 |
| H | -1.04381200 | 1.63282200 | 0.78999800 |

Frequencies

| | | |
|---|---|---|
| 23.8081 | 34.7649 | 59.5491 |
| 69.1687 | 94.3106 | 128.3362 |
| 147.6660 | 187.4533 | 271.2007 |
| 325.7493 | 340.1134 | 371.9597 |
| 378.8800 | 399.1040 | 548.5756 |
| 647.1111 | 652.0870 | 685.7470 |
| 726.0070 | 759.6246 | 806.0436 |
| 828.4667 | 830.3339 | 858.7900 |
| 882.1644 | 915.9486 | 925.7754 |
| 959.9159 | 970.3775 | 1036.7849 |
| 1062.2537 | 1067.1189 | 1096.4858 |
| 1109.7967 | 1152.9710 | 1159.4751 |
| 1186.8710 | 1219.6201 | 1230.7243 |
| 1284.0077 | 1289.6336 | 1302.9598 |
| 1330.4930 | 1356.9524 | 1394.9064 |
| 1430.4935 | 1439.3888 | 1445.1178 |
| 1458.1346 | 1463.1913 | 1495.5034 |
| 1504.0341 | 1530.8461 | 1576.8935 |
| 1592.4062 | 1751.8330 | 1820.6494 |
| 3081.5941 | 3096.5570 | 3107.3638 |
| 3142.7446 | 3152.8760 | 3168.0652 |
| 3171.9771 | 3198.5661 | 3237.0955 |
| 3264.7592 | 3287.4844 | 3294.5304 |