# Electronic supporting information

## Experimental and theoretical study of the mechanism and rate constants of the sequential 5-*exo*-*trig* spirocyclization involving vinyl, aryl and *N*-alkoxyaminyl radicals

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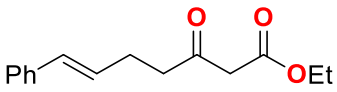
# 1. Experimental procedures

### General information

Reactions were monitored by thin layer chromatography (TLC) on 0.2 mm silica gel F254 plates (Merck); the spots were visualized under UV light (254 nm). Column chromatography and flash column chromatography were conducted under silica gel (Merck, 70−230 mesh). All the reagents and solvents were commercially available and used as received. $^{1}H$ and $^{13}C$ NMR spectra were acquired on a Bruker Avance spectrometer (300 and 75 MHz, respectively) in $CDCl_3$. All chemical shifts are quoted in respect to residual proton signals of $CDCl_3$ (7.28 ppm for $^{1}H$ and 77.0 ppm for $^{13}C$). Chemical shifts were assigned with the help of HSQC, HMBC, and COSY experiments. The assignment of *trans*/*cis* configuration was made by NOESY experiments. High-resolution mass spectra (HRMS) were recorded on a Shimadzu LC-MS QTOF 9030 Nexera X2 system using electrospray ionization (ESI).

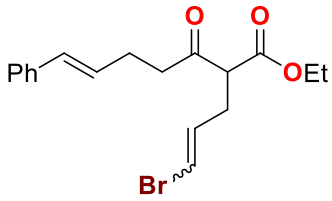
### Ethyl (*E*)-3-oxo-7-phenylhept-6-enoate (11)




Ethyl acetoacetate (**9**) (1.8 mL, 14.2 mmol) was added dropwise to a suspension of NaH (739 mg, 18.5 mmol) in anhydrous THF (7.9 mL) at room temperature. After 20 minutes stirring under argon, *n*-butyllithium (6.8 mL, 17.1 mmol) was added at -78 °C. The mixture was kept at that temperature for 30 min. Then, the cinnamyl bromide (**10**) (3466 mg, 17.1 mmol) was added slowly. The reaction mixture was stirred under argon for 2 h at 0 °C and quenched by adding a saturated solution of $NH_4Cl$. Subsequently, extractions were carried out with ethyl acetate, and the organic phase was dried with $Na_2SO_4$ and concentrated under reduced pressure. Purification by flash column chromatography (CCR) (70-230 mesh silica gel, hexane-$CH_2Cl_2$) yielded 2136 mg (61%) of ethyl (*E*)-3-oxo-7-phenylhept-6-enoate (**11**) as a pale yellow oil.

$^{1}H$ NMR (300 MHz, $CDCl_3$): $\delta$ (ppm) 1.30 (t, *J* = 7.2 Hz, 3H), 2.47 – 2.58 (m, 2H), 2.75 (t, *J* = 7.2 Hz, 2H), 3.48 (s, 2H), 4.22 (q, *J* = 7.2 Hz, 2H), 6.21 (dt, *J* = 6.8, 15.8 Hz, 1H), 6.44 (d, *J* = 15.8 Hz, 1H), 7.18 – 7.26 (m, 1H), 7.27 – 7.40 (m, 4H); $^{13}C$ NMR (75 MHz, $CDCl_3$): $\delta$ (ppm) 14.2, 26.8, 42.5, 49.4, 61.4, 126.0, 127.2, 128.4, 128.5, 131.0, 137.3, 167.2, 202.1. HRMS (ESI) calcd for $C_{15}H_{18}O_3$ ($M + H^+$): 247.13287, found: 247.13229.

### Ethyl (6*E*)-2-(3-bromoallyl)-3-oxo-7-phenylhept-6-enoate (13)

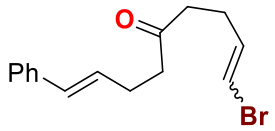



To a suspension of potassium *tert*-butoxide (719 mg, 6.1 mmol) in anhydrous THF (20.3 mL) at 20 °C was added dropwise ethyl (*E*)-3-oxo-7-phenylhept-6-enoate (**11**) (1500 mg, 6.1 mmol) and the mixture was stirred under argon for 10 min. After this time 1,3-dibromopropene, mixture of cis and trans (**12**) (0.62 mL, 6.1 mmol) was added and the reaction mixture was stirred under argon overnight at room temperature. The reaction was quenched by the addition of saturated NaCl solution, extracted with ethyl acetate, and the organic phase was dried over $Na_2SO_4$ and concentrated under reduced pressure. Purification by CCR with 70-230 mesh silica gel using $CH_2Cl_2$/hexanes as eluent afforded 1157 mg (52%) of oxoester **13** as a pale yellow oil.

$^{1}H$ NMR (300 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 1.28 (t, *J* = 7.1 Hz, 6H), 2.47 – 2.89 (m, 12H), 3.56 (t, *J* = 7.3 Hz, 1H), 3.64 (t, *J* = 7.3 Hz, 1H), 4.21 (q, *J* = 7.0 Hz, 4H), 6.03 – 6.29 (m, 6H), 6.44 (d, *J* = 15.8 Hz, 2H), 7.19 – 7.27 (m, 1H), 7.27 – 7.38 (m, 2H); $^{13}C$ NMR (75 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 14.1, 14.1, 26.8, 26.9, 28.2, 31.2, 41.6, 41.9, 57.4, 57.9, 61.7, 61.8, 107.7, 110.6, 126.0, 127.2,

127.2, 128.2, 128.3, 128.5, 130.7, 131.1, 131.1, 133.5, 137.3, 137.3, 168.6, 168.9, 203.1, 203.5. HRMS (ESI) calcd for $C_{18}H_{21}BrO_3$ (M + $H^+$): 365.07468, found: 365.07449.

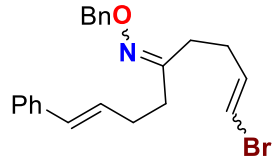
**(1*EZ*,8*E*)-1-Bromo-9-phenylnona-1,8-dien-5-one (14)**




A mixture of compound **13** (1000 mg, 2.7 mmol), lithium chloride (237 mg, 5.5 mmol), and $H_2O$ (49 mg, 2.7 mmol) in 11 mL of DMSO was heated at 180 °C for 1 hour. When the mixture reached room temperature, saturated NaCl solution was added, and it was extracted several times with hexane. The combined organics were dried over $Na_2SO_4$ and evaporated to dryness. Purification by CCR with 70-230 mesh silica, using a $CH_2Cl_2$/hexanes solution as eluant, yielded 554 mg (69%) of (1*EZ*,8*E*)-1-bromo-9-phenylnona-1,8-dien-5-one (**14**) as a yellow oil.

$^1$H NMR (300 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 2.35 (2 H, dt, *J* 8.0, 6.7), 2.45 – 2.66 (m, 14 H), 6.06 – 6.28 (m, 2H), 6.44 (d, *J* 15.8, 6H), 7.19 – 7.27 (m, 2H), 7.27 – 7.39 (m, 8H); $^{13}$C NMR (75 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 24.0, 26.9, 27.1, 27.1, 40.9, 41.4, 42.2, 42.4, 105.6, 108.9, 126.0, 127.2, 127.2, 128.6, 128.7, 128.8, 130.8, 130.9, 133.3, 136.3, 137.3, 137.4, 208.4, 208.8. HRMS (ESI) calcd for $C_{15}H_{17}BrO$ (M + $H^+$): 293.05355, found: 293.05318.

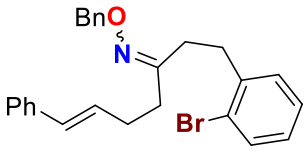
**(1*EZ*,5*EZ*,8*E*)-1-Bromo-9-phenylnona-1,8-dien-5-one *O*-benzyl oxime (15)**




A solution of ketone **14** (500 mg, 1.7 mmol), *O*-benzylhydroxylamine hydrochloride (330 mg, 2.0 mmol), and dry pyridine (0.4 mL, 5.1 mmol) in $CH_2Cl_2$ (6.8 mL) was stirred at room temperature for 5 hours. Purification by CCR (silica gel 70-230 mesh, hexane-$CH_2Cl_2$) yielded (1*EZ*,5*EZ*,8*E*)-1-bromo-9-phenylnona-1,8-dien-5-one *O*-benzyl oxime (**15**) as a pale yellow oil (550 mg, 81%).

$^1$H NMR (300 MHz, $CDCl_3$), measurement was performed using a mixture of four isomers: $\delta$ (ppm) 2.26 – 2.61 (32 H, m), 5.13 (4 H, s), 5.14 (4 H, s), 6.02 – 6.31 (12 H, m), 6.37 – 6.50 (4 H, m), 7.21 – 7.44 (40 H, m); $^{13}$C NMR (75 MHz, $CDCl_3$), measurement was performed using a mixture of four isomers: $\delta$ (ppm) 26.17, 26.53, 26.83, 27.71, 28.28, 28.55, 29.17, 29.22, 29.44, 29.54, 29.76, 29.81, 32.70, 33.42, 34.07, 34.23, 75.53, 75.58, 105.32, 105.36, 108.53, 108.73, 126.08, 126.14, 127.06, 127.10, 127.14, 127.65, 127.70, 128.06, 128.33, 128.39, 128.54, 129.23, 129.29, 129.33, 129.40, 130.63, 130.66, 130.69, 133.59, 133.68, 136.75, 136.84, 137.49, 137.57, 138.29, 138.36, 158.98, 159.03, 159.34, 159.39; HRMS (ESI) calcd for $C_{22}H_{24}BrNO$ (M + $H^+$): 398.11140, found: 398.11108.

**(3*EZ*,6*E*)-1-(2-Bromophenyl)-7-phenylhept-6-en-3-one *O*-benzyl oxime (5c)**




Oxime ether **5c** was prepared according to previously reported procedures.[1] A solution of (*E*)-1-(2-bromophenyl)-7-phenylhept-6-en-3-one (250 mg, 0.7 mmol), *O*-benzylhydroxylamine hydrochloride (141 mg, 0.9 mmol), and dry pyridine (0.2 mL, 2.2 mmol) in

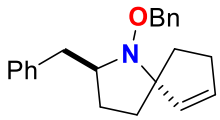
$CH_2Cl_2$ (2.9 mL) was stirred at room temperature for 5 hours. Purification by CCR (silica gel 70-230 mesh, hexane-$CH_2Cl_2$) yielded (3*EZ*,6*E*)-1-(2-bromophenyl)-7-phenylhept-6-en-3-one *O*-benzyl oxime (**5c**) as a pale yellow oil (245 mg, 75%).

$^1$H NMR (300 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 2.32 – 2.77 (m, 12H), 2.98 – 3.09 (m, 4H), 5.20 (s, 4H), 6.18 – 6.32 (m, 2H), 6.32 – 6.51 (m, 2H), 7.05 – 7.52 (m, 28H), 7.59 (d, *J* = 7.4 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 28.60, 29.00, 29.34, 29.76, 32.24, 33.13, 34.48, 34.56, 75.58, 75.60, 124.36, 124.42, 126.00, 126.13, 127.08, 127.59, 127.70, 127.89, 127.99, 128.14, 128.40, 128.57, 129.40, 130.57, 130.66, 132.86, 137.55, 137.63, 138.40, 140.62, 140.75, 159.64. Other spectroscopic data were previously reported in the literature.[20]

### Radical reaction of oxime ethers 15

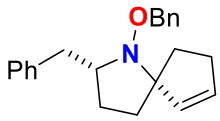
A flask was charged with the oxime ether 15 (300 mg, 0.75 mmol), tributyltin hydride (0.23 mL, 0.83 mmol), and AIBN (37.9 mg, 0.23 mmol) with benzene (25.1 mL) to reach a 0.03 M solution. The mixture was degassed with argon by cycles of freezing and thawing with liquid nitrogen, and the contents were placed into a mineral oil bath heated at 80 °C. The reaction mixture was stirred until the starting material was consumed (monitored by TLC).
After removal of benzene, the residue was dissolved in ethyl acetate (3 mL), mixed with 2 mL of an aqueous solution of KF (10%), and stirred overnight. The white solid was filtered, the liquid phase extracted with ethyl acetate, and the combined organic extracts dried with anhydrous sodium sulphate. Finally, the solvent was removed under reduced pressure and the crude product filtered on a short column charged with a silica gel 70−230 mesh and eluted with hexane to remove organotin by-products. After evaporation of the solvent, the crude product was purified by preparative plate chromatography (silica gel, 1000 µm, 10 cm × 20 cm) with two elutions with 40% DCM/hexane obtaining the corresponding spirocyclic (**16**) and reduced (**17**) compounds.

### *trans*-2-Benzyl-1-(benzyloxy)-1-azaspiro[4.4]non-6-ene (16)




Pale yellow oil (96.24 mg, 40%). $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ (ppm) 1.53 (ddd, *J* = 6.2, 11.2, 14.5 Hz, 1H), 1.66 – 1.83 (m, 2H), 2.38 – 2.21 (m, 0H), 1.84 – 2.02 (m, 0H), 2.21 – 2.38 (m, 2H), 2.42 – 2.55 (m, 1H), 2.66 (dd, *J* = 9.8, 12.9 Hz, 1H), 3.26 (dd, *J* = 4.4, 12.9 Hz, 1H), 3.42 (qd, *J* = 4.4, 9.2 Hz, 1H), 4.80 (d, *J* = 10.5 Hz, 1H), 4.84 (d, *J* = 10.5 Hz, 1H), 5.86 – 5.91 (m, 1H), 5.93 – 5.98 (m, 1H), 7.17 – 7.40 (m, 10H); $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ (ppm) 25.68, 31.02, 33.62, 35.67, 41.26, 67.26, 78.31, 80.35, 126.03, 128.27, 127.88, 128.69, 129.19, 133.00, 137.57, 139.79; HRMS (ESI) calcd for $C_{22}H_{25}NO$ ($M + H^+$): 320.20089, found: 320.20084.

### *cis*-2-Benzyl-1-(benzyloxy)-1-azaspiro[4.4]non-6-ene (16)




Pale yellow oil (60.14 mg, 25%). $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ (ppm) 1.44 – 1.81 (m, 4H) 1.97 (td, *J* = 11.5, 11.1, 6.1 Hz, 1H), 2.34 – 2.59 (m, 3H), 2.67 (dd, *J* = 10.5, 10.8, 1H), 3.23 – 3.35 (m, 2H), 4.73 (d, *J* = 10.2, 1H), 4.77 (d, *J* = 9.9, 1H), 5.73 – 5.81 (m, 1H), 5.94 – 5.99 (m, 1H), 7.21 – 7.43 (m, 10H); $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ (ppm) 24.57, 29.05, 32.36, 32.70, 41.06, 65.53, 77.84, 126.01, 127.91, 128.33, 128.92, 129.19, 133.63, 135.75, 137.49, 139.83; HRMS (ESI) calcd for $C_{22}H_{25}NO$ ($M + H^+$): 320.20089, found: 320.20082.

The *trans*/*cis* configuration assignment of spyrocyclic compounds **16** was carried out on the basis of NOESY-2D experiments, the space couplings of protons are shown in Figure 1. The *trans* and *cis* diastereomers displayed marked differences in the chemical shift of the C**H** at the pyrrolidinic ring and the OC**H$_2$**Ph group in the $^1$H NMR spectra. On the other hand, the methylene diastereotopic protons of the benzyloxy groups appeared as two doublets at 4.80 and 4.84 ppm for the *trans* diastereomer and at

4.73 and 4.77 ppm for the *cis* diastereomer. With respect to the uncyclized product **17**, the methylenic protons of the benzyloxy group appeared as a singlet at 5.12 ppm and the terminal vinyl protons (=$CH_2$) as a multiplet between 4.96 and 5.15 ppm.

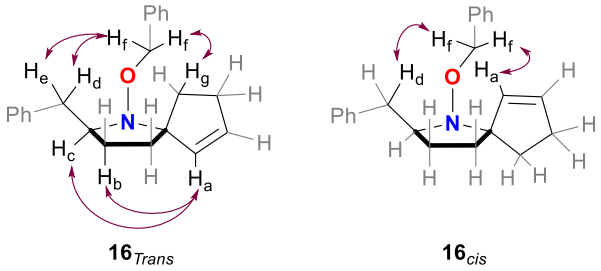
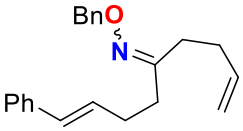



**Figure 1:** NOESY-2D couplings of the *trans* and *cis* diastereomers **16**.

**(1*E*, 5*EZ*)-1-Phenylnona-1,8-dien-5-one *O*-benzyl oxime (17)**




Pale yellow oil (45.71 mg, 19%). $^1$H NMR (300 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 2.25 – 2.56 ( m, 16H), 4.96 – 5.15 (m, 8H), 5.84 (ddt, *J* 16.6, 9.9, 6.4, 2H), 6.22 (dtd, *J* 16.0, 6.4, 3.3, 2H), 6.36 – 6.49 (m, 2H), 7.18 – 7.43 (m, 20H). $^{13}$C NMR (75 MHz, $CDCl_3$), *E*,*Z* isomers: $\delta$ (ppm) 27.91, 28.26, 29.20, 29.82, 29.86, 30.58, 33.77, 34.12, 75.37, 75.42, 115.15, 115.21, 126.04, 127.02, 127.05, 127.58, 127.91, 127.98, 128.30, 160.05, 128.51, 129.44,129.47, 129.51, 130.48, 137.50, 137.57, 138.34, 138.44, 160.08; HRMS (ESI) calcd for $C_{22}H_{25}NO$ (M + $H^+$): 320.20089, found: 320.20085.

**Determination of kinetic constants by competition experiment**

In five 1 mL volumetric flasks, 0.023 mmol of the oxime ether **15** were added along with 7 eq (41 µL, 0.161 mmol), 9 eq (53 µL, 0.207 mmol), 11 eq (65 µL, 0.253 mmol), 13 eq (76 µL, 0.299 mmol) and 15 eq (91 µL, 0.345 mmol) of $Bu_3SnH$ respectively and the volume was completed with benzene. The contents of each flask were placed in 2 mL vials and degassed by freeze-thaw cycles with liquid nitrogen and sealed under argon. Finally, the vials were heated at 80°C in an oil bath for 5 hours. After this time, the samples were concentrated under reduced pressure until dryness and placed in 1 mL volumetric flasks together with 30 µL (0.005 mmol) of an anisole solution (internal standard) and the volume was completed with deuterated chloroform. Samples were quantitatively analyzed by $^1$H NMR as previously explained.

Subsequently, with the same methodology, another five competition experiments were carried out with a concentration 0.030 M of oxime ether **15**.

Competition experiments with the oxime ether **5c** were performed using the same methodology.

## 2. Computational methodology

The formation mechanisms for 2-benzyl-1-(benzyloxy)-1-azaspiro[4,4]non-6-ene (**16**) and 5'-benzyl-1'-(benzyloxy)-2,3-dihydrospiro[indene-1,2'-pyrrolidine] (**6c**) from the vinyl radical **18a** and the aryl radical **18b**, respectively, have been investigated using density functional theory (DFT) calculations. An exhaustive search of the optimized structural parameters, harmonic vibration frequencies and zero-point energies (ZPE) for all reported reactants, transition states and products were obtained at B3LYP, M06-2X, mPW1PW91 and TPSSh functionals combined with the 6-311+G(*d,p*) basis set on the reaction pathway. For calculations involving a tin atom, the functional M06-2X was used together with the effective core potential LanL2DZ.

DFT calculations for systems **6c**, **16**, **18a,b**, **19a,b** and **21a,b** included the solvent effect (benzene solvent; ε = 2.27) according to the implicit model SMD,[2] while calculations for systems **19c-h**, **20a** and **22-27** were performed in the gas phase. Electronic structure

calculations were carried out with Gaussian09 program.[3] Transition state (TS) geometries were identified by the existence of only one imaginary frequency in the normal mode coordinate analysis.

To evaluate the influence of spin contamination on the energy barriers, single-point calculations were performed on the optimized geometries of the structures involved in the double cyclization of the vinyl radical **18a** and the aryl radical **18b** with the ROM06-2X/6-311+G(*d*,*p*) approach in benzene phase. Grimme-type quasi-harmonic correction calculations with a cut-off (Grimme-type) of 100 $cm^{-1}$ were performed using the GoodVibes script created by Dr. Robert Paton and Dr. Ignacio Funes-Ardoiz.[4]

Rate constants were calculated in solution[5] ($k_{c1a,b}$, $k_{c2a,b}$ and $k_{ra,b}$) or in gas phase ($k_{c\text{-}trans}$ and $k_{HSn}$) using the conventional transition state theory (TST)[5-7] as shown in Equation 1.

$$k = \sigma\kappa\frac{k_B T}{h}e^{-(\Delta G^{\ddagger})/RT} \qquad eq\ (1)$$

Where $\sigma$ is the reaction symmetry number which represents reaction path degeneracy, in this case, the value is 1 due to point a group of reactive and transition state, $\kappa$ correspond to tunneling corrections which were calculated using Eckart barrier,[8] $k_B$ and $h$ consist in Boltzmann and Planck constants, $\Delta G^{\neq}$ is Gibbs free energy of activation of the studied reaction. The main advantage of using conventional TST is that it requires very limited information of the potential energy surface (only on reactants and the transition state) and has been shown to be good enough to reproduce experimental rate constants for medium size systems.[9] All kinetic calculations were performed employing Eyringpy code.[10] Arrhenius plots were obtained at different temperatures to report a general Arrhenius equation for each studied system.

Finally, reactivity and radical stabilization energy calculations were performed using the M06-2X/6-311+G(*d*,*p*) approach in gas phase. The Fukui local reactivity index for the attack of a nucleophilic specie ($f_k^+$) was calculated for systems **19a,c-g**, using the frontier molecular orbital method as implemented in UCA-FUKUI code.[11] The stabilization energy of the *N*-alkoxyaminyl radical was calculated from the enthalpy of an isodesmic hydrogen transfer reaction at 25 °C using $NH_3$ as reference.

## 3. Effect of spin contamination on energy barriers

Single-point calculations were performed on the optimized geometries for the structures involved in the double cyclization of the vinyl radical **18a** using ROM06-2X/6-311+G(*d*,*p*) (Table 1). The energy data were compared with those obtained with UM06-X/6-311+G(*d*,*p*) and it was found that the energy difference does not exceed 0.0047 Hartrees. Analysis of the spin contaminations showed that values obtained using UM06-2X are very close to 0.750.

**Table 1.** Energies and spin contaminations for the double cyclization of **18a** system calculated using UM06-2X/6-311+G(*d*,*p*) and ROM06-2X/6-311+G(*d*,*p*).

| Vinyl radical cyclization system **18a** | | | | | | |
|---|---|---|---|---|---|---|
| Compound | UM06-2X/6-311+G(*d*,*p*) | | ROM06-2X/6-311+G(*d*,*p*) | | $\Delta$ (*E*(UM06-2X) − *E*(ROM06-2X)) Hartrees | Difference (%) |
| | S^2 | *E*(UM062X) Hartrees | S^2 | *E*(ROM062X) Hartrees | | |
| 18a | 0.7501 | -982.443486 | 0.7500 | -982.441519 | -0.0020 | -0.0002 |
| 18a´ (TS1) | 0.7509 | -982.431381 | 0.7500 | -982.426707 | -0.0047 | -0.0005 |
| 19a | 0.7500 | -982.493250 | 0.7500 | -982.491721 | -0.0015 | -0.0002 |
| 19a´(TS2$_{trans}$) | 0.7508 | -982.471647 | 0.7500 | -982.467055 | -0.0046 | -0.0005 |
| 19a´´(TS2$_{cis}$) | 0.7508 | -982.475649 | 0.7500 | -982.470977 | -0.0047 | -0.0005 |
| 21a *trans* | 0.7504 | -982.503648 | 0.7500 | -982.500655 | -0.0030 | -0.0003 |
| 21a *cis* | 0.7504 | -982.501110 | 0.7500 | -982.497990 | -0.0031 | -0.0003 |

In the same way, single point calculations were performed using ROM06-2X/6-311+G(*d*,*p*) for the optimized structures of the double cyclization of the aryl radical **18b**. As shown in Table 2, the energy difference does not exceed 0.0048 Hartrees and the spin contamination is around 0.750. Thus, we found that the influence of spin contamination on the energy barriers in the studied systems is not significant.

**Table 2:** Energies and spin contaminations for the double cyclization of **18b** system calculated using UM06-2X/6-311+G(*d*,*p*) and ROM06-2X/6-311+G(*d*,*p*).

| Aryl radical cyclization system **18b** | | | | | | |
|---|---|---|---|---|---|---|
| Compound | UM06-2X/6-311+G(*d*,*p*) | | ROM06-2X/6-311+G(*d*,*p*) | | $\Delta$ (*E*(UM06-2X) − *E*(ROM06-2X)) Hartrees | Difference (%) |
| | S^2 | *E*(UM062X) Hartrees | S^2 | *E*(ROM062X) Hartrees | | |
| 18b | 0.7501 | -1136.08198 | 0.7500 | -1136.07990 | -0.0021 | -0.0002 |
| 18b´ (TS1) | 0.7507 | -1136.06974 | 0.7500 | -1136.06517 | -0.0046 | -0.0004 |
| 19b | 0.7500 | -1136.13306 | 0.7500 | -1136.13107 | -0.0020 | -0.0002 |
| 19b´(TS2$_{trans}$) | 0.7507 | -1136.11070 | 0.7500 | -1136.10606 | -0.0046 | -0.0004 |
| 19b´´(TS2$_{cis}$) | 0.7508 | -1136.11318 | 0.7500 | -1136.10839 | -0.0048 | -0.0004 |
| 21b *trans* | 0.7504 | -1136.14303 | 0.7500 | -1136.13997 | -0.0031 | -0.0003 |
| 21b *cis* | 0.7504 | -1136.13781 | 0.7500 | -1136.13492 | -0.0029 | -0.0003 |

## 4. Grimme-type quasi-harmonic correction

Using the GoodVibes script,[4] a Grimme-type quasi-harmonic (qh) correction was performed with a Grimme-type cut-off of 100 $cm^{-1}$ for the structures involved in the **18a** vinyl radical cyclization system. Table 3 shows the thermochemical data (in Hartrees) without quasi-harmonic correction obtained with the M06-2X/6-311+G(*d*,*p*) approach, while Table 4 shows the data (in Hartrees) with the quasi-harmonic correction applied. When comparing the values of entropy (S), enthalpy (H) and Gibbs free energy (G), it is observed (Table 5) that the variation of S, H y G are 0.005 Hartree (6.5%), 0.012 Hartree (less than 0.00119%) and 0.008 Hartree (less than 0.00084%) respectively.

**Table 3:** Thermochemical data (in Hartrees) obtained with the M06-2X/6-311+G(*d*,*p*) approach without quasi-harmonic correction.

| Compound | EE | ZPE | EE + ZPE | *H* | *G* | T.*S* |
|---|---|---|---|---|---|---|
| 18a | -982.4435 | 0.4050 | -982.0385 | -982.0146 | -982.0952 | 0.081 |
| 18a´ (TS1) | -982.4314 | 0.4040 | -982.0274 | -982.0044 | -982.0829 | 0.079 |
| 19a | -982.4933 | 0.4080 | -982.0853 | -982.0627 | -982.1402 | 0.078 |
| 19a´(TS2$_{trans}$) | -982.4716 | 0.4070 | -982.0646 | -982.0430 | -982.1178 | 0.075 |
| 21a *trans* | -982.5036 | 0.4090 | -982.0947 | -982.0731 | -982.1476 | 0.074 |
| 19a´´(TS2$_{cis}$) | -982.4756 | 0.4077 | -982.0680 | -982.0467 | -982.1195 | 0.073 |
| 21a *cis* | -982.5011 | 0.4091 | -982.0920 | -982.0703 | -982.1454 | 0.075 |

**Table 4:** Thermochemical data (in Hartrees) obtained with the M06-2X/6-311+G(*d*,*p*) approach with quasi-harmonic correction.

| Compound | EE | ZPE | EE + ZPE | *H* | *S* | | *G*(T) | qh-*G*(T) |
|---|---|---|---|---|---|---|---|---|
| | | | | | T.*S* | T.qh-*S* | | |
| 18a | -982.4435 | 0.3929 | -982.0506 | -982.0262 | 0.0818 | 0.076 | -982.1080 | -982.1018 |
| 18a´ (TS1) | -982.4314 | 0.3918 | -982.0395 | -982.0160 | 0.0797 | 0.074 | -982.0957 | -982.0898 |
| 19a | -982.4933 | 0.3957 | -982.0975 | -982.0743 | 0.0787 | 0.073 | -982.1530 | -982.1472 |
| 19a´(TS2$_{trans}$) | -982.4716 | 0.3948 | -982.0769 | -982.0547 | 0.0759 | 0.071 | -982.1306 | -982.1252 |
| 21a $_{trans}$ | -982.5036 | 0.3967 | -982.1070 | -982.0848 | 0.0756 | 0.070 | -982.1604 | -982.1552 |
| 19a´´(TS2$_{cis}$) | -982.4756 | 0.3954 | -982.0802 | -982.0584 | 0.0739 | 0.069 | -982.1323 | -982.1277 |
| 21a $_{cis}$ | -982.5011 | 0.3968 | -982.1043 | -982.0820 | 0.0762 | 0.071 | -982.1583 | -982.1530 |

**Table 5:** Comparison between thermochemical data without quasi-harmonic correction and with quasi-harmonic correction.

| Compound | *S* | | *H* | | *G* | |
|---|---|---|---|---|---|---|
| | Difference | | Difference | | Difference | |
| | Hartrees | (%) | Hartrees | (%) | Hartrees | (%) |
| 18a | 0.005 | 6.5 | 0.012 | 0.00118 | 0.007 | 0.00068 |
| 18a´ (TS1) | 0.005 | 6.3 | 0.012 | 0.00118 | 0.007 | 0.00070 |
| 19a | 0.005 | 6.3 | 0.012 | 0.00119 | 0.007 | 0.00072 |
| 19a´(TS2$_{trans}$) | 0.004 | 5.9 | 0.012 | 0.00119 | 0.007 | 0.00076 |
| 21a $_{trans}$ | 0.004 | 5.7 | 0.012 | 0.00119 | 0.008 | 0.00078 |
| 19a´´(TS2$_{cis}$) | 0.003 | 4.9 | 0.012 | 0.00119 | 0.008 | 0.00084 |
| 21a $_{cis}$ | 0.004 | 5.8 | 0.012 | 0.00119 | 0.008 | 0.00077 |

Additionally, the reaction coordinate for the double cyclization of compound **18a** was plotted using the data without quasi-harmonic correction and the data without quasi-harmonic correction (Table 6). As shown in Figure 2, no significant changes in energy barriers were found (differences in energy barriers are less than 1 kcal mol$^{-1}$).

**Table 6:** Energy data of the vinyl radical cyclization system **18a** obtained with the M06-2X/6-311+G(*d*,*p*) approach without quasi-harmonic correction and with quasi-harmonic correction.

| Compound | No quasi-harmonic correction | | | | | Quasi-harmonic correction | | | | | Difference kcal mol$^{-1}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | EE Hartrees | ZPE Hartrees | EE + ZPE Hartrees | EE + ZPE kcal mol$^{-1}$ | *Δ* Energy values kcal mol$^{-1}$ | EE Hartrees | ZPE Hartrees | EE + ZPE Hartrees | EE + ZPE kcal mol$^{-1}$ | *Δ* Energy values kcal mol$^{-1}$ | |
| 18a | -982.4435 | 0.4050 | -982.0384 | -1.5650 | 0.0 | -982.4435 | 0.3929 | -982.0506 | -1.5650 | 0.00 | 0.00 |
| 18a´ (TS1) | -982.4314 | 0.4040 | -982.0274 | -1.5650 | 6.93 | -982.4314 | 0.3918 | -982.0395 | -1.5650 | 6.95 | 0.02 |
| 19a | -982.4932 | 0.4079 | -982.0853 | -1.5651 | -29.39 | -982.4932 | 0.3957 | -982.0975 | -1.5651 | -29.45 | 0.06 |
| 19a´(TS2$_{trans}$) | -982.4716 | 0.4070 | -982.0646 | -1.5650 | -16.44 | -982.4716 | 0.3948 | -982.0769 | -1.5650 | -16.47 | 0.04 |
| 21a $_{trans}$ | -982.5036 | 0.4090 | -982.0947 | -1.5651 | -35.29 | -982.5036 | 0.3967 | -982.1070 | -1.5651 | -35.36 | 0.07 |
| 19a´´(TS2$_{cis}$) | -982.4756 | 0.4077 | -982.0680 | -1.5650 | -18.53 | -982.4756 | 0.3954 | -982.0802 | -1.5650 | -18.57 | 0.05 |
| 21a $_{cis}$ | -982.5011 | 0.4091 | -982.0920 | -1.5651 | -33.60 | -982.5011 | 0.3968 | -982.1043 | -1.5651 | -33.68 | 0.08 |
| 16 $_{cis}$ | -983.1512 | 0.4226 | -982.7286 | -1.5661 | -120.70 | -983.1512 | 0.4099 | -982.7413 | -1.5661 | -121.03 | 0.33 |
| 16 $_{trans}$ | -983.1538 | 0.4230 | -982.7307 | -1.5661 | -122.03 | -983.1538 | 0.4103 | -982.7434 | -1.5661 | -122.37 | 0.34 |

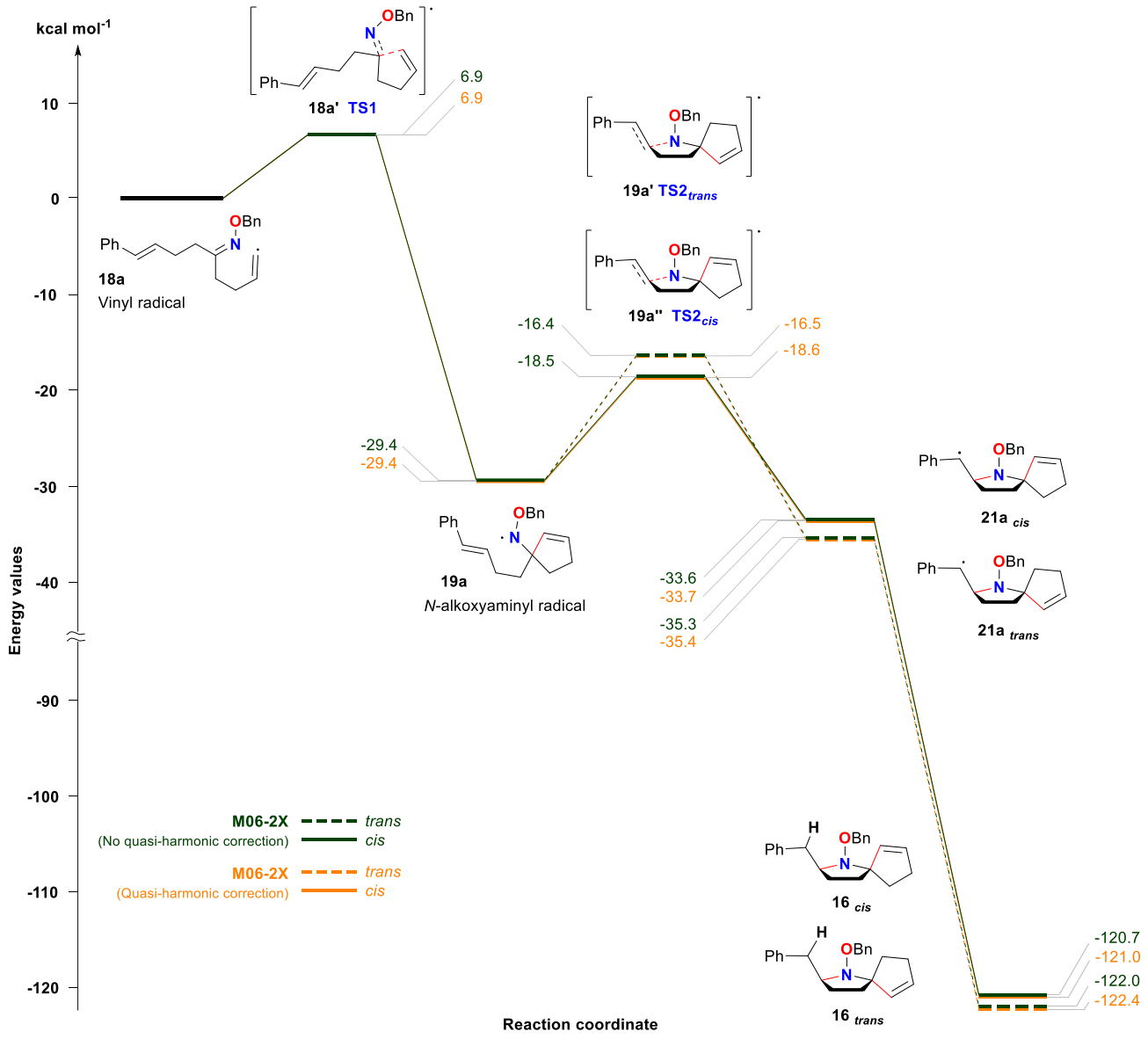



**Figure 2.** Calculated spirocyclization pathway for **18a** using thermochemical data obtained with the M06-2X/6-311+G(*d*,*p*) approach without quasi-harmonic correction and with quasi-harmonic correction.

Subsequently, to verify the impact of the quasi-harmonic correction of the Gibbs free energy on the cyclization constants, the vinyl radical **18a** cyclization constant at 353.15 K (80 °C) was calculated, finding no significant variation of the constant (the order of the magnitude is maintained) as shown in Table 7.

**Table 7:** Calculated Gibbs free energies and **18a** cyclization rate constant at 80 °C using corrected and uncorrected quasi-harmonic data.

| Compound | qh-*G*[a] | *G*[b] |
|---|---|---|
| 18a | -982.115618 | -982.095213 |
| 18a´ (TS1) | -982.103372 | -982.082946 |
| 19a | -982.160599 | -982.140196 |
| **Rate constant** | | |
| $K_{c1}$ (80 °C) | 1.7 x $10^8$ $s^{-1}$ | 1.1 x $10^8$ $s^{-1}$ |

[a] Gibbs free energies with quasi-harmonic correction. [b]Gibbs free energies without quasi-harmonic correction.

In this way, we consider that the quasi-harmonic thermochemical corrections made with GoodVibes (although necessary in other molecular systems), do not affect in a high level the energetic and kinetic values used to calculate the rate constants reported in our work.

## 5. Optimized structures of the vinyl (18a), aryl (18b) and *N*-alkoxyaminyl (19a and 19b) radicals

The structures shown in Figures 3 and 4 where hydrogens are not explicitly shown, were calculated with the M06-2X functional, which showed excellent agreement with experimental systems when comparing both structural and thermochemical results.[12]

**Optimized structures of 18a vinyl and 18b aryl radicals.**

The vinyl radical **18a** (*Z* isomer), for which a structure with a conformation close to a *pseudo*-chair was calculated with the four functionals, where the vinyl radical ($C_4$) is about 3.2 Å from the oxymic carbon $C_5$, with the M06-2X functional predicting the shortest distance at 3.133 Å as shown in Figure 3. The aryl radical **18b** (*E* isomer), whose calculated structure also shows a *pseudo*-chair conformation where the shortest distance between $C_4$ and $C_5$ aryl radicals (3.166 Å) is again predicted by M06-2X. IRC calculations showed that the calculated structures for **18a** vinyl and **18b** aryl radicals connect to the respective transition states (TS1).

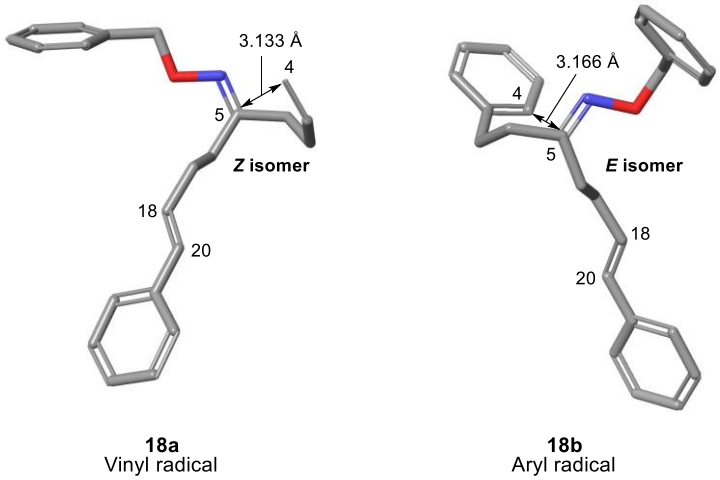


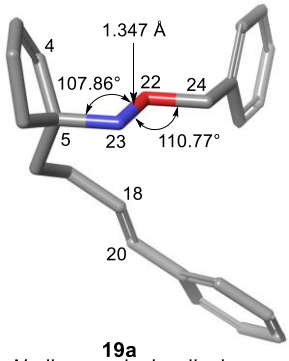

**Figure 3.** Optimized structures of **18a** vinyl and **18b** aryl radicals with the M06-2X/6-311+G(*d*,*p*) approach. All hydrogen atoms are hidden.

**Optimized structures of 19a and 19b *N*-alkoxyaminyl radicals.**

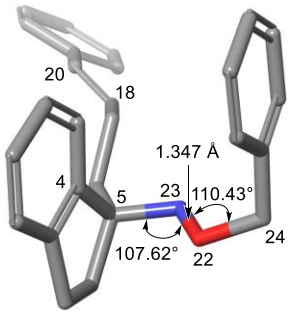
The optimized geometries for **19a** and **19b** *N*-alkoxyaminyl radicals obtained with the M06-2X functional are shown in Figure 4. Structure **19a** shows that N and O atoms are coplanar with $C_{24}$ and quaternary carbon $C_5$ at a dihedral angle of -178.50°, while $C_5$-N-O y N-O-$C_{24}$ bond angles are 107.86° and 110.77°, respectively. The *N*-alkoxyaminyl radical **19b** shows that the $C_5$-N-O-$C_{24}$ residue approaches a coplanar structure with a dihedral angle of -162.78°, and the $C_5$-N-O y N-O-$C_{24}$ bond angles are 107.62° and 110.43°, respectively. In both structures the N-O bond length (1.347 Å) is found to be shorter than the typical bonds N($sp^2$) - O (1.397 Å) of oxime ethers, or N($sp^3$)-O (1.463 Å) in alkoxyamines.[13] This N-O bond length in *N*-alkoxyaminyl radicals is consistent with the characteristics of a two-center, three-electron bond in which the unpaired electron is accommodated in the anti-bonding orbital,[14] as reported in previous studies.[15, 16]

On the other hand, $C_5$ quaternary centers and benzyl groups, although they do not allow the unpaired electron to delocalize, offer steric protection that contributes to the stability of the radical. In the structural parameters for the **19a** and **19b** *N*-alkoxyaminyl

radicals obtained with the B3LYP, mPW1PW91 and TPSSh functionals, no significant variations were found compared to those obtained with M06-2X.




**19a**
*N*-alkoxyaminyl radical




**19b**
*N*-alkoxyaminyl radical

**Figure 4.** Optimized structures of **19a** and **19b** *N*-alkoxyaminyl radicals with the M06-2X/6-311+G(*d*,*p*) approach. All hydrogen atoms are hidden.

## 6. Cartesian coordinates and energy values of optimized structures

### 18a

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.405032
Thermal correction to Energy= 0.427931
Thermal correction to Enthalpy= 0.428876
Thermal correction to Gibbs Free Energy= 0.348273

Sum of electronic and zero-point Energies= -982.038453
Sum of electronic and thermal Energies= -982.015554
Sum of electronic and thermal Enthalpies= -982.014610
Sum of electronic and thermal Free Energies= -982.095213

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.04531900 | 3.75591000 | -1.11179100 |
| C | 0.06686000 | 4.32699400 | -0.22672800 |
| C | -0.22310000 | 4.28016500 | 1.25293900 |
| C | -1.29622400 | 3.77262100 | 1.80604200 |
| C | -1.25067300 | 2.27400800 | -0.94475100 |
| H | -0.78065600 | 3.94201700 | -2.15863900 |
| H | 0.24425300 | 5.36943500 | -0.51035100 |
| H | 1.01375000 | 3.80670600 | -0.41744500 |
| H | 0.54502100 | 4.71650400 | 1.89950000 |
| H | -1.67425100 | 3.64727800 | 2.81009100 |
| H | -1.98876300 | 4.26614500 | -0.90613100 |
| C | -0.09223800 | 1.33785900 | -1.16459100 |
| H | -0.43199900 | 0.48366600 | -1.75620400 |
| H | 0.68608700 | 1.85472700 | -1.73209700 |
| C | 0.49943800 | 0.82413600 | 0.16471200 |
| H | -0.29234500 | 0.29331400 | 0.70177400 |
| H | 0.80950600 | 1.66668800 | 0.78813300 |
| C | 1.66161700 | -0.08905300 | -0.07767500 |
| H | 1.44788500 | -0.98661700 | -0.65569900 |
| C | 2.90247300 | 0.15729400 | 0.34827600 |
| H | 3.07829400 | 1.07103800 | 0.91443600 |
| O | -2.51001000 | 0.50850500 | -0.50137500 |
| N | -2.42312300 | 1.89270500 | -0.61910300 |

| | | | |
|---|---|---|---|
| C | -3.84776800 | 0.15694500 | -0.15286400 |
| H | -4.13151200 | 0.70416100 | 0.75166400 |
| H | -4.52456800 | 0.44579900 | -0.96245700 |
| C | 4.10039800 | -0.67468800 | 0.13398700 |
| C | 4.06588300 | -1.92198200 | -0.50383900 |
| C | 5.33577300 | -0.19997000 | 0.58803600 |
| C | 5.22868500 | -2.65656800 | -0.68861300 |
| H | 3.12364200 | -2.32503200 | -0.85720700 |
| C | 6.50180000 | -0.93509900 | 0.40457000 |
| H | 5.37878700 | 0.76180400 | 1.08910300 |
| C | 6.45344800 | -2.16744800 | -0.23663000 |
| H | 5.18046800 | -3.61894800 | -1.18545400 |
| H | 7.44711400 | -0.54507800 | 0.76461200 |
| H | 7.35942100 | -2.74380000 | -0.38295600 |
| C | -3.88255500 | -1.32792900 | 0.07818000 |
| C | -4.51123400 | -2.17846900 | -0.82789000 |
| C | -3.26577700 | -1.87173400 | 1.20657200 |
| C | -4.53108700 | -3.55378800 | -0.60961900 |
| H | -4.98762700 | -1.76134300 | -1.70899900 |
| C | -3.27805400 | -3.24374100 | 1.42427000 |
| H | -2.77795900 | -1.21103200 | 1.91630000 |
| C | -3.91385400 | -4.08762900 | 0.51572300 |
| H | -5.02628100 | -4.20657400 | -1.31922700 |
| H | -2.79904500 | -3.65715500 | 2.30437000 |
| H | -3.92823000 | -5.15768500 | 0.68770900 |

**Vibrational frequencies**

14.64, 24.95, 38.26, 42.58, 52.24, 53.01, 56.46, 72.94, 80.18, 95.97, 104.74, 126.24, 151.44, 185.99, 192.68, 233.1, 250.86, 271.82, 284.29, 313.85, 325.36, 370.03, 374.69, 382.1, 412.05, 413, 426.86, 463.59, 498.77, 528.44, 562.11, 574.57, 602.83, 624.32, 631.91, 632.37, 639.33, 673.95, 707.21, 716.28, 768.74, 777.25, 789.25, 798.24, 838.36, 853.76, 864.6, 867.13, 874.67, 880.6, 884.31, 912.12, 945.55, 949.81, 959.94, 987.43, 1004.55, 1008.53, 1009.1, 1013.19, 1016.45, 1020.99, 1024.8, 1026.41, 1026.97, 1030.62, 1044.49, 1062.99, 1064.5, 1096.58, 1104.84, 1114.12, 1117.26, 1125.48, 1174.39, 1177.16, 1179.64, 1199.05, 1201.55, 1205.68, 1229.01, 1243.01, 1253.65, 1259.48, 1261.45, 1275.61, 1301.03, 1312.39, 1330.2, 1335.74, 1347.07, 1352.54, 1354.22, 1360.85, 1377.84, 1380.96, 1395.03, 1423.02, 1469.29, 1474.06, 1488.3, 1492.93, 1498.35, 1499.51, 1521.57, 1541.73, 1546.03, 1653.44, 1669.1, 1683.77, 1689.55, 1694.85, 1738.81, 1751.6, 3038.36, 3052.57, 3056.38, 3061.74, 3067.67, 3077.17, 3078.63, 3105.36, 3111.97, 3116.53, 3131.17, 3134.51, 3157.09, 3169.96, 3174.78, 3177.82, 3178.13, 3189.18, 3192.14, 3195.61, 3207.72, 3211.47, 3217.33, 3272.24.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.400330
Thermal correction to Energy= 0.423599
Thermal correction to Enthalpy= 0.424544
Thermal correction to Gibbs Free Energy= 0.342559

Sum of electronic and zero-point Energies= -982.480276
Sum of electronic and thermal Energies= -982.457007
Sum of electronic and thermal Enthalpies= -982.456062
Sum of electronic and thermal Free Energies= -982.538047

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.19554000 | 3.71496100 | -1.20037600 |
| C | -0.11444300 | 4.46557000 | -0.40513100 |
| C | -0.36738300 | 4.60893300 | 1.07813600 |
| C | -1.40368600 | 4.18155000 | 1.75336500 |
| C | -1.30150400 | 2.23462700 | -0.91777600 |
| H | -0.96352300 | 3.83031700 | -2.26684500 |
| H | -0.01143000 | 5.47201900 | -0.82867900 |
| H | 0.86580100 | 3.99457200 | -0.54911200 |

| | | | |
|---|---|---|---|
| H | 0.42063800 | 5.14482200 | 1.62413200 |
| H | -1.75369100 | 4.18634700 | 2.77547900 |
| H | -2.17211500 | 4.17313000 | -1.02757600 |
| C | -0.10048500 | 1.34220600 | -1.12521300 |
| H | -0.41644100 | 0.46473500 | -1.69748000 |
| H | 0.64303600 | 1.87552900 | -1.72369200 |
| C | 0.55420700 | 0.86278300 | 0.19642900 |
| H | -0.20651900 | 0.32516500 | 0.77085500 |
| H | 0.86289000 | 1.72328100 | 0.79614800 |
| C | 1.72721900 | -0.03718200 | -0.05602900 |
| H | 1.51136100 | -0.94347100 | -0.61948200 |
| C | 2.97583000 | 0.20617400 | 0.36377600 |
| H | 3.14971600 | 1.11036700 | 0.94560300 |
| O | -2.49927600 | 0.42414000 | -0.37202900 |
| N | -2.45918100 | 1.82047500 | -0.55825700 |
| C | -3.83372400 | 0.04484600 | 0.01894100 |
| H | -4.07996800 | 0.53320100 | 0.96681000 |
| H | -4.53839000 | 0.39221800 | -0.74266700 |
| C | 4.17162900 | -0.62592600 | 0.15056400 |
| C | 4.20327100 | -1.72045000 | -0.73170700 |
| C | 5.34724700 | -0.31830400 | 0.85518700 |
| C | 5.35833500 | -2.47777500 | -0.88983700 |
| H | 3.32141300 | -1.97597500 | -1.30782100 |
| C | 6.50494300 | -1.07699400 | 0.69810700 |
| H | 5.34831000 | 0.52531600 | 1.53820000 |
| C | 6.51598700 | -2.16288000 | -0.17458200 |
| H | 5.35913300 | -3.31572100 | -1.57878900 |
| H | 7.39756000 | -0.81902600 | 1.25776700 |
| H | 7.41578600 | -2.75425100 | -0.30236600 |
| C | -3.86935100 | -1.45399100 | 0.15160000 |
| C | -4.16069200 | -2.25673200 | -0.95634800 |
| C | -3.58986600 | -2.06851700 | 1.37631500 |
| C | -4.17428600 | -3.64537800 | -0.84348800 |
| H | -4.38030000 | -1.78856200 | -1.91050100 |
| C | -3.60257400 | -3.45739500 | 1.49336500 |
| H | -3.36443500 | -1.45486600 | 2.24263000 |
| C | -3.89500000 | -4.24826300 | 0.38275900 |
| H | -4.40536600 | -4.25604700 | -1.70948200 |
| H | -3.38757600 | -3.92177400 | 2.44954000 |
| H | -3.90821800 | -5.32893300 | 0.47302700 |

**Vibrational frequencies**

11.12, 22.41, 37.25, 39.27, 44.01, 50.5, 61.33, 67.48, 74.08, 89.81, 108.86, 127.7, 153.76, 165.85, 183.08, 222.64, 247.49, 260.19, 269.31, 302.64, 332.91, 344.55, 364.55, 372.8, 411.3, 414.85, 419.57, 472.24, 498.37, 522.5, 555.32, 562.1, 590.56, 622.2, 631.69, 633.82, 635.46, 658.49, 705.21, 713.13, 758.13, 770.98, 774.37, 776.3, 809.62, 834.76, 842.73, 852.18, 858.16, 862.27, 862.78, 888.42, 928.59, 933.58, 944.8, 963.89, 973.46, 988.46, 990.93, 992.72, 997.93, 1003.33, 1009.29, 1010.38, 1014.36, 1017.82, 1020.54, 1047.27, 1049.13, 1050.3, 1080.66, 1089.25, 1105.31, 1107.85, 1166.64, 1177.52, 1178.05, 1197.76, 1199.34, 1200.55, 1228.91, 1230.02, 1235.56, 1244.11, 1252.88, 1274.99, 1290.61, 1305.93, 1326.07, 1336.82, 1342.19, 1352.5, 1356.08, 1358.25, 1370.43, 1374.96, 1379.59, 1404.5, 1466.7, 1467.66, 1476.72, 1480.13, 1481.87, 1491.01, 1513.34, 1523.71, 1527.39, 1613.62, 1625.09, 1639.08, 1645.89, 1672.6, 1686.41, 1701.09, 2999.61, 3011.6, 3020.77, 3030.17, 3033.67, 3036.3, 3043.69, 3069.54, 3073.35, 3086.23, 3090.05, 3117.57, 3130.06, 3156.93, 3160.06, 3163.34, 3163.96, 3171.86, 3173.77, 3180.04, 3182.94, 3189.89, 3190.54, 3241.23.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.389924
Thermal correction to Energy= 0.413809
Thermal correction to Enthalpy= 0.414753
Thermal correction to Gibbs Free Energy= 0.331602
Sum of electronic and zero-point Energies= -982.334115
Sum of electronic and thermal Energies= -982.310230
Sum of electronic and thermal Enthalpies= -982.309286
Sum of electronic and thermal Free Energies= -982.392437

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.16502200 | 3.73026800 | -1.19956000 |
| C | -0.07467700 | 4.46781500 | -0.40083400 |
| C | -0.32409500 | 4.58620200 | 1.08601000 |
| C | -1.35710100 | 4.12740500 | 1.75905200 |
| C | -1.28029400 | 2.24958100 | -0.92091500 |
| H | -0.93488800 | 3.85170700 | -2.27287300 |
| H | 0.03339400 | 5.48590900 | -0.81279300 |
| H | 0.90972000 | 3.99266600 | -0.55751900 |
| H | 0.46340100 | 5.12908900 | 1.64098800 |
| H | -1.70678600 | 4.10880200 | 2.78799200 |
| H | -2.14372700 | 4.19766800 | -1.01828800 |
| C | -0.08864900 | 1.34560200 | -1.13061600 |
| H | -0.41524500 | 0.46738100 | -1.71005900 |
| H | 0.66803000 | 1.87465800 | -1.72888300 |
| C | 0.55739000 | 0.85154600 | 0.19476000 |
| H | -0.21768400 | 0.31226400 | 0.76214500 |
| H | 0.86656400 | 1.71196400 | 0.80643200 |
| C | 1.72621600 | -0.05293600 | -0.05818300 |
| H | 1.50885600 | -0.96081500 | -0.63243400 |
| C | 2.98309400 | 0.18541800 | 0.36939700 |
| H | 3.15632400 | 1.09156200 | 0.96207500 |
| O | -2.49998300 | 0.43930100 | -0.37149200 |
| N | -2.45338100 | 1.84569300 | -0.55593000 |
| C | -3.84882700 | 0.07547800 | 0.02431900 |
| H | -4.08623200 | 0.56809200 | 0.98045200 |
| H | -4.55408900 | 0.43712600 | -0.74037600 |
| C | 4.17694700 | -0.64584900 | 0.15349200 |
| C | 4.20825800 | -1.74523200 | -0.73312300 |
| C | 5.36031200 | -0.33685900 | 0.85851500 |
| C | 5.36815900 | -2.50374500 | -0.89512100 |
| H | 3.31910900 | -2.00187900 | -1.31099800 |
| C | 6.52224200 | -1.09710600 | 0.69745800 |
| H | 5.36102400 | 0.51194900 | 1.54624500 |
| C | 6.53207200 | -2.18702000 | -0.17966500 |
| H | 5.36834000 | -3.34615900 | -1.58938000 |
| H | 7.42175700 | -0.83722700 | 1.25841100 |
| H | 7.43785600 | -2.78084500 | -0.31133800 |
| C | -3.89941900 | -1.42434600 | 0.15229500 |
| C | -4.20187400 | -2.22404400 | -0.96241900 |
| C | -3.62203000 | -2.04771400 | 1.37992300 |
| C | -4.23108900 | -3.61800300 | -0.85235600 |
| H | -4.41938700 | -1.74680100 | -1.92037100 |
| C | -3.65037500 | -3.44190500 | 1.49361800 |
| H | -3.38726500 | -1.43395300 | 2.25231100 |

| | | | |
|---|---|---|---|
| C | -3.95527900 | -4.22928500 | 0.37684500 |
| H | -4.47228200 | -4.22783800 | -1.72466000 |
| H | -3.43773400 | -3.91449300 | 2.45400200 |
| H | -3.98127700 | -5.31670700 | 0.46500700 |

**Vibrational frequencies**

10.54, 22.55, 35.31, 41.05, 43.31, 48.51, 64.12, 66.04, 70.48, 86.3, 105.23, 126.71, 149.74, 162.65, 175.83, 214.45, 238.09, 252.92, 263.48, 292.2, 319.95, 331.33, 352.05, 359.34, 394.14, 397.65, 405.72, 455.92, 480.29, 504.97, 535.64, 545.87, 571.03, 603.1, 612.35, 613.6, 615.66, 636.34, 680.99, 690.08, 732.84, 745.11, 750.18, 750.99, 779.01, 809.99, 819.84, 820.87, 831.12, 832.21, 837.69, 865.35, 887.25, 896.8, 903.52, 928.28, 943.28, 948.99, 953.34, 959.84, 960.07, 969.19, 970.2, 976.94, 986.22, 987.23, 990.68, 1005.88, 1024.25, 1026, 1053.33, 1061.85, 1077.33, 1079.95, 1131.97, 1147.2, 1147.81, 1159.15, 1165.71, 1165.96, 1185.18, 1202.07, 1202.79, 1205.95, 1211.49, 1231.3, 1245.61, 1268.88, 1290.55, 1295.12, 1306.53, 1311.14, 1322.1, 1322.86, 1330.71, 1346.69, 1348.03, 1353.01, 1415.1, 1416.13, 1428.53, 1434.61, 1438.01, 1440.76, 1462.76, 1478.85, 1484.38, 1569.54, 1583.05, 1595.93, 1602.31, 1613.06, 1632.96, 1649.59, 2933.99, 2952.97, 2960.4, 2966.24, 2971.63, 2981.2, 2982.21, 3012.26, 3012.66, 3027.17, 3032.73, 3052.41, 3066.26, 3095.95, 3100.75, 3103.52, 3105.72, 3112.26, 3113.12, 3120.69, 3121.46, 3130.41, 3130.86, 3185.48.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.399395
Thermal correction to Energy= 0.422864
Thermal correction to Enthalpy= 0.423809
Thermal correction to Gibbs Free Energy= 0.341557
Sum of electronic and zero-point Energies= -982.538334
Sum of electronic and thermal Energies= -982.514864
Sum of electronic and thermal Enthalpies= -982.513920
Sum of electronic and thermal Free Energies= -982.596171

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.17344300 | 3.72514800 | -1.19205700 |
| C | -0.07546800 | 4.44706200 | -0.39276200 |
| C | -0.32476800 | 4.55002100 | 1.09370500 |
| C | -1.37226000 | 4.10143200 | 1.74663400 |
| C | -1.28947700 | 2.24475100 | -0.92075200 |
| H | -0.94739100 | 3.85105500 | -2.25932400 |
| H | 0.03424200 | 5.46312300 | -0.79263300 |
| H | 0.89764400 | 3.96487800 | -0.55521200 |
| H | 0.46347800 | 5.06397800 | 1.66007300 |
| H | -1.72430500 | 4.07668600 | 2.76940200 |
| H | -2.14399800 | 4.19096100 | -1.00034400 |
| C | -0.10109800 | 1.34003200 | -1.13525800 |
| H | -0.43024700 | 0.46459200 | -1.70493700 |
| H | 0.65021600 | 1.86699100 | -1.73142100 |
| C | 0.54175200 | 0.85464500 | 0.19160900 |
| H | -0.22901700 | 0.31931800 | 0.75626600 |
| H | 0.85238500 | 1.71404000 | 0.79313700 |
| C | 1.71130500 | -0.04893900 | -0.06084200 |
| H | 1.49738000 | -0.95430800 | -0.62845600 |
| C | 2.96139300 | 0.19667400 | 0.36394900 |
| H | 3.13325600 | 1.10004100 | 0.94969100 |
| O | -2.49073800 | 0.43795200 | -0.37457100 |
| N | -2.45296100 | 1.84023700 | -0.55329300 |
| C | -3.82987300 | 0.07119200 | 0.02804300 |
| H | -4.05868600 | 0.55854800 | 0.98122600 |
| H | -4.53473600 | 0.42794700 | -0.72962600 |
| C | 4.15596700 | -0.63368400 | 0.14962600 |
| C | 4.18635300 | -1.73199300 | -0.73009600 |
| C | 5.33376500 | -0.32094000 | 0.85124700 |

| | | | |
|---|---|---|---|
| C | 5.34353100 | -2.48797400 | -0.88883700 |
| H | 3.30133600 | -1.99016400 | -1.30253000 |
| C | 6.49321600 | -1.07863400 | 0.69367900 |
| H | 5.33322300 | 0.52605000 | 1.53183000 |
| C | 6.50356800 | -2.16835200 | -0.17668700 |
| H | 5.34429000 | -3.32869700 | -1.57577600 |
| H | 7.38758500 | -0.81741400 | 1.25070000 |
| H | 7.40471200 | -2.75911300 | -0.30526700 |
| C | -3.87077900 | -1.42774600 | 0.15404400 |
| C | -4.16905400 | -2.22445200 | -0.95793000 |
| C | -3.58980900 | -2.04805600 | 1.37687300 |
| C | -4.18923400 | -3.61460300 | -0.85008500 |
| H | -4.38944700 | -1.75000800 | -1.90986900 |
| C | -3.60933300 | -3.43849300 | 1.48854500 |
| H | -3.35913400 | -1.43733600 | 2.24508900 |
| C | -3.90928100 | -4.22389200 | 0.37440000 |
| H | -4.42605800 | -4.22158500 | -1.71819500 |
| H | -3.39386200 | -3.90836300 | 2.44290800 |
| H | -3.92808800 | -5.30568400 | 0.46059800 |

**Vibrational frequencies**

10.82, 25.5, 37.27, 39.6, 45.11, 51.22, 65.23, 66.32, 72.43, 86.95, 108.19, 124.81, 150.12, 164.28, 178.28, 217.1, 239.86, 256.23, 266.17, 299.6, 320.36, 335.69, 355.04, 364.58, 404.64, 407.55, 409.47, 461.42, 490.17, 516.39, 548.37, 554.78, 586.41, 612.27, 622.15, 624.09, 624.7, 648.54, 700.38, 709.19, 752.71, 766.02, 769.39, 778.17, 811.18, 829.38, 836.83, 848.01, 854.67, 859.37, 863.5, 888.85, 919.95, 929.03, 937.83, 954.97, 968.46, 985.29, 987.41, 990.25, 995.34, 998.51, 1005.41, 1008.45, 1009.33, 1012.49, 1015.59, 1038.53, 1046.38, 1047.96, 1079, 1086.83, 1102.62, 1107.02, 1160.53, 1176.81, 1177.57, 1192.99, 1197.07, 1197.92, 1223.41, 1228.38, 1233.54, 1236.28, 1245.72, 1272.07, 1285.69, 1304.83, 1327, 1334.02, 1350.74, 1355.15, 1357.08, 1357.35, 1365.37, 1370.95, 1374.75, 1395.86, 1471.09, 1472.52, 1476.47, 1482.11, 1484.53, 1496.06, 1519.75, 1522.67, 1527.77, 1612.72, 1625.34, 1637.47, 1644.88, 1661.34, 1670.15, 1692.94, 3004.97, 3011.83, 3020.83, 3030.37, 3031.97, 3039.4, 3041.64, 3071.58, 3077.63, 3086.5, 3092.11, 3114.49, 3127.88, 3153.88, 3158.85, 3161.42, 3162.07, 3171.15, 3172.19, 3180.27, 3180.75, 3189.9, 3190.59, 3237.08.

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## 18a' TS1

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.403967
Thermal correction to Energy= 0.426017
Thermal correction to Enthalpy= 0.426961
Thermal correction to Gibbs Free Energy= 0.348435

Sum of electronic and zero-point Energies= -982.027415
Sum of electronic and thermal Energies= -982.005364
Sum of electronic and thermal Enthalpies= -982.004420
Sum of electronic and thermal Free Energies= -982.082946

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.24573900 | -0.18295700 | -1.54466200 |
| C | -0.64088500 | 0.50033200 | -0.49954100 |
| C | 0.12120500 | 0.55479200 | 0.80141700 |
| C | 1.42689200 | 0.44749600 | 0.77723500 |
| C | 1.68547200 | 0.28110200 | -1.48319700 |
| H | -0.13465300 | 0.01039800 | -2.55314900 |
| H | -1.58173600 | -0.04314700 | -0.38448200 |
| H | -0.90745600 | 1.51834200 | -0.80735900 |
| H | -0.42595400 | 0.70503800 | 1.73394800 |
| H | 2.23833700 | 0.44942100 | 1.49097000 |
| H | 0.24059100 | -1.26257300 | -1.38372600 |
| C | 2.00441800 | 1.71561200 | -1.87025100 |

| | | | |
|---|---|---|---|
| H | 2.50820000 | 1.66760800 | -2.84270500 |
| H | 1.06109200 | 2.24807100 | -2.02390900 |
| C | 2.89137900 | 2.52756900 | -0.91138500 |
| H | 2.34013500 | 2.69572400 | 0.01867700 |
| H | 3.78961100 | 1.95883900 | -0.66857600 |
| C | 3.26221300 | 3.85111200 | -1.51024100 |
| H | 2.43668900 | 4.52458700 | -1.73868900 |
| C | 4.51336000 | 4.22031300 | -1.79206800 |
| H | 5.31767600 | 3.51351800 | -1.59366500 |
| O | 3.84739200 | -0.18857300 | -1.72437700 |
| N | 2.56189900 | -0.68108700 | -1.56545100 |
| C | 4.74216500 | -1.26886600 | -1.91958800 |
| H | 5.73639300 | -0.83731000 | -1.77631000 |
| H | 4.57579700 | -2.02409200 | -1.14548100 |
| C | 4.93244600 | 5.50517200 | -2.38202900 |
| C | 6.19120100 | 5.59932300 | -2.98583500 |
| C | 4.12057800 | 6.64672600 | -2.36075400 |
| C | 6.62010400 | 6.78612400 | -3.56967700 |
| H | 6.83602600 | 4.72650100 | -3.00001700 |
| C | 4.54723500 | 7.83238400 | -2.94373800 |
| H | 3.15586600 | 6.61191200 | -1.86743400 |
| C | 5.79719700 | 7.90731000 | -3.55456200 |
| H | 7.59763500 | 6.83534300 | -4.03567800 |
| H | 3.90653700 | 8.70651000 | -2.91422200 |
| H | 6.12979500 | 8.83534600 | -4.00477600 |
| C | 4.64005400 | -1.89281200 | -3.29274400 |
| C | 5.22329200 | -3.13943300 | -3.51966000 |
| C | 4.00898000 | -1.23668300 | -4.34691900 |
| C | 5.18468300 | -3.71960400 | -4.78229700 |
| H | 5.70862100 | -3.66043300 | -2.69958100 |
| C | 3.96350100 | -1.81971400 | -5.61008600 |
| H | 3.54969100 | -0.26988100 | -4.17520500 |
| C | 4.55212900 | -3.06018400 | -5.83295500 |
| H | 5.64169100 | -4.68934300 | -4.94431700 |
| H | 3.46537300 | -1.30278600 | -6.42267800 |
| H | 4.51423200 | -3.51288600 | -6.81694700 |

**Vibrational frequencies**

561.76*i*, 13.22, 25.47, 33.86, 38.96, 44.28, 50.55, 71.29, 82.62, 95.5, 109.6, 156.72, 169.6, 194.68, 208.31, 224.12, 240.95, 258.89, 289.35, 295.04, 332.26, 377.38, 387.37, 411.8, 413.8, 418.17, 434.92, 469.51, 487.94, 508.6, 532.76, 583.57, 600.12, 626.31, 630.13, 630.92, 642.63, 680.92, 706.64, 712.68, 751.52, 765.11, 768.2, 806.5, 819.28, 844.32, 857.85, 869.76, 876.09, 879.33, 889.82, 907.03, 920.29, 934.4, 945.03, 977.94, 994.43, 1000.28, 1006.66, 1011.87, 1016.08, 1018.27, 1019.32, 1024.06, 1024.83, 1056.62, 1060.56, 1062.91, 1063.68, 1068.24, 1102.86, 1109.3, 1116.55, 1130.85, 1173.37, 1175.44, 1176.32, 1193.22, 1201.14, 1202.39, 1209.66, 1239.96, 1242.28, 1243.5, 1260.71, 1284.68, 1314.27, 1322.7, 1324.21, 1331.09, 1342.47, 1349.65, 1352.02, 1352.56, 1360.3, 1374.47, 1397.96, 1417.45, 1465.51, 1468.76, 1484.94, 1486.39, 1490.15, 1495.47, 1495.96, 1537.3, 1543.7, 1548.77, 1653.77, 1660.82, 1678, 1680.87, 1687.23, 1744.41, 3041.18, 3044.91, 3056.95, 3061.69, 3080.94, 3090.91, 3092.17, 3098.5, 3121.85, 3131.19, 3132.56, 3140.16, 3151.37, 3177.91, 3181.7, 3182.45, 3190.62, 3192.64, 3199.59, 3201.4, 3209.65, 3210.05, 3220.89, 3254.61.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.399689
Thermal correction to Energy= 0.422057
Thermal correction to Enthalpy= 0.423001
Thermal correction to Gibbs Free Energy= 0.343209
Sum of electronic and zero-point Energies= -982.471454
Sum of electronic and thermal Energies= -982.449087

Sum of electronic and thermal Enthalpies= -982.448143 Sum of electronic and thermal Free Energies= -982.527934

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.67053800 | -0.08143200 | -1.02292000 |
| C | 0.11883400 | 0.70728100 | 0.17661500 |
| C | 1.14402800 | 0.69769400 | 1.28517500 |
| C | 2.40009600 | 0.44518100 | 1.00772900 |
| C | 2.13464400 | 0.19178500 | -1.31739600 |
| H | 0.08989900 | 0.15135700 | -1.92349000 |
| H | -0.82716000 | 0.26901000 | 0.51036600 |
| H | -0.11005000 | 1.74496400 | -0.09850100 |
| H | 0.81320400 | 0.92787500 | 2.30216800 |
| H | 3.33323100 | 0.36973900 | 1.54802500 |
| H | 0.56599000 | -1.15180300 | -0.83334600 |
| C | 2.52058300 | 1.56119100 | -1.86125700 |
| H | 2.75329900 | 1.41215000 | -2.92299900 |
| H | 1.64034800 | 2.20820100 | -1.82053700 |
| C | 3.70491000 | 2.30260400 | -1.20117400 |
| H | 3.44727500 | 2.56616400 | -0.17299400 |
| H | 4.56225900 | 1.62476000 | -1.16114600 |
| C | 4.07683800 | 3.53648100 | -1.97105700 |
| H | 4.37848700 | 3.36974700 | -3.00397100 |
| C | 4.05619500 | 4.78199100 | -1.47812500 |
| H | 3.75670800 | 4.91434100 | -0.43938900 |
| O | 4.11455800 | -0.60487800 | -2.01976100 |
| N | 2.83987100 | -0.89238500 | -1.52716200 |
| C | 4.80753800 | -1.82919200 | -2.34316300 |
| H | 5.86282900 | -1.55027200 | -2.32456900 |
| H | 4.61784500 | -2.55276400 | -1.54697000 |
| C | 4.40183900 | 6.02967900 | -2.17957900 |
| C | 4.39043800 | 7.23694700 | -1.46147500 |
| C | 4.74215600 | 6.08260600 | -3.54323500 |
| C | 4.70585600 | 8.44777900 | -2.07439400 |
| H | 4.12929100 | 7.22162600 | -0.40797000 |
| C | 5.05675500 | 7.28990700 | -4.15597000 |
| H | 4.75599600 | 5.17348000 | -4.13303000 |
| C | 5.04148800 | 8.48073800 | -3.42594300 |
| H | 4.68874000 | 9.36479000 | -1.49527100 |
| H | 5.31430700 | 7.30456200 | -5.20964800 |
| H | 5.28594100 | 9.42071900 | -3.90799600 |
| C | 4.42841800 | -2.38293300 | -3.69537900 |
| C | 3.35211900 | -3.26660000 | -3.83422700 |
| C | 5.14457000 | -2.00811700 | -4.83747300 |
| C | 2.99466400 | -3.75649700 | -5.08910600 |
| H | 2.79152000 | -3.56609800 | -2.95585400 |
| C | 4.79097700 | -2.49803800 | -6.09352000 |
| H | 5.98605300 | -1.32893400 | -4.74186800 |
| C | 3.71373800 | -3.37396700 | -6.22135100 |
| H | 2.15850200 | -4.44093800 | -5.18287400 |
| H | 5.35792900 | -2.20124800 | -6.96922100 |
| H | 3.43799600 | -3.75861100 | -7.19719600 |

**Vibrational frequencies**

366.74*i*, 9.58, 25.51, 28.22, 34.36, 47.89, 52.05, 67.78, 77.14, 101.2, 108.52, 137.96, 150.28, 161.93, 192.67, 227.4, 249.56, 264.65, 280.66, 302.33, 333.22, 366, 369.87, 387.85, 414.48, 414.67, 433.37, 466.6, 500.91, 507.95, 528.45, 577.06, 594.22, 622.15, 629.81, 633.29, 635.42, 663.71, 704, 709.57, 754.89, 767.59, 775.06, 792.11, 831.4, 835.16, 848.98, 850.65, 854.17, 858.08, 866.97, 889.11, 904.09, 931.79, 933.44, 940.58, 985.18, 988.05, 989.1, 992.48, 998.46, 1001.47, 1006.3, 1012.25, 1013.5, 1017.75, 1032.34, 1035.56, 1046.3, 1049.08, 1050.19, 1089.72, 1106.85, 1108.15, 1162.89, 1176.45, 1177.15, 1183.6, 1197.27, 1200.89, 1203.57, 1226.74, 1228.63, 1233.29, 1245.9, 1275.71, 1288.06, 1305.48, 1327.89, 1333.05, 1340.84, 1343.28, 1354.37, 1358.95, 1360.77, 1370.79, 1376.84, 1387.42, 1461.68, 1468.63, 1476.17, 1476.83, 1482.03, 1482.46, 1489.13, 1510.27, 1524.3, 1524.48, 1612.89, 1624.18, 1639.04, 1642.98, 1657.17, 1700.99, 3009.15, 3016.05, 3027.25, 3046.53, 3049.85, 3055.98, 3058.94, 3064.77, 3091.73, 3092.56, 3109.57, 3118.73, 3127.2, 3157.68, 3158.12, 3164.74, 3165.37, 3173.69, 3173.91, 3181.77, 3182.73, 3189.76, 3190.8, 3234.17.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.389235
Thermal correction to Energy= 0.412271
Thermal correction to Enthalpy= 0.413216
Thermal correction to Gibbs Free Energy= 0.331912
Sum of electronic and zero-point Energies= -982.329803
Sum of electronic and thermal Energies= -982.306766
Sum of electronic and thermal Enthalpies= -982.305822
Sum of electronic and thermal Free Energies= -982.387125

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.70884000 | -0.02284700 | -1.09080800 |
| C | 0.18848600 | 0.82215600 | 0.08663300 |
| C | 1.19557100 | 0.79734000 | 1.21353300 |
| C | 2.45807800 | 0.50602700 | 0.97585000 |
| C | 2.16660600 | 0.21882600 | -1.43380900 |
| H | 0.10436400 | 0.18320500 | -1.99085800 |
| H | -0.78823600 | 0.43840100 | 0.42119800 |
| H | 0.01053300 | 1.86847100 | -0.22001000 |
| H | 0.84268700 | 1.05218500 | 2.22613600 |
| H | 3.38128800 | 0.41107500 | 1.54283000 |
| H | 0.59465100 | -1.09037700 | -0.85530400 |
| C | 2.57562200 | 1.57159000 | -1.99715500 |
| H | 2.84568000 | 1.39983800 | -3.05390000 |
| H | 1.69510300 | 2.23097000 | -1.99788800 |
| C | 3.74822000 | 2.31197800 | -1.30733300 |
| H | 3.47978200 | 2.53269700 | -0.26449800 |
| H | 4.61860800 | 1.63748400 | -1.28632900 |
| C | 4.10378700 | 3.57919800 | -2.02856800 |
| H | 4.41475600 | 3.46196400 | -3.07321700 |
| C | 4.05596400 | 4.81030600 | -1.47908800 |
| H | 3.74996700 | 4.88789800 | -0.42893000 |
| O | 4.14290900 | -0.62413600 | -2.12047500 |
| N | 2.86019300 | -0.88564400 | -1.60410500 |
| C | 4.82406900 | -1.88392700 | -2.37480500 |
| H | 5.88827600 | -1.61085600 | -2.37979700 |
| H | 4.62853800 | -2.55689800 | -1.52756100 |
| C | 4.37597400 | 6.09500600 | -2.11900800 |
| C | 4.35070200 | 7.26928900 | -1.33558900 |
| C | 4.70468000 | 6.22629400 | -3.48683100 |
| C | 4.64380000 | 8.51966300 | -1.88764900 |
| H | 4.09587600 | 7.19248300 | -0.27602600 |
| C | 4.99665000 | 7.47396100 | -4.03884800 |
| H | 4.72546500 | 5.34381400 | -4.12794500 |

| | | | |
|---|---|---|---|
| C | 4.96956800 | 8.62912000 | -3.24373700 |
| H | 4.61701200 | 9.41005900 | -1.25694600 |
| H | 5.24605200 | 7.54882400 | -5.09892700 |
| H | 5.19770800 | 9.60280800 | -3.67996100 |
| C | 4.42452500 | -2.51155600 | -3.68867200 |
| C | 3.33865800 | -3.40077200 | -3.76095800 |
| C | 5.11921400 | -2.19139700 | -4.86754700 |
| C | 2.95153400 | -3.95128300 | -4.98755000 |
| H | 2.79381700 | -3.65444000 | -2.85011000 |
| C | 4.73550300 | -2.74233500 | -6.09481100 |
| H | 5.96799300 | -1.50504400 | -4.82092500 |
| C | 3.64938900 | -3.62369200 | -6.15654800 |
| H | 2.10716300 | -4.64152600 | -5.03088900 |
| H | 5.28657300 | -2.48890900 | -7.00216500 |
| H | 3.34989300 | -4.05665100 | -7.11253100 |

**Vibrational frequencies**

263.68*i*, 8.51, 24.06, 25.34, 28.73, 48, 63.46, 69.39, 73.27, 93.1, 101.38, 132.11, 143.21, 150.95, 185.18, 222.37, 237.64, 252.99, 264.66, 290.53, 325.58, 353.73, 357.97, 373.9, 396.66, 397.68, 421.5, 453.72, 485.06, 502.97, 509.75, 552.42, 566.89, 599.6, 609.81, 612.85, 614.24, 637.45, 679.32, 686.87, 728.15, 744.43, 748.38, 756.24, 803.37, 808.65, 811.47, 818.38, 827.21, 831.06, 838.71, 861.24, 880.01, 894.12, 901.75, 908.09, 942.54, 947.68, 952.81, 953.51, 958.76, 966.4, 967.4, 972.54, 984.57, 990.2, 998.09, 1007.97, 1022.08, 1023.66, 1024.57, 1061.82, 1077.25, 1080.69, 1127.65, 1143.94, 1145.3, 1147.75, 1160.64, 1163.61, 1165.38, 1192.41, 1197.74, 1201.66, 1209.9, 1236.09, 1244.55, 1268.72, 1286.24, 1292.8, 1296.44, 1312.48, 1314.47, 1320.88, 1326.41, 1337.29, 1346.46, 1346.62, 1413.16, 1416.31, 1428.19, 1429.02, 1433.1, 1438.92, 1439.62, 1478.4, 1480.35, 1493.24, 1568.57, 1581.87, 1594.79, 1599.12, 1616.79, 1647.64, 2949.44, 2958.36, 2967.11, 2974.64, 2980.95, 2992.92, 3000.53, 3008.58, 3031.78, 3032.48, 3051.68, 3052.67, 3061.95, 3096.07, 3096.39, 3103, 3103.62, 3111.37, 3113.49, 3118.96, 3122.18, 3128.67, 3129.37, 3177.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.398663
Thermal correction to Energy= 0.421286
Thermal correction to Enthalpy= 0.422231
Thermal correction to Gibbs Free Energy= 0.341854
Sum of electronic and zero-point Energies= -982.532786
Sum of electronic and thermal Energies= -982.510163
Sum of electronic and thermal Enthalpies= -982.509219
Sum of electronic and thermal Free Energies= -982.589595

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.72552800 | -0.03605200 | -1.12538500 |
| C | 0.18748800 | 0.81024600 | 0.04024000 |
| C | 1.19216800 | 0.79530600 | 1.16681300 |
| C | 2.44930300 | 0.50028100 | 0.91997900 |
| C | 2.18618400 | 0.21593100 | -1.44287600 |
| H | 0.13923900 | 0.16402700 | -2.03133200 |
| H | -0.78049200 | 0.41784900 | 0.37038800 |
| H | 0.00597300 | 1.84732500 | -0.27325100 |
| H | 0.84975600 | 1.05673300 | 2.17333000 |
| H | 3.37013100 | 0.41128600 | 1.48169600 |
| H | 0.61808900 | -1.09727200 | -0.88664100 |
| C | 2.59604300 | 1.57043000 | -1.99861000 |
| H | 2.86820400 | 1.40272600 | -3.04887600 |
| H | 1.71983900 | 2.22575400 | -1.99342100 |
| C | 3.76638300 | 2.30235400 | -1.30148600 |
| H | 3.49371500 | 2.52617100 | -0.26683100 |
| H | 4.63056300 | 1.63039400 | -1.28104100 |
| C | 4.12150400 | 3.56984300 | -2.02252800 |

| | | | |
|---|---|---|---|
| H | 4.44102500 | 3.45484200 | -3.05826300 |
| C | 4.05809400 | 4.79432600 | -1.47428700 |
| H | 3.74293700 | 4.87167700 | -0.43339100 |
| O | 4.16606500 | -0.60230900 | -2.11036700 |
| N | 2.88489100 | -0.87868900 | -1.61208000 |
| C | 4.85082100 | -1.85126700 | -2.37175600 |
| H | 5.90566500 | -1.57039900 | -2.40196900 |
| H | 4.67571500 | -2.51844000 | -1.52380700 |
| C | 4.37474700 | 6.07973200 | -2.11416200 |
| C | 4.32739600 | 7.25040600 | -1.33644200 |
| C | 4.72118400 | 6.20767900 | -3.47252300 |
| C | 4.61615600 | 8.49851100 | -1.88630300 |
| H | 4.05951400 | 7.17420900 | -0.28617000 |
| C | 5.00901600 | 7.45275700 | -4.02243200 |
| H | 4.76025700 | 5.32756400 | -4.10600700 |
| C | 4.95977900 | 8.60630400 | -3.23353500 |
| H | 4.57208900 | 9.38560900 | -1.26224100 |
| H | 5.27219100 | 7.52636400 | -5.07312500 |
| H | 5.18436600 | 9.57543400 | -3.66704800 |
| C | 4.42523100 | -2.48410700 | -3.67334300 |
| C | 3.33842900 | -3.36640900 | -3.71872000 |
| C | 5.09690100 | -2.17417500 | -4.86239200 |
| C | 2.92648800 | -3.92037100 | -4.93088600 |
| H | 2.81343900 | -3.61109800 | -2.80093800 |
| C | 4.68870200 | -2.72886600 | -6.07548100 |
| H | 5.94429800 | -1.49446700 | -4.83588300 |
| C | 3.60107800 | -3.60301600 | -6.11127700 |
| H | 2.08294500 | -4.60323700 | -4.95424400 |
| H | 5.22034900 | -2.48412300 | -6.98970500 |
| H | 3.28272500 | -4.03712600 | -7.05382100 |

**Vibrational frequencies**

299.58*i*, 10.31, 24.46, 26.75, 30.21, 49.09, 62.63, 66.01, 74.53, 94.44, 103.98, 133.3, 144.71, 153.89, 186.3, 222.92, 240.63, 255.76, 270.56, 297.05, 324.82, 360.21, 361.84, 378.81, 408.04, 409.07, 425.29, 459.14, 491.77, 508.11, 521.1, 563.32, 582.29, 614.82, 618.02, 622.48, 623.83, 656.89, 699.17, 706.95, 747.8, 762.8, 767.01, 787.55, 825.58, 829.58, 843.66, 845.48, 852.78, 859.54, 861.03, 885.16, 903.46, 926.78, 928.2, 936.01, 979.15, 981.28, 985.1, 988.31, 993.14, 995.7, 1001.53, 1007.41, 1009.55, 1012.34, 1025.07, 1031.84, 1045.58, 1046.43, 1047.53, 1085.86, 1102.18, 1107.1, 1158.28, 1173.97, 1177.15, 1177.53, 1196.19, 1197.57, 1202.36, 1224.83, 1225.78, 1231.95, 1246.66, 1272.15, 1282.8, 1304.79, 1327.04, 1330.73, 1339.55, 1355.27, 1356.37, 1357.58, 1359.47, 1367.7, 1369.71, 1381.46, 1466.07, 1471.77, 1475.43, 1481.78, 1484.73, 1485.75, 1494.96, 1522.76, 1524.22, 1525.31, 1611.88, 1623.93, 1637.16, 1641.63, 1646.97, 1690.93, 3007.42, 3016.71, 3024.31, 3042.08, 3047.47, 3054.79, 3058.63, 3066.1, 3090.31, 3092.47, 3114.19, 3115.06, 3122.64, 3154.25, 3154.65, 3161.6, 3162.05, 3170.84, 3172.84, 3179.36, 3182.48, 3188.76, 3189.72, 3230.93.

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## 19a

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.407954
Thermal correction to Energy= 0.429652
Thermal correction to Enthalpy= 0.430596
Thermal correction to Gibbs Free Energy= 0.353054

Sum of electronic and zero-point Energies= -982.085296
Sum of electronic and thermal Energies= -982.063599
Sum of electronic and thermal Enthalpies= -982.062654
Sum of electronic and thermal Free Energies= -982.140196

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.96591000 | -2.08776700 | -0.71128400 |

| | | | |
|---|---|---|---|
| C | 5.22268900 | -1.19963700 | -0.76834000 |
| C | 5.01105200 | -0.25742600 | 0.39122500 |
| C | 3.75945900 | -0.28488100 | 0.83969200 |
| C | 2.90505800 | -1.25781800 | 0.04282800 |
| H | 4.18275100 | -2.98800700 | -0.13033600 |
| H | 5.28026000 | -0.63563500 | -1.70589200 |
| H | 6.14714700 | -1.77558100 | -0.68356800 |
| H | 5.79191000 | 0.38787400 | 0.77823200 |
| H | 3.35749000 | 0.33457400 | 1.63194200 |
| H | 3.59762300 | -2.39346600 | -1.69193800 |
| C | 1.99931800 | -2.15589900 | 0.91340700 |
| H | 1.63050900 | -2.97979300 | 0.29268600 |
| H | 2.65314200 | -2.59721000 | 1.67158900 |
| C | 0.81438600 | -1.45816900 | 1.60317300 |
| H | 0.57485800 | -1.98136300 | 2.53255600 |
| H | 1.10331700 | -0.43773600 | 1.87901600 |
| C | -0.41946400 | -1.40102300 | 0.74882900 |
| H | -0.26860700 | -1.12525300 | -0.29164500 |
| C | -1.65429300 | -1.65626200 | 1.18584300 |
| H | -1.79722300 | -1.91658500 | 2.23338200 |
| O | 1.58732200 | 0.54385600 | -0.42238500 |
| N | 2.11197800 | -0.56256200 | -0.98426100 |
| C | 0.76830800 | 1.25536800 | -1.36575900 |
| H | 1.41893400 | 1.65572400 | -2.14743100 |
| H | 0.06675900 | 0.54778900 | -1.81568800 |
| C | -2.88865000 | -1.57428200 | 0.38303800 |
| C | -4.12474800 | -1.54342800 | 1.03821600 |
| C | -2.88213600 | -1.51575100 | -1.01763900 |
| C | -5.31442000 | -1.44065600 | 0.32503700 |
| H | -4.14859600 | -1.59631500 | 2.12205200 |
| C | -4.06884600 | -1.41140400 | -1.73056800 |
| H | -1.94311200 | -1.57403900 | -1.55727700 |
| C | -5.29159000 | -1.37067300 | -1.06348000 |
| H | -6.25953600 | -1.41605800 | 0.85553600 |
| H | -4.04156100 | -1.37168700 | -2.81367000 |
| H | -6.21669200 | -1.29278700 | -1.62257600 |
| C | 0.05405800 | 2.34352000 | -0.61882000 |
| C | -1.19135300 | 2.09886700 | -0.04040300 |
| C | 0.64911200 | 3.59481600 | -0.46115500 |
| C | -1.83526000 | 3.09541700 | 0.68552000 |
| H | -1.65905500 | 1.12606000 | -0.16026900 |
| C | 0.00699700 | 4.59259900 | 0.26413200 |
| H | 1.61890600 | 3.78416500 | -0.91041300 |
| C | -1.23602200 | 4.34268400 | 0.83849900 |
| H | -2.80449700 | 2.89863900 | 1.12922600 |
| H | 0.47440300 | 5.56371800 | 0.38027700 |
| H | -1.73894700 | 5.12088700 | 1.40117500 |

**Vibrational frequencies**

14.9, 21.5, 29.92, 39.02, 44.99, 53.81, 73.03, 81.74, 95.19, 136.4, 160.77, 163.19, 187.93, 199.33, 237.2, 263.35, 276.83, 293.86, 319.58, 347.94, 363.12, 382.49, 409.95, 411.09, 417.58, 452.18, 495.26, 504.75, 530.6, 552.24, 615.78, 616.59, 631.38, 632.2, 648.94, 708.69, 713.68, 725.87, 758.07, 767.2, 779.05, 822.89, 835.37, 849.97, 854.48, 860.37, 869.17, 874.38, 896.11, 934.28, 946.53, 951.32, 954.58, 979.15, 990.57, 992.72, 1001.47, 1004.6, 1007.11, 1010.52, 1016.93, 1020.09, 1020.94, 1024.72, 1044.65, 1062.27, 1064.81, 1072.08,

1079.85, 1110.84, 1112.58, 1122.1, 1127.01, 1145.13, 1171.09, 1176.12, 1179.23, 1186.26, 1201.83, 1206.19, 1206.94, 1234.12, 1239.97, 1255.22, 1256.21, 1256.35, 1282.12, 1316.88, 1324.24, 1330.06, 1340.94, 1342.12, 1347.24, 1361.69, 1363.35, 1368.65, 1384.1, 1389.2, 1414.67, 1470.45, 1471.36, 1475.24, 1489.94, 1490.11, 1500.49, 1515.49, 1540.94, 1545.31, 1653.41, 1664.99, 1680.18, 1684.57, 1693.93, 1737.01, 3044.25, 3050.47, 3051.01, 3076.15, 3081.46, 3094.49, 3096.17, 3097.2, 3132.06, 3136.39, 3138.82, 3165.62, 3175.82, 3182.74, 3183.87, 3185.5, 3186.87, 3190.37, 3197.43, 3197.69, 3205.46, 3207.41, 3211.58, 3217.08.

**M06-2X/6-311+G(*d*,*p*) (gas phase)**

Zero-point correction= 0.408028
Thermal correction to Energy= 0.429371
Thermal correction to Enthalpy= 0.430315
Thermal correction to Gibbs Free Energy= 0.355755
Sum of electronic and zero-point Energies= -982.065527
Sum of electronic and thermal Energies= -982.044184
Sum of electronic and thermal Enthalpies= -982.043240
Sum of electronic and thermal Free Energies=-982.11780

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 4.20178800 | -1.84765100 | -0.82246900 |
| C | 5.20537800 | -0.68095200 | -0.86346200 |
| C | 4.81396800 | 0.13133700 | 0.34749800 |
| C | 3.62238800 | -0.21754600 | 0.82258000 |
| C | 2.99977600 | -1.33357700 | 0.00337600 |
| H | 4.65180800 | -2.69605900 | -0.30048700 |
| H | 5.09446400 | -0.07912700 | -1.77199300 |
| H | 6.24288100 | -1.02092800 | -0.82900200 |
| H | 5.42871000 | 0.92992000 | 0.74649200 |
| H | 3.11583700 | 0.25709600 | 1.65334000 |
| H | 3.87741300 | -2.18425900 | -1.80791800 |
| C | 2.37946900 | -2.47135600 | 0.83947000 |
| H | 2.13106500 | -3.29330500 | 0.15781600 |
| H | 3.17001000 | -2.83585500 | 1.50264100 |
| C | 1.14559300 | -2.12446600 | 1.68246400 |
| H | 1.01353800 | -2.94029000 | 2.40394200 |
| H | 1.32293000 | -1.21948100 | 2.27251800 |
| C | -0.13319800 | -1.97716400 | 0.90556200 |
| H | -0.27486500 | -2.68038200 | 0.08651100 |
| C | -1.07086900 | -1.07184100 | 1.18677500 |
| H | -0.89134700 | -0.38635600 | 2.01332300 |
| O | 1.39714300 | 0.23498300 | -0.45091300 |
| N | 2.00062100 | -0.85245900 | -0.96490500 |
| C | 0.33037100 | 0.65009800 | -1.29887000 |
| H | 0.75702300 | 1.04895000 | -2.22501700 |
| H | -0.27580300 | -0.22736700 | -1.54379800 |
| C | -2.33459000 | -0.84320400 | 0.46574500 |
| C | -3.24616400 | 0.08342600 | 0.98074300 |
| C | -2.64255100 | -1.46811800 | -0.74976300 |
| C | -4.42945900 | 0.37523100 | 0.31257500 |
| H | -3.00855900 | 0.59780400 | 1.90619900 |
| C | -3.82149800 | -1.17479500 | -1.42101000 |
| H | -1.94990300 | -2.18133300 | -1.18338000 |
| C | -4.72207300 | -0.25071200 | -0.89322500 |
| H | -5.11571100 | 1.10423200 | 0.72839500 |
| H | -4.03889100 | -1.66634800 | -2.36240700 |
| H | -5.63987900 | -0.02123700 | -1.42147100 |
| C | -0.51228600 | 1.68140400 | -0.60017400 |
| C | -1.65642400 | 2.14783200 | -1.24820500 |

| | | | |
|---|---|---|---|
| C | -0.20862800 | 2.15411200 | 0.67335900 |
| C | -2.48685200 | 3.07372800 | -0.63244800 |
| H | -1.90959400 | 1.76382100 | -2.23196700 |
| C | -1.04431300 | 3.08170600 | 1.29187200 |
| H | 0.67765000 | 1.78991300 | 1.17855100 |
| C | -2.18358200 | 3.54337400 | 0.64318100 |
| H | -3.37970100 | 3.41773900 | -1.14144800 |
| H | -0.80101400 | 3.44354400 | 2.28442700 |
| H | -2.83302500 | 4.26332100 | 1.12729000 |

**Vibrational frequencies**

18.67, 31.72, 43.21, 47.39, 59.45, 81.96, 86.94, 102.87, 131.23, 152.54, 170.36, 186.47, 204.2, 214.99, 228.72, 238.12, 284.39, 291.44, 306.26, 330.42, 362.25, 403.16, 405.99, 412.65, 430.11, 467.85, 478.05, 495.28, 533.01, 561.23, 611.86, 617.99, 627.43, 632.05, 640.53, 700.85, 709.11, 726.7, 746.24, 754.78, 767.74, 818.3, 826.47, 849.68, 851.86, 857.44, 862.47, 869.46, 895.67, 926.23, 929.65, 942.63, 951.59, 979.73, 990.19, 998.37, 1001.58, 1007.46, 1011.95, 1017.59, 1019.69, 1020.24, 1021.47, 1035.5, 1056.01, 1058.92, 1061.56, 1070.31, 1087.37, 1103.66, 1115.14, 1118.97, 1125.06, 1158.11, 1168.71, 1174.47, 1183.78, 1196.73, 1197.77, 1210.51, 1212.42, 1228.96, 1243.35, 1246.44, 1260.3, 1277.5, 1289.06, 1310.92, 1323.74, 1327.76, 1331.47, 1338.9, 1346.75, 1350.02, 1366.36, 1375.02, 1389.49, 1394.71, 1412.76, 1470.6, 1477.31, 1480.18, 1490.04, 1497.7, 1498.22, 1502.23, 1541.75, 1546, 1655.22, 1662.78, 1684.42, 1686.83, 1697, 1743.12, 3026.07, 3036.11, 3043.49, 3064.84, 3070.52, 3075.58, 3088.11, 3099.36, 3111.95, 3132.86, 3140.29, 3149.27, 3165.07, 3177.89, 3179, 3183.11, 3189.3, 3189.39, 3197, 3199.95, 3204.53, 3206.5, 3214.88, 3230.61.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.403441
Thermal correction to Energy= 0.425579
Thermal correction to Enthalpy= 0.426523
Thermal correction to Gibbs Free Energy= 0.347758
Sum of electronic and zero-point Energies= -982.520669
Sum of electronic and thermal Energies= -982.498531
Sum of electronic and thermal Enthalpies= -982.497586
Sum of electronic and thermal Free Energies= -982.576351

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.89994900 | -3.16841700 | -0.84059700 |
| C | 4.41378700 | -2.87072900 | -0.73957800 |
| C | 4.50096300 | -1.96802200 | 0.46570900 |
| C | 3.30745900 | -1.52966400 | 0.86383700 |
| C | 2.18224700 | -2.05828800 | -0.01681300 |
| H | 2.68547600 | -4.13990600 | -0.38800500 |
| H | 4.79547200 | -2.35946600 | -1.63200200 |
| H | 5.00908900 | -3.78217200 | -0.62558800 |
| H | 5.44388500 | -1.69595100 | 0.92890400 |
| H | 3.13351800 | -0.84501800 | 1.68401200 |
| H | 2.52854700 | -3.19030600 | -1.86661300 |
| C | 0.98436600 | -2.65096900 | 0.77970000 |
| H | 0.38252700 | -3.25821700 | 0.09516100 |
| H | 1.42246700 | -3.34432100 | 1.50454000 |
| C | 0.05995800 | -1.66008800 | 1.52770100 |
| H | -0.30151100 | -2.13418300 | 2.44550000 |
| H | 0.63986600 | -0.78376500 | 1.83852100 |
| C | -1.12292900 | -1.21527900 | 0.71439500 |
| H | -0.89758300 | -0.83858200 | -0.27950100 |
| C | -2.39540300 | -1.27472700 | 1.12858300 |
| H | -2.59048300 | -1.65099200 | 2.13186900 |
| O | 1.67000300 | 0.16558400 | -0.37607600 |
| N | 1.71990800 | -1.05106500 | -0.99682500 |
| C | 1.29694500 | 1.20757700 | -1.31773500 |

| | | | |
|---|---|---|---|
| H | 2.03558300 | 1.20771700 | -2.12311900 |
| H | 0.31912600 | 0.96148700 | -1.73862500 |
| C | -3.59819000 | -0.87754700 | 0.37755100 |
| C | -4.83943800 | -0.87151900 | 1.03529300 |
| C | -3.57582700 | -0.50942700 | -0.97988500 |
| C | -6.00944300 | -0.50759300 | 0.37204600 |
| H | -4.88321300 | -1.15696700 | 2.08169000 |
| C | -4.74253100 | -0.14647500 | -1.64293400 |
| H | -2.64046300 | -0.51984800 | -1.52746700 |
| C | -5.96728700 | -0.14159100 | -0.97146800 |
| H | -6.95392700 | -0.51193100 | 0.90547800 |
| H | -4.69915500 | 0.12911900 | -2.69131800 |
| H | -6.87568000 | 0.13883000 | -1.49285600 |
| C | 1.27382700 | 2.51873400 | -0.58257600 |
| C | 0.07901700 | 3.02324000 | -0.06019100 |
| C | 2.45671800 | 3.24132000 | -0.39157800 |
| C | 0.06401700 | 4.23167500 | 0.63469000 |
| H | -0.84368800 | 2.46931400 | -0.19872900 |
| C | 2.44526200 | 4.44694400 | 0.30584200 |
| H | 3.38883500 | 2.85745400 | -0.79350400 |
| C | 1.24763400 | 4.94441200 | 0.81994800 |
| H | -0.86981000 | 4.61465500 | 1.03109400 |
| H | 3.36797300 | 4.99925300 | 0.44597100 |
| H | 1.23716200 | 5.88518500 | 1.35932500 |

**Vibrational frequencies**

14.01, 28.55, 31.42, 39.36, 48.38, 50.1, 67.44, 69.64, 87.72, 116.21, 133.36, 140.45, 163.23, 183.02, 223.39, 257.03, 273.34, 283.87, 323.48, 334.1, 341.72, 373.16, 412.17, 415.59, 417.74, 446.66, 480.84, 503.56, 532.02, 543.84, 614.49, 619.28, 634.33, 635.98, 646.86, 703.67, 713.68, 722.8, 752.16, 757.98, 774.23, 813.06, 823.05, 832.66, 843.45, 851.5, 859.51, 866.77, 876.18, 921.27, 928.12, 932.07, 937.84, 960.44, 971.79, 976.8, 978.85, 989.67, 992.63, 997.23, 1003.79, 1005.75, 1013.3, 1014.92, 1018.59, 1033.16, 1049.46, 1050.27, 1052.58, 1081.82, 1087.26, 1098.61, 1108.48, 1115.46, 1128.32, 1159.95, 1177.95, 1179.87, 1188.12, 1199.63, 1201.91, 1223.22, 1228.05, 1233.86, 1237, 1241.46, 1274.98, 1307.28, 1315.91, 1319.52, 1329.75, 1341.7, 1345.15, 1354.78, 1357.18, 1359.47, 1377.48, 1380.77, 1391.36, 1469.58, 1471.73, 1476.09, 1478.19, 1482.71, 1488.83, 1505.44, 1525.34, 1529.04, 1613.17, 1625.36, 1639.54, 1646.52, 1668.81, 1698.98, 3014.87, 3021.3, 3023.35, 3042.44, 3048.95, 3055.96, 3057.63, 3065, 3096.17, 3100.83, 3117.41, 3150.32, 3159.15, 3163.1, 3164.21, 3167.04, 3167.43, 3174.22, 3174.38, 3182.92, 3183.6, 3190.56, 3192.19, 3205.79.

### mPWPW91/6-311+G(*d*,*p*)

Zero-point correction= 0.393045
Thermal correction to Energy= 0.415718
Thermal correction to Enthalpy= 0.416663
Thermal correction to Gibbs Free Energy= 0.337420

Sum of electronic and zero-point Energies= -982.376778
Sum of electronic and thermal Energies= -982.354104
Sum of electronic and thermal Enthalpies= -982.353160
Sum of electronic and thermal Free Energies= -982.432403

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.89097000 | -3.18109100 | -0.83903800 |
| C | 4.40682600 | -2.88122000 | -0.75762500 |
| C | 4.51138800 | -1.98218900 | 0.44968900 |
| C | 3.31540000 | -1.54260700 | 0.86696900 |
| C | 2.18144300 | -2.06792400 | -0.00668900 |
| H | 2.67967600 | -4.15706300 | -0.37778200 |
| H | 4.77808400 | -2.36306800 | -1.65896500 |
| H | 5.01015500 | -3.79704000 | -0.65722200 |
| H | 5.46627800 | -1.70874100 | 0.90350100 |

| | | | |
|---|---|---|---|
| H | 3.14941300 | -0.85542000 | 1.69576100 |
| H | 2.50174200 | -3.20488000 | -1.86563400 |
| C | 0.98690500 | -2.66045400 | 0.80307500 |
| H | 0.38308900 | -3.28365900 | 0.12373000 |
| H | 1.43466300 | -3.34602300 | 1.54000600 |
| C | 0.06111900 | -1.65814300 | 1.53642900 |
| H | -0.29861400 | -2.11271200 | 2.47279800 |
| H | 0.64613500 | -0.76929000 | 1.82864000 |
| C | -1.12172200 | -1.23099600 | 0.71409400 |
| H | -0.89538100 | -0.90134000 | -0.30444300 |
| C | -2.40079000 | -1.25281100 | 1.14111300 |
| H | -2.59404400 | -1.58822000 | 2.16700500 |
| O | 1.68891400 | 0.16840700 | -0.36267200 |
| N | 1.71128300 | -1.06205900 | -0.98926000 |
| C | 1.30471400 | 1.20923400 | -1.31652500 |
| H | 2.04649100 | 1.20515500 | -2.12914600 |
| H | 0.32046400 | 0.95233100 | -1.73477300 |
| C | -3.60139600 | -0.86778900 | 0.38350100 |
| C | -4.85039100 | -0.85503600 | 1.04148600 |
| C | -3.57818600 | -0.51418800 | -0.98455900 |
| C | -6.02420600 | -0.50188600 | 0.36887200 |
| H | -4.89419800 | -1.12853200 | 2.09834100 |
| C | -4.74919200 | -0.16237600 | -1.65662200 |
| H | -2.63520400 | -0.52700600 | -1.53322200 |
| C | -5.98038200 | -0.15241100 | -0.98508900 |
| H | -6.97561700 | -0.50147000 | 0.90387600 |
| H | -4.70425900 | 0.10219200 | -2.71481400 |
| H | -6.89422900 | 0.12022100 | -1.51513400 |
| C | 1.27984800 | 2.52379700 | -0.58583300 |
| C | 0.07981900 | 3.02870100 | -0.05930300 |
| C | 2.46674600 | 3.25241200 | -0.39865000 |
| C | 0.06368700 | 4.24434600 | 0.63341700 |
| H | -0.84709400 | 2.46758600 | -0.19498300 |
| C | 2.45362900 | 4.46495800 | 0.29754200 |
| H | 3.40413900 | 2.86633800 | -0.80472900 |
| C | 1.25102600 | 4.96318300 | 0.81414100 |
| H | -0.87586000 | 4.62935100 | 1.03291800 |
| H | 3.38101200 | 5.02343800 | 0.43492800 |
| H | 1.23934100 | 5.91195200 | 1.35317400 |

**Vibrational frequencies**

16.5, 29.93, 32.49, 45.28, 46.89, 52.53, 66.09, 77.8, 87.8, 119.16, 127.61, 135.2, 156.47, 182.1, 215.92, 247.87, 266.5, 276.19, 312.41, 321.75, 329.9, 359.6, 399.3, 399.79, 401.89, 431.92, 465.75, 486.53, 515.62, 526.49, 593.84, 599.86, 614.4, 616.05, 625.8, 680.9, 690.59, 700.83, 726.52, 732.32, 748, 789.14, 798.62, 807.66, 819.64, 824.38, 832.07, 836.43, 850.4, 890.74, 898.89, 901.19, 912.92, 927.87, 934.49, 943.35, 950.36, 951.36, 958.15, 959.27, 961.53, 969.06, 975.34, 985.12, 991.13, 1002.08, 1021.03, 1021.42, 1026.71, 1026.8, 1049.58, 1070.64, 1080.82, 1084.08, 1095.72, 1121.79, 1147.37, 1148.17, 1149.71, 1167.24, 1168.75, 1181.72, 1190.17, 1194.74, 1206.07, 1208.64, 1230.29, 1262.21, 1270.44, 1280.38, 1289.96, 1300.79, 1309.97, 1311.67, 1327.55, 1332.16, 1337.64, 1346.94, 1349.17, 1417.12, 1420.44, 1426.52, 1435.76, 1437.04, 1440.3, 1453.24, 1480.9, 1484.74, 1569.79, 1583.6, 1595.92, 1602.75, 1620.61, 1649.32, 2956.3, 2957.79, 2964.15, 2982.41, 2985.6, 2998.16, 2999.53, 3009.82, 3031.58, 3045.37, 3053.31, 3079.86, 3097.67, 3103.52, 3104.15, 3106.89, 3107.38, 3113.51, 3114.45, 3121.17, 3124.02, 3130.53, 3132.69, 3144.84.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.402410
Thermal correction to Energy= 0.424767
Thermal correction to Enthalpy= 0.425711
Thermal correction to Gibbs Free Energy= 0.346876
Sum of electronic and zero-point Energies= -982.583242
Sum of electronic and thermal Energies= -982.560885
Sum of electronic and thermal Enthalpies= -982.559941
Sum of electronic and thermal Free Energies= -982.638777

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -2.92456300 | -3.14290000 | 0.82490000 |
| C | -4.42928000 | -2.79761100 | 0.77393100 |
| C | -4.52375200 | -1.89128400 | -0.42752500 |
| C | -3.32668200 | -1.47991500 | -0.85257800 |
| C | -2.20091800 | -2.04007900 | 0.00260900 |
| H | -2.75265500 | -4.10925600 | 0.34111500 |
| H | -4.76310100 | -2.27221100 | 1.67825100 |
| H | -5.05702200 | -3.69018100 | 0.67955700 |
| H | -5.47150900 | -1.59221100 | -0.86588500 |
| H | -3.15142100 | -0.79453000 | -1.67341500 |
| H | -2.52242200 | -3.19633600 | 1.83928800 |
| C | -1.02552900 | -2.64355000 | -0.81578400 |
| H | -0.42472800 | -3.27153300 | -0.14780100 |
| H | -1.48629400 | -3.31386900 | -1.54985200 |
| C | -0.09929500 | -1.64534000 | -1.55132300 |
| H | 0.25974500 | -2.10403800 | -2.47874900 |
| H | -0.67867100 | -0.75940200 | -1.83967200 |
| C | 1.08385600 | -1.22538500 | -0.72642700 |
| H | 0.85972600 | -0.87549200 | 0.27903100 |
| C | 2.35835500 | -1.27860000 | -1.14576000 |
| H | 2.55276100 | -1.62922000 | -2.15955200 |
| O | -1.65896700 | 0.17261900 | 0.36331200 |
| N | -1.70735700 | -1.05069900 | 0.98796300 |
| C | -1.25312800 | 1.20040200 | 1.31326800 |
| H | -1.98575800 | 1.20629300 | 2.12484500 |
| H | -0.27410500 | 0.92997300 | 1.71707900 |
| C | 3.55878400 | -0.90254500 | -0.38349900 |
| C | 4.80504900 | -0.89876900 | -1.03477700 |
| C | 3.53031800 | -0.55075300 | 0.97951800 |
| C | 5.97487900 | -0.55307600 | -0.35922600 |
| H | 4.85109600 | -1.17172900 | -2.08556700 |
| C | 4.69696800 | -0.20619100 | 1.65461000 |
| H | 2.58972000 | -0.56008100 | 1.52065300 |
| C | 5.92709600 | -0.20344300 | 0.99003700 |
| H | 6.92340300 | -0.55869800 | -0.88723500 |
| H | 4.64947400 | 0.05692100 | 2.70691600 |
| H | 6.83527900 | 0.06269100 | 1.52101900 |
| C | -1.21471600 | 2.51335300 | 0.58244400 |
| C | -0.01164400 | 3.00765700 | 0.06600600 |
| C | -2.39152600 | 3.24789800 | 0.39040100 |
| C | 0.01744500 | 4.22023300 | -0.62364800 |
| H | 0.90546100 | 2.44286000 | 0.20632500 |

| | | | |
|---|---|---|---|
| C | -2.36559000 | 4.45727800 | -0.30247800 |
| H | -3.32901100 | 2.87026500 | 0.78824000 |
| C | -1.15988900 | 4.94561500 | -0.81007500 |
| H | 0.95700500 | 4.59652600 | -1.01520700 |
| H | -3.28297800 | 5.01969900 | -0.44398500 |
| H | -1.13820200 | 5.88951800 | -1.34538600 |

**Vibrational frequencies**

18.67, 31.36, 33.44, 43.58, 45.67, 51.03, 63, 69.61, 86.87, 112.5, 128.16, 135.23, 159.03, 180.85, 215.88, 249.7, 269.17, 281.69, 314.06, 317.28, 330.32, 363.07, 403.69, 409.37, 412.01, 436.16, 470.4, 494.8, 526.66, 534.86, 604.13, 607.56, 623.71, 625.03, 636.31, 699.47, 709.46, 715.26, 749.64, 755.62, 768.93, 807.39, 817.06, 830.7, 838.25, 848.17, 858.47, 867.23, 870.67, 916.48, 928.15, 929.33, 935.25, 954.65, 969.01, 970.77, 976.44, 987.17, 993.81, 994.83, 996.27, 1005.21, 1007.91, 1009.79, 1013.06, 1028.11, 1046.9, 1048.38, 1050.21, 1061.7, 1084.55, 1094.79, 1107.39, 1113.31, 1126.41, 1157.35, 1176.98, 1179.58, 1183.11, 1199.2, 1199.71, 1220.15, 1224.07, 1225.82, 1234.32, 1237.74, 1269.2, 1303.93, 1313.88, 1317.14, 1326.16, 1342.65, 1352.6, 1355.63, 1357.59, 1360, 1374.92, 1379.21, 1383.21, 1472.27, 1474.51, 1477.66, 1481.87, 1482.88, 1491.72, 1509.9, 1524.29, 1528.95, 1612.27, 1625.9, 1638.03, 1645.39, 1662.61, 1691.75, 3011.02, 3017.22, 3020.81, 3040.52, 3047.62, 3054.03, 3058.3, 3065.38, 3098.82, 3099.35, 3114.79, 3140.27, 3155.99, 3161.42, 3162.58, 3164.52, 3165.3, 3172.15, 3172.81, 3180.16, 3183.38, 3190.39, 3192.46, 3203.25.

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## 19a' TS2*trans*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.406998
Thermal correction to Energy= 0.427666
Thermal correction to Enthalpy= 0.428610
Thermal correction to Gibbs Free Energy= 0.353854
Sum of electronic and zero-point Energies= -982.064649
Sum of electronic and thermal Energies= -982.043981
Sum of electronic and thermal Enthalpies= -982.043037
Sum of electronic and thermal Free Energies= -982.117793

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.66234200 | 0.81690100 | -0.01958900 |
| C | 4.70977500 | 0.25939500 | 0.96248100 |
| C | 3.86351300 | -0.48961100 | 1.96240600 |
| C | 2.61847800 | -0.66652300 | 1.53161100 |
| C | 2.42384500 | -0.10174700 | 0.13360400 |
| H | 4.00615200 | 0.86433400 | -1.05405700 |
| H | 5.30866600 | 1.04812700 | 1.42392400 |
| H | 5.40942100 | -0.42556800 | 0.46978000 |
| H | 4.25217900 | -0.86313300 | 2.90340900 |
| H | 1.84374000 | -1.20165000 | 2.06870100 |
| H | 3.37464000 | 1.82414900 | 0.29188000 |
| C | 2.33051500 | -1.20052500 | -0.92676300 |
| H | 2.36810400 | -0.72018500 | -1.90835200 |
| H | 3.17195600 | -1.89233300 | -0.85226300 |
| C | 0.97381500 | -1.90695000 | -0.74694000 |
| H | 0.60717800 | -2.28695900 | -1.70250000 |
| H | 1.08337100 | -2.76602900 | -0.07877300 |
| C | -0.03821700 | -0.95466800 | -0.13798100 |
| H | -0.05344400 | -0.92920800 | 0.94751300 |
| C | -1.22071600 | -0.63725600 | -0.77609000 |
| H | -1.30867700 | -0.85598500 | -1.83775000 |
| O | 0.86967300 | 1.38424800 | 0.99245300 |
| N | 1.19457300 | 0.65438500 | -0.12314300 |

| | | | |
|---|---|---|---|
| C | 0.18660700 | 2.58433000 | 0.59831200 |
| H | -0.57470900 | 2.33025000 | -0.14298700 |
| H | -0.29998900 | 2.94322000 | 1.50679600 |
| C | -2.35306700 | 0.03200200 | -0.16306200 |
| C | -3.50901400 | 0.27404300 | -0.92759300 |
| C | -2.35149800 | 0.46929600 | 1.17622300 |
| C | -4.61487900 | 0.90997800 | -0.38101200 |
| H | -3.52969300 | -0.04935300 | -1.96347200 |
| C | -3.45741400 | 1.10627100 | 1.71843700 |
| H | -1.47012400 | 0.32295400 | 1.79024100 |
| C | -4.59692400 | 1.33008800 | 0.94673600 |
| H | -5.49381800 | 1.08197800 | -0.99210500 |
| H | -3.43158800 | 1.43459700 | 2.75167600 |
| H | -5.45905700 | 1.82655500 | 1.37620100 |
| C | 1.16061200 | 3.60005800 | 0.06215500 |
| C | 1.43012700 | 3.67506000 | -1.30421300 |
| C | 1.86764600 | 4.42045100 | 0.94120900 |
| C | 2.39416500 | 4.55668500 | -1.78436900 |
| H | 0.88900000 | 3.02939100 | -1.98755100 |
| C | 2.83178400 | 5.30279800 | 0.46465900 |
| H | 1.66451600 | 4.36074100 | 2.00590700 |
| C | 3.09722900 | 5.36996000 | -0.90048000 |
| H | 2.59861700 | 4.60719800 | -2.84776600 |
| H | 3.37481000 | 5.93735800 | 1.15570700 |
| H | 3.84771900 | 6.05691500 | -1.27476900 |

**Vibrational frequencies**

630.41*i*, 15.64, 25.69, 29.19, 36.51, 44.25, 65.64, 74.53, 105.94, 123.87, 148.39, 156.93, 194.65, 210.82, 254.44, 275.54, 301.33, 316.66, 345.04, 375.62, 402.4, 409.87, 412.29, 415.96, 427.77, 461.97, 498.56, 508.15, 528.65, 598.9, 615.32, 627.36, 629.17, 631.08, 692.34, 702, 713.48, 715.66, 759.31, 773.09, 782.91, 788.35, 822.52, 833.86, 842.95, 856.39, 858.72, 860.48, 869.79, 932.41, 935.04, 946.13, 949.43, 975.22, 981.19, 998.73, 1000.67, 1003.83, 1004.54, 1008.3, 1013.2, 1016.26, 1019.81, 1023.55, 1024.89, 1039.26, 1058.81, 1061.17, 1069, 1082.75, 1109.74, 1111.87, 1115.42, 1126.58, 1146.83, 1163.24, 1171.36, 1177.56, 1195.75, 1198.55, 1214.43, 1219.83, 1239.47, 1246.93, 1255.1, 1272.82, 1293.99, 1305.02, 1318.06, 1321.66, 1325.81, 1336.86, 1342.31, 1345.72, 1354.33, 1357.72, 1369.91, 1395.99, 1401.24, 1473.07, 1474.67, 1479.03, 1480.98, 1490.62, 1493.48, 1497.72, 1527.12, 1540.11, 1552.41, 1638.66, 1663.44, 1666.72, 1681.14, 1698.71, 3042.17, 3060.42, 3061.47, 3074.13, 3080.74, 3092.15, 3115.49, 3126.77, 3131.95, 3143.47, 3151.45, 3164.92, 3174.69, 3175.25, 3179.69, 3179.95, 3189.84, 3190.7, 3194.83, 3196.22, 3203.26, 3206.65, 3212.01, 3226.89.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.402850
Thermal correction to Energy= 0.423814
Thermal correction to Enthalpy= 0.424758
Thermal correction to Gibbs Free Energy= 0.349616

Sum of electronic and zero-point Energies= -982.497645
Sum of electronic and thermal Energies= -982.476680
Sum of electronic and thermal Enthalpies= -982.475736
Sum of electronic and thermal Free Energies= -982.550878

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.80202100 | -0.35828600 | -1.20011100 |
| C | 5.04869300 | -0.47681100 | -0.29037600 |
| C | 4.46717600 | -0.44735600 | 1.10083200 |
| C | 3.14051900 | -0.55816000 | 1.09962000 |
| C | 2.57408400 | -0.72191100 | -0.30426000 |
| H | 3.85475100 | -0.99384100 | -2.08602600 |
| H | 5.76718400 | 0.33154500 | -0.46066500 |
| H | 5.59309000 | -1.41417900 | -0.46223300 |

| | | | |
|---|---|---|---|
| H | 5.08130600 | -0.37044600 | 1.99202400 |
| H | 2.51882600 | -0.57718000 | 1.98676100 |
| H | 3.68975000 | 0.67294000 | -1.53901000 |
| C | 2.03012800 | -2.13596400 | -0.55829400 |
| H | 1.83253700 | -2.23549200 | -1.62990900 |
| H | 2.76455700 | -2.89633100 | -0.28339800 |
| C | 0.71322200 | -2.28719500 | 0.22645400 |
| H | 0.05362300 | -3.00203300 | -0.27120100 |
| H | 0.91098800 | -2.68695400 | 1.22591500 |
| C | 0.01571100 | -0.94095400 | 0.37530600 |
| H | 0.24546200 | -0.40472100 | 1.29075200 |
| C | -1.26416500 | -0.75873100 | -0.15070900 |
| H | -1.56324500 | -1.41739600 | -0.96357000 |
| O | 1.56962000 | 1.36353400 | -0.06393200 |
| N | 1.40676700 | 0.11176600 | -0.65558500 |
| C | 0.85696600 | 2.36598600 | -0.82000500 |
| H | 1.15769800 | 2.27437200 | -1.86902300 |
| H | -0.21744900 | 2.17971500 | -0.75615000 |
| C | -2.24334600 | 0.22864000 | 0.23875600 |
| C | -3.46779900 | 0.29862700 | -0.46727900 |
| C | -2.06507800 | 1.12903000 | 1.31593500 |
| C | -4.45509100 | 1.21100800 | -0.11873700 |
| H | -3.63178000 | -0.37938100 | -1.29871700 |
| C | -3.05564300 | 2.03866200 | 1.66126700 |
| H | -1.14664800 | 1.10956300 | 1.89024200 |
| C | -4.25772300 | 2.08897900 | 0.94915100 |
| H | -5.38310900 | 1.23883100 | -0.67979000 |
| H | -2.89307800 | 2.71352900 | 2.49495500 |
| H | -5.02912700 | 2.79893900 | 1.22529000 |
| C | 1.20003600 | 3.72637500 | -0.26942800 |
| C | 2.53283300 | 4.14791300 | -0.18363400 |
| C | 0.18925200 | 4.60238600 | 0.13457600 |
| C | 2.84495800 | 5.41628800 | 0.29746200 |
| H | 3.32720700 | 3.47604200 | -0.48859900 |
| C | 0.49915400 | 5.87829100 | 0.60721600 |
| H | -0.84688800 | 4.28659800 | 0.07611600 |
| C | 1.82782800 | 6.28709500 | 0.69238700 |
| H | 3.88174100 | 5.72836500 | 0.36172500 |
| H | -0.29748700 | 6.54768100 | 0.91331900 |
| H | 2.07190900 | 7.27665200 | 1.06301600 |

**Vibrational frequencies**

531.3*i*, 20.27, 23.04, 32.99, 40.99, 47.5, 58.85, 86.2, 90.62, 122.15, 141.94, 154.8, 179.43, 209, 241.1, 250.72, 284.18, 313.8, 332.17, 355.06, 366.98, 402.94, 411.37, 417.03, 441.58, 463.4, 492.14, 504.77, 527.9, 597.22, 620.35, 628.6, 631.8, 635.21, 685.91, 692.57, 709.59, 712.29, 749.96, 756.76, 764.97, 782.38, 808.42, 821.23, 839.45, 845.69, 847.28, 859.93, 861.05, 913.87, 922.4, 926.68, 929.74, 964.27, 969.91, 983.57, 985.12, 991.56, 992.52, 995.12, 996.85, 1003.86, 1005.22, 1006.7, 1013.28, 1018.09, 1032.24, 1042.31, 1049.53, 1056.57, 1075.04, 1098.41, 1106.77, 1109.24, 1127.5, 1145.9, 1172.58, 1178.86, 1191.72, 1198.7, 1199.99, 1212.02, 1222.99, 1230.93, 1243.91, 1250.17, 1261.54, 1278.5, 1302.11, 1309.96, 1318.07, 1333.62, 1334.99, 1341.5, 1351.75, 1353.88, 1369.56, 1380.08, 1400.89, 1462.38, 1476.29, 1479.25, 1481.35, 1492.81, 1496.27, 1504.7, 1509.26, 1516.54, 1527.9, 1595.04, 1619.07, 1624.46, 1646.11, 1674.52, 3008.43, 3028.47, 3033.25, 3041, 3042.63, 3063.44, 3074.64, 3083.85, 3091.97, 3104.81, 3128.07, 3145.24, 3158.24, 3161.53, 3164.62, 3165.71, 3168.16, 3174.21, 3176.61, 3183.97, 3184.87, 3190.98, 3191.31, 3194.43.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.392869
Thermal correction to Energy= 0.414314
Thermal correction to Enthalpy= 0.415258
Thermal correction to Gibbs Free Energy= 0.339914

Sum of electronic and zero-point Energies= -982.362727
Sum of electronic and thermal Energies= -982.341282
Sum of electronic and thermal Enthalpies= -982.340338
Sum of electronic and thermal Free Energies= -982.415682

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.77717900 | -0.30197000 | -1.12918900 |
| C | 5.03191500 | -0.41135700 | -0.22732400 |
| C | 4.46214000 | -0.36975900 | 1.16894800 |
| C | 3.12787000 | -0.49123500 | 1.17827800 |
| C | 2.55584600 | -0.67325500 | -0.22189600 |
| H | 3.82524200 | -0.93855400 | -2.02282600 |
| H | 5.75357100 | 0.39991900 | -0.41262200 |
| H | 5.58011300 | -1.35535800 | -0.39577300 |
| H | 5.08635600 | -0.27873800 | 2.06005800 |
| H | 2.50616500 | -0.50657200 | 2.07391500 |
| H | 3.65251000 | 0.73691300 | -1.46263700 |
| C | 2.02372400 | -2.09705400 | -0.45910800 |
| H | 1.79714300 | -2.20172400 | -1.53180500 |
| H | 2.78099300 | -2.85038500 | -0.20080100 |
| C | 0.73020400 | -2.25949600 | 0.36323400 |
| H | 0.08722300 | -3.03162100 | -0.08333600 |
| H | 0.96890400 | -2.60062300 | 1.38255100 |
| C | -0.02096400 | -0.93517800 | 0.45514000 |
| H | 0.16554700 | -0.35512600 | 1.36334000 |
| C | -1.29272100 | -0.81958800 | -0.12070800 |
| H | -1.52832900 | -1.50775000 | -0.93987100 |
| O | 1.54989900 | 1.40905600 | 0.00508300 |
| N | 1.37583400 | 0.14798000 | -0.58040400 |
| C | 0.76531900 | 2.40703300 | -0.71735000 |
| H | 0.92455400 | 2.24830200 | -1.79396700 |
| H | -0.30064700 | 2.25755700 | -0.49109300 |
| C | -2.32594000 | 0.13661100 | 0.19765700 |
| C | -3.48874600 | 0.19534400 | -0.61876900 |
| C | -2.26893000 | 1.02409800 | 1.30731500 |
| C | -4.52019200 | 1.09464800 | -0.35591900 |
| H | -3.56278400 | -0.48019700 | -1.47395600 |
| C | -3.30424900 | 1.92025100 | 1.56698400 |
| H | -1.40873800 | 0.99762800 | 1.97799400 |
| C | -4.43665300 | 1.96760300 | 0.73849800 |
| H | -5.39669300 | 1.11704800 | -1.00622000 |
| H | -3.23566300 | 2.58584200 | 2.42984500 |
| H | -5.24434300 | 2.67021300 | 0.94801700 |
| C | 1.23647100 | 3.76828700 | -0.27788600 |
| C | 2.33088800 | 4.38222000 | -0.91043600 |
| C | 0.60721600 | 4.43580100 | 0.78514800 |
| C | 2.78762600 | 5.63485100 | -0.48863000 |
| H | 2.82537500 | 3.87429200 | -1.74127900 |
| C | 1.06152500 | 5.68919800 | 1.20997500 |

| | | | |
|---|---|---|---|
| H | -0.24830000 | 3.97099500 | 1.27852400 |
| C | 2.15369700 | 6.29055800 | 0.57423500 |
| H | 3.63647500 | 6.10214000 | -0.99078100 |
| H | 0.56095000 | 6.19780500 | 2.03569000 |
| H | 2.50735900 | 7.26937600 | 0.90259400 |

**Vibrational frequencies**

365.4*i*, 22.25, 30.42, 36.24, 45.09, 52.78, 65.19, 77.85, 96.01, 121.04, 133.72, 152.38, 173.49, 205.9, 232.6, 249.55, 287.65, 319.89, 327.47, 331, 357.26, 390.97, 398.74, 399.93, 418.87, 450.91, 479.07, 491.9, 512.63, 575.83, 597.76, 610.54, 613.29, 617.19, 661.67, 673.5, 683.72, 690.38, 724.05, 733.42, 743.32, 760.01, 784.96, 797.8, 817.13, 819.26, 825.6, 826.97, 839.6, 880.36, 892.74, 897.06, 913.87, 926.82, 929.98, 944.93, 946.91, 949.48, 955.02, 958.84, 963.89, 965.26, 972.6, 974.61, 976.4, 983.9, 991.23, 1020.65, 1027.71, 1030.72, 1037.68, 1070.51, 1075.18, 1084.79, 1092.29, 1104.85, 1145.86, 1151.08, 1162.1, 1162.57, 1168.97, 1173.89, 1196.46, 1198.37, 1205.9, 1207.55, 1222.45, 1248.66, 1260.73, 1271.3, 1280.78, 1290.52, 1300.62, 1315.08, 1319.09, 1331.58, 1342.1, 1345.35, 1348.12, 1424.59, 1426.08, 1428.37, 1441.58, 1442.74, 1444.27, 1462.52, 1466.05, 1485.12, 1485.43, 1552.12, 1579.5, 1584.52, 1602.24, 1625.67, 2949.91, 2977.51, 2980.76, 2981.67, 2988.38, 3005.99, 3018.35, 3032.5, 3036.63, 3051.82, 3060.43, 3076.1, 3094.53, 3099.89, 3100.87, 3105.55, 3105.66, 3110.74, 3114.65, 3117.66, 3121.81, 3128.66, 3131.79, 3132.64.

### TPSSh/6-311+G(*d*,*p*)

Zero-point correction= 0.402181
Thermal correction to Energy= 0.423233
Thermal correction to Enthalpy= 0.424177
Thermal correction to Gibbs Free Energy= 0.349656
Sum of electronic and zero-point Energies= -982.565604
Sum of electronic and thermal Energies= -982.544553
Sum of electronic and thermal Enthalpies= -982.543609
Sum of electronic and thermal Free Energies= -982.618129

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.75172000 | -0.28056200 | -1.13309000 |
| C | 5.00697200 | -0.41374000 | -0.24041800 |
| C | 4.43963400 | -0.35702600 | 1.15561200 |
| C | 3.11036100 | -0.47220000 | 1.16688200 |
| C | 2.54210300 | -0.66649100 | -0.22889400 |
| H | 3.79322700 | -0.89320200 | -2.03693600 |
| H | 5.73736300 | 0.38027200 | -0.43019800 |
| H | 5.52898200 | -1.36580300 | -0.40740600 |
| H | 5.06241500 | -0.26162200 | 2.04012400 |
| H | 2.49053400 | -0.47802000 | 2.05705500 |
| H | 3.62924700 | 0.76274100 | -1.43345500 |
| C | 2.02289300 | -2.09125500 | -0.46023900 |
| H | 1.77853500 | -2.19569100 | -1.52299700 |
| H | 2.78312200 | -2.83639000 | -0.21140300 |
| C | 0.74672400 | -2.25427300 | 0.38437400 |
| H | 0.10163200 | -3.02783300 | -0.04144500 |
| H | 1.00558800 | -2.57719000 | 1.39820600 |
| C | -0.00496100 | -0.93105500 | 0.47130500 |
| H | 0.18751700 | -0.34279400 | 1.36512500 |
| C | -1.27660800 | -0.82564700 | -0.09958800 |
| H | -1.51458600 | -1.51843400 | -0.90582400 |
| O | 1.52255200 | 1.39804500 | 0.00291000 |
| N | 1.35564000 | 0.14011200 | -0.58463200 |
| C | 0.75325200 | 2.39084100 | -0.72821500 |
| H | 0.93064400 | 2.23482300 | -1.79559700 |
| H | -0.30938800 | 2.24449100 | -0.51726900 |
| C | -2.30284800 | 0.14274800 | 0.20600100 |
| C | -3.45414100 | 0.20409100 | -0.61580000 |
| C | -2.24250000 | 1.03257600 | 1.30593100 |

| | | | |
|---|---|---|---|
| C | -4.47565500 | 1.11341200 | -0.36774100 |
| H | -3.52820600 | -0.47380100 | -1.46148900 |
| C | -3.26770400 | 1.93851400 | 1.55161300 |
| H | -1.39004900 | 1.00270900 | 1.97677700 |
| C | -4.39012200 | 1.99051000 | 0.71732500 |
| H | -5.34274700 | 1.13988000 | -1.02045400 |
| H | -3.19835100 | 2.60641200 | 2.40501000 |
| H | -5.18743700 | 2.69933500 | 0.91489400 |
| C | 1.22162400 | 3.74883700 | -0.27896100 |
| C | 2.31594000 | 4.36325500 | -0.90033800 |
| C | 0.58829000 | 4.40812300 | 0.78048400 |
| C | 2.77025900 | 5.60924800 | -0.46987800 |
| H | 2.81186500 | 3.86260900 | -1.72698500 |
| C | 1.04025500 | 5.65467900 | 1.21444500 |
| H | -0.26572300 | 3.94378200 | 1.26393700 |
| C | 2.13332800 | 6.25692900 | 0.59044100 |
| H | 3.61769000 | 6.07609900 | -0.96194800 |
| H | 0.53849200 | 6.15610600 | 2.03604600 |
| H | 2.48456800 | 7.22787800 | 0.92514300 |

**Vibrational frequencies**

468.31*i*, 26.46, 29.91, 36.32, 45.45, 55.47, 65.61, 80.02, 99.3, 121.45, 134.86, 154.28, 176.48, 208.59, 232.96, 249.98, 291.7, 321.51, 329.42, 332.32, 356.38, 396.32, 409.66, 411.23, 423.35, 452.75, 488.38, 503.09, 519.29, 583.74, 608.78, 620.45, 621.09, 626.74, 671.66, 694.76, 701.15, 704.38, 745.82, 756.2, 764.38, 778.32, 803.65, 816.25, 836.13, 847.01, 848.92, 856.64, 858.39, 912.56, 918.54, 926.56, 930.27, 954.04, 964.7, 977.16, 982.55, 983.55, 986.09, 989.28, 991.1, 997.21, 998.95, 1000.07, 1000.87, 1012.5, 1014.21, 1043.22, 1050.55, 1053.81, 1069.31, 1097.93, 1105.43, 1111.25, 1121.58, 1140.44, 1175.54, 1180.51, 1191.62, 1196.89, 1200.73, 1208.93, 1222.28, 1231.61, 1234.74, 1242.93, 1258.16, 1279.21, 1303.82, 1312.24, 1316.81, 1332.91, 1340.39, 1357.92, 1358.45, 1359.17, 1364.79, 1378.36, 1387.45, 1465.49, 1480.81, 1482.67, 1485.48, 1497.53, 1498.48, 1507.94, 1520.31, 1521.56, 1529.42, 1596.99, 1618.54, 1627.1, 1645, 1667.02, 3005.37, 3033.78, 3036.13, 3044.57, 3045.83, 3059.85, 3075.28, 3091.08, 3096.47, 3105.06, 3121.25, 3138.27, 3153.8, 3159.18, 3159.58, 3163.13, 3163.66, 3170.6, 3172.92, 3177.75, 3181.08, 3188.62, 3191.58, 3191.82.

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## 19a'' TS2*cis*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.407673
Thermal correction to Energy= 0.428006
Thermal correction to Enthalpy= 0.428950
Thermal correction to Gibbs Free Energy= 0.356170

Sum of electronic and zero-point Energies= -982.067976
Sum of electronic and thermal Energies= -982.047643
Sum of electronic and thermal Enthalpies= -982.046699
Sum of electronic and thermal Free Energies= -982.119478

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.97225200 | 2.20425000 | 0.12917100 |
| C | -2.23701900 | 3.18340000 | 1.28913600 |
| C | -0.95432800 | 3.11138600 | 2.08186000 |
| C | 0.02132800 | 2.52175900 | 1.39826100 |
| C | -0.43052100 | 2.13967200 | -0.00121500 |
| H | -2.44819700 | 2.49034000 | -0.81028200 |
| H | -3.11357700 | 2.90422500 | 1.87852800 |
| H | -2.40589000 | 4.20529100 | 0.92953100 |
| H | -0.85265900 | 3.52357800 | 3.07961200 |
| H | 1.03417000 | 2.36266700 | 1.74926500 |
| H | -2.32864300 | 1.20904800 | 0.40710900 |

| | | | |
|---|---|---|---|
| C | 0.14132300 | 3.07890700 | -1.06595000 |
| H | -0.33920000 | 2.84904600 | -2.02234000 |
| H | -0.06094800 | 4.12411400 | -0.82249400 |
| C | 1.64144500 | 2.77959500 | -1.13909600 |
| H | 2.08231500 | 3.19561000 | -2.04852200 |
| H | 2.15371400 | 3.23914800 | -0.28936800 |
| C | 1.84557000 | 1.27970400 | -1.09796400 |
| H | 1.69678800 | 0.76558900 | -2.04168000 |
| C | 2.70339600 | 0.71156900 | -0.16902000 |
| H | 2.97429200 | 1.30565000 | 0.70069600 |
| O | 0.01216700 | -0.05104600 | 0.56551600 |
| N | -0.00504600 | 0.82631600 | -0.48713000 |
| C | -0.28488800 | -1.37653500 | 0.11019100 |
| H | 0.24788200 | -1.56116000 | -0.82515900 |
| H | 0.11247100 | -2.03812600 | 0.88213400 |
| C | 3.11347700 | -0.67580800 | -0.13762400 |
| C | 3.67350000 | -1.20074200 | 1.04264600 |
| C | 2.96387700 | -1.54798700 | -1.23363700 |
| C | 4.04590000 | -2.53387100 | 1.13296700 |
| H | 3.79964900 | -0.54422500 | 1.89744300 |
| C | 3.33947100 | -2.87951800 | -1.14143700 |
| H | 2.55760200 | -1.17600900 | -2.16753500 |
| C | 3.87758600 | -3.38411700 | 0.04227000 |
| H | 4.46625000 | -2.91379900 | 2.05742600 |
| H | 3.21637000 | -3.53173600 | -1.99882400 |
| H | 4.16798900 | -4.42590800 | 0.10999100 |
| C | -1.77034100 | -1.55613100 | -0.06007400 |
| C | -2.37880700 | -1.32959700 | -1.29450300 |
| C | -2.56654800 | -1.86573600 | 1.04326200 |
| C | -3.76207300 | -1.41189500 | -1.42490900 |
| H | -1.76288700 | -1.07718100 | -2.15125600 |
| C | -3.94887700 | -1.94944500 | 0.91670100 |
| H | -2.09690200 | -2.03508400 | 2.00722400 |
| C | -4.54879000 | -1.72011500 | -0.31881700 |
| H | -4.22676000 | -1.23486800 | -2.38828600 |
| H | -4.55771900 | -2.19358300 | 1.77985400 |
| H | -5.62627600 | -1.78460100 | -0.41977800 |

**Vibrational frequencies**

589.42*i*, 31.28, 33.67, 34.65, 44.58, 48.58, 52.61, 99.59, 109.51, 133.22, 141.21, 176.78, 208.9, 216.94, 262.91, 289.8, 310.93, 338.41, 359.46, 377.83, 410.45, 413.97, 416.65, 424.98, 434.41, 489.35, 504.43, 518.32, 533.53, 592.03, 610.85, 620.08, 628.85, 631.22, 688.65, 700.59, 713.3, 719.22, 758.18, 764.27, 785.45, 797.54, 821.7, 841.82, 849.81, 859.33, 862.85, 872.64, 884.18, 922.06, 934.28, 945.92, 951.34, 959.98, 980.02, 995.38, 996.12, 1000.85, 1007.25, 1010.87, 1014.68, 1017.81, 1019.54, 1027.1, 1028.7, 1045.38, 1056.52, 1062.56, 1063.77, 1084.79, 1100.92, 1109.43, 1117.89, 1124.27, 1152.33, 1160.23, 1172.34, 1173.08, 1193.92, 1203.03, 1217.01, 1223.79, 1236.53, 1246.57, 1249.25, 1268.68, 1284.44, 1292.98, 1310.86, 1320.85, 1327.75, 1337.51, 1343.38, 1350.88, 1354.65, 1361.96, 1377.72, 1387.28, 1400.74, 1468.7, 1476.26, 1478.91, 1482.41, 1491.84, 1493.5, 1494.87, 1524.86, 1543.12, 1546.25, 1637.65, 1659.2, 1661.3, 1682.42, 1702.93, 3042.62, 3057.88, 3065.14, 3068.46, 3082.89, 3109.71, 3111.3, 3124.93, 3127.44, 3141.53, 3168.29, 3172.43, 3174.52, 3181.87, 3185.73, 3190.91, 3192.18, 3195.97, 3199.29, 3209.73, 3210.69, 3212.83, 3215.6, 3216.78.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.403179

Thermal correction to Enthalpy= 0.424827

Thermal correction to Energy= 0.423882

Thermal correction to Gibbs Free Energy= 0.350655

Sum of electronic and zero-point Energies= -982.500891
Sum of electronic and thermal Energies= -982.480188
Sum of electronic and thermal Enthalpies= -982.479244
Sum of electronic and thermal Free Energies= -982.553415

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -2.02740100 | 2.44916100 | 0.10559100 |
| C | -2.33953800 | 3.43162000 | 1.25938400 |
| C | -1.09683700 | 3.36408500 | 2.11226000 |
| C | -0.09883300 | 2.72637600 | 1.50368600 |
| C | -0.47543100 | 2.27973300 | 0.09636800 |
| H | -2.40214800 | 2.78536000 | -0.86301700 |
| H | -3.24328300 | 3.15237800 | 1.81055000 |
| H | -2.50256600 | 4.45433000 | 0.89493900 |
| H | -1.03552500 | 3.81434300 | 3.09762100 |
| H | 0.88791900 | 2.56910500 | 1.92154200 |
| H | -2.47799400 | 1.47880700 | 0.31939900 |
| C | 0.23018400 | 3.11598800 | -0.98593700 |
| H | -0.23511200 | 2.90064400 | -1.95379700 |
| H | 0.12290100 | 4.18579000 | -0.79353700 |
| C | 1.69590700 | 2.67042100 | -0.99334400 |
| H | 2.21200400 | 3.02733900 | -1.89080800 |
| H | 2.22448600 | 3.09455900 | -0.13469000 |
| C | 1.75661600 | 1.15541200 | -0.93245300 |
| H | 1.54810200 | 0.66613900 | -1.87766100 |
| C | 2.68001200 | 0.52809800 | -0.08601200 |
| H | 3.01871800 | 1.08695300 | 0.78319100 |
| O | -0.20465500 | 0.09557400 | 0.84473800 |
| N | -0.10096100 | 0.90411100 | -0.28262300 |
| C | -0.46980200 | -1.27788200 | 0.47665200 |
| H | 0.19109500 | -1.56240000 | -0.34346500 |
| H | -0.18414600 | -1.84530900 | 1.36454900 |
| C | 3.18067100 | -0.81869700 | -0.19112700 |
| C | 4.02252300 | -1.32562800 | 0.82845800 |
| C | 2.89736300 | -1.67749300 | -1.28139300 |
| C | 4.54687200 | -2.60956700 | 0.76496800 |
| H | 4.25718000 | -0.68947900 | 1.67603900 |
| C | 3.42344600 | -2.96077900 | -1.33971000 |
| H | 2.26826900 | -1.32931100 | -2.09236400 |
| C | 4.25068500 | -3.43925500 | -0.31927000 |
| H | 5.18878000 | -2.96826700 | 1.56253700 |
| H | 3.19160300 | -3.59529000 | -2.18874600 |
| H | 4.65955500 | -4.44197000 | -0.37075800 |
| C | -1.91504900 | -1.52443200 | 0.12053700 |
| C | -2.32667300 | -1.57222500 | -1.21492700 |
| C | -2.87450400 | -1.68497200 | 1.12731500 |
| C | -3.66765100 | -1.77428300 | -1.53993000 |
| H | -1.59161900 | -1.44768900 | -2.00270700 |
| C | -4.21533000 | -1.88600400 | 0.80680200 |
| H | -2.56787700 | -1.65201200 | 2.16820400 |
| C | -4.61510100 | -1.93016300 | -0.52932100 |
| H | -3.97188300 | -1.80988200 | -2.58049300 |
| H | -4.94746500 | -2.01188200 | 1.59718100 |
| H | -5.65812300 | -2.08941300 | -0.78052500 |

**Vibrational frequencies**

497.19*i*, 23.24, 27.13, 32.67, 40.91, 46.04, 59.21, 85.32, 106.74, 126.7, 139.35, 169.95, 201.2, 206.87, 252.59, 288.51, 291.48, 322.47, 348.73, 369.58, 399.72, 414.09, 415.07, 422.22, 426.31, 490.2, 501.44, 513.22, 529.49, 587.34, 608.64, 615.28, 629.86, 634.7, 683.96, 694.6, 703.07, 708.45, 748.19, 754.37, 768.49, 787.62, 805.58, 831.28, 839.6, 841.47, 846.8, 855.25, 857.81, 909.84, 914.14, 924.73, 929.37, 938.7, 967.35, 974.31, 980.31, 984.22, 988, 990.99, 996.17, 997.37, 1002.69, 1004.92, 1017.54, 1020.81, 1036, 1043.97, 1048.38, 1054.3, 1077.51, 1097.65, 1104.47, 1108.24, 1141.29, 1144.51, 1173, 1177.41, 1192.24, 1196.28, 1199.37, 1208.61, 1220.74, 1226.38, 1234.95, 1259.67, 1272.87, 1281.17, 1306.66, 1308.08, 1319.52, 1333.89, 1342.71, 1343.99, 1353.96, 1359, 1371.35, 1379.93, 1386.75, 1462.45, 1475.48, 1478.87, 1480.17, 1483.07, 1486.9, 1494.09, 1506.97, 1516.88, 1524.31, 1593.38, 1616.81, 1623.87, 1642.06, 1671.55, 3005.04, 3029.49, 3032.59, 3046.25, 3065.13, 3066.15, 3066.86, 3089.66, 3108.99, 3117.17, 3133.07, 3156.09, 3158.21, 3158.57, 3164.29, 3164.77, 3166.62, 3173.19, 3174.02, 3180.76, 3183.24, 3189.43, 3190.87, 3198.76.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.393065
Thermal correction to Energy= 0.414332
Thermal correction to Enthalpy= 0.415276
Thermal correction to Gibbs Free Energy= 0.340246
Sum of electronic and zero-point Energies= -982.366591
Sum of electronic and thermal Energies= -982.345324
Sum of electronic and thermal Enthalpies= -982.344380
Sum of electronic and thermal Free Energies= -982.419409

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -2.02825900 | 2.49191100 | 0.08923200 |
| C | -2.34330500 | 3.49350000 | 1.22757500 |
| C | -1.10743500 | 3.43546200 | 2.09136600 |
| C | -0.10186800 | 2.77870100 | 1.49705900 |
| C | -0.47400900 | 2.30773000 | 0.09549800 |
| H | -2.39323200 | 2.81740000 | -0.89399100 |
| H | -3.25868800 | 3.22714600 | 1.77947700 |
| H | -2.50105200 | 4.51781400 | 0.84509700 |
| H | -1.04933700 | 3.90781000 | 3.07409700 |
| H | 0.88886000 | 2.62437500 | 1.92423600 |
| H | -2.48824600 | 1.52025100 | 0.31343900 |
| C | 0.25353900 | 3.11201000 | -1.00089600 |
| H | -0.20830600 | 2.87790200 | -1.97377100 |
| H | 0.15377300 | 4.19313300 | -0.83193600 |
| C | 1.71552100 | 2.64785200 | -0.98255300 |
| H | 2.25337700 | 2.99808100 | -1.87832700 |
| H | 2.23982400 | 3.07197200 | -0.11237700 |
| C | 1.75896600 | 1.13199100 | -0.91645600 |
| H | 1.53037300 | 0.63778700 | -1.86353100 |
| C | 2.68437300 | 0.49202500 | -0.07435100 |
| H | 3.03685600 | 1.04975700 | 0.79947800 |
| O | -0.23908800 | 0.13957400 | 0.89993800 |
| N | -0.11726600 | 0.91568900 | -0.25482800 |
| C | -0.47506600 | -1.25854800 | 0.55302500 |
| H | 0.22161600 | -1.54996800 | -0.24435900 |
| H | -0.20730100 | -1.79994800 | 1.47052900 |
| C | 3.17377100 | -0.85810500 | -0.18975700 |
| C | 4.02689300 | -1.38088500 | 0.82220900 |
| C | 2.86971400 | -1.71501900 | -1.28511300 |
| C | 4.54094900 | -2.67357800 | 0.74654300 |
| H | 4.27755700 | -0.74566400 | 1.67501300 |
| C | 3.38539900 | -3.00736100 | -1.35472500 |
| H | 2.23279400 | -1.35405200 | -2.09418700 |
| C | 4.22348200 | -3.50016500 | -0.34198900 |
| H | 5.19328000 | -3.04345700 | 1.53991300 |

| | | | |
|---|---|---|---|
| H | 3.13716600 | -3.63976400 | -2.20951000 |
| H | 4.62550400 | -4.51239500 | -0.40299200 |
| C | -1.90755800 | -1.52069900 | 0.15996600 |
| C | -2.28940000 | -1.54178100 | -1.19160300 |
| C | -2.89297200 | -1.70769000 | 1.14514000 |
| C | -3.62675500 | -1.74264500 | -1.55238500 |
| H | -1.53090800 | -1.39815700 | -1.96309600 |
| C | -4.23014500 | -1.90888100 | 0.78791500 |
| H | -2.60779600 | -1.69597400 | 2.19970000 |
| C | -4.60012500 | -1.92458300 | -0.56302600 |
| H | -3.90901800 | -1.75790300 | -2.60664700 |
| H | -4.98422100 | -2.05673500 | 1.56303200 |
| H | -5.64285200 | -2.08387200 | -0.84317600 |

**Vibrational frequencies**

335.37*i*, 22.84, 26.52, 37.33, 42.02, 49, 56.41, 80.52, 103.73, 121.92, 137.52, 165.62, 197.05, 201.71, 243.1, 280, 285.88, 316.22, 339.33, 358.61, 386.01, 398.06, 399.13, 408.96, 413.96, 476.94, 485.56, 499.68, 511.38, 569.12, 588.58, 595.51, 609.82, 615.04, 662.31, 670.52, 684.41, 686.62, 723.24, 732.29, 746.38, 765.35, 780.76, 808.86, 811.99, 819.36, 821.51, 827.75, 829.29, 874.5, 888.16, 892.41, 910.12, 914.92, 924.95, 930.87, 943.91, 949.18, 950.4, 953.99, 963.21, 966.42, 967.44, 974.81, 989.25, 990.76, 1006.89, 1016.15, 1022.76, 1025.07, 1043.15, 1066.14, 1071.44, 1081.54, 1106.98, 1111.27, 1142.38, 1146.29, 1158.57, 1161.79, 1163.85, 1171.31, 1191.6, 1197.89, 1200.41, 1218.15, 1238.84, 1243.01, 1261.9, 1268.89, 1278, 1294.33, 1301.35, 1314.44, 1321.77, 1333.29, 1334.18, 1345.55, 1346.16, 1422.52, 1426.27, 1428.43, 1429.38, 1436.35, 1440.01, 1443.33, 1463.47, 1480.65, 1485.27, 1548.65, 1577.7, 1581.89, 1598.12, 1623.48, 2948.54, 2970.69, 2974.02, 2990.82, 3002.89, 3006.34, 3009.71, 3036.15, 3053.06, 3058.09, 3067.85, 3087.38, 3096.2, 3098.74, 3102.97, 3105.4, 3107.57, 3112.53, 3114.27, 3119.84, 3122.09, 3130.48, 3130.87, 3139.38.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.402400
Thermal correction to Energy= 0.423260
Thermal correction to Enthalpy= 0.424205
Thermal correction to Gibbs Free Energy= 0.350074
Sum of electronic and zero-point Energies= -982.569409
Sum of electronic and thermal Energies= -982.548549
Sum of electronic and thermal Enthalpies= -982.547604
Sum of electronic and thermal Free Energies= -982.621735

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -2.03891400 | 2.42690900 | 0.12907600 |
| C | -2.33995500 | 3.43450600 | 1.26205700 |
| C | -1.08986500 | 3.38142000 | 2.10391700 |
| C | -0.09413800 | 2.73759300 | 1.49158100 |
| C | -0.48815600 | 2.27541900 | 0.09766700 |
| H | -2.43511600 | 2.73205000 | -0.84238000 |
| H | -3.24022700 | 3.16778200 | 1.82650000 |
| H | -2.50200100 | 4.45005400 | 0.87551000 |
| H | -1.01959500 | 3.84665800 | 3.08282000 |
| H | 0.90006200 | 2.58817000 | 1.89760000 |
| H | -2.46872100 | 1.45447900 | 0.38082400 |
| C | 0.19956000 | 3.09673400 | -1.00540700 |
| H | -0.26531300 | 2.85070700 | -1.96714000 |
| H | 0.08024000 | 4.16967700 | -0.83393500 |
| C | 1.66965000 | 2.66519600 | -1.00184100 |
| H | 2.18979700 | 3.02532600 | -1.89671300 |
| H | 2.18586000 | 3.09258500 | -0.13601000 |
| C | 1.74227300 | 1.15177400 | -0.94019700 |
| H | 1.51993800 | 0.65483800 | -1.87966600 |
| C | 2.66961100 | 0.52970800 | -0.09399100 |

| | | | |
|---|---|---|---|
| H | 3.01175200 | 1.09033000 | 0.77441200 |
| O | -0.19951900 | 0.11728100 | 0.88508700 |
| N | -0.11487200 | 0.89559700 | -0.26862400 |
| C | -0.44129100 | -1.27126200 | 0.53727100 |
| H | 0.24383600 | -1.55792600 | -0.26305800 |
| H | -0.17495200 | -1.81472700 | 1.44612900 |
| C | 3.16293100 | -0.82075000 | -0.19975900 |
| C | 4.00114000 | -1.33518600 | 0.82000700 |
| C | 2.87256100 | -1.67556900 | -1.29248500 |
| C | 4.51479500 | -2.62501200 | 0.75518900 |
| H | 4.24027100 | -0.70024400 | 1.66870300 |
| C | 3.38727200 | -2.96478300 | -1.35197800 |
| H | 2.24698700 | -1.31861200 | -2.10429100 |
| C | 4.21058100 | -3.45215600 | -0.33064500 |
| H | 5.15409600 | -2.99030800 | 1.55308300 |
| H | 3.15021600 | -3.59656000 | -2.20273900 |
| H | 4.61071700 | -4.45932500 | -0.38291800 |
| C | -1.87631700 | -1.52189700 | 0.14940700 |
| C | -2.25983100 | -1.53991800 | -1.19653900 |
| C | -2.85627500 | -1.70312700 | 1.13427300 |
| C | -3.59525300 | -1.73237100 | -1.55325300 |
| H | -1.50667300 | -1.40009300 | -1.96567700 |
| C | -4.19164100 | -1.89597500 | 0.78146300 |
| H | -2.56979000 | -1.69327700 | 2.18234100 |
| C | -4.56403700 | -1.90897600 | -0.56443700 |
| H | -3.87893400 | -1.74479000 | -2.60105200 |
| H | -4.94059200 | -2.03885400 | 1.55419500 |
| H | -5.60278200 | -2.06105200 | -0.84047800 |

**Vibrational frequencies**

434.49*i*, 23.64, 28.06, 38.7, 45.35, 52.77, 58.45, 84.33, 103.91, 123.29, 136.8, 168.17, 197.46, 203.52, 248.49, 282.26, 287.42, 315.93, 341.11, 360.11, 390.63, 408.57, 409.65, 412.71, 418.48, 484.17, 495.34, 507.27, 518.29, 575.68, 598, 606.21, 618.57, 624.43, 673.35, 691.36, 698.13, 707.25, 744.15, 755.03, 765.75, 783.15, 798.97, 826.9, 835.07, 837.33, 846.4, 851.44, 860.49, 905.32, 909.5, 921.85, 930.88, 934.06, 962.98, 966.74, 976.73, 981.18, 986.36, 987.33, 990.28, 992.92, 997.64, 1001.93, 1012.42, 1016.49, 1030.18, 1039.67, 1046.1, 1047.96, 1074.46, 1094.07, 1101.27, 1108.05, 1138.76, 1141.53, 1171.8, 1176.06, 1190.22, 1195.76, 1196.3, 1206.91, 1220.69, 1226.4, 1231.92, 1256, 1271.84, 1277.24, 1305.03, 1306.67, 1317.74, 1334.72, 1340.15, 1355.85, 1356.94, 1360.34, 1368.16, 1378, 1380.88, 1462.81, 1479.97, 1482.07, 1483.5, 1488.48, 1491.37, 1499.02, 1506.5, 1520.53, 1525.41, 1593.18, 1616.02, 1624.6, 1641.25, 1664.64, 3004.54, 3026.61, 3030.16, 3047.56, 3060.79, 3064.79, 3066.53, 3090.07, 3106.99, 3120.55, 3128.69, 3153.51, 3155.26, 3157.73, 3162.22, 3164.05, 3164.81, 3171.68, 3173.34, 3179.23, 3182, 3190.18, 3190.83, 3196.98.

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## **21a** trans

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.408962
Thermal correction to Energy= 0.429648
Thermal correction to Enthalpy= 0.430592
Thermal correction to Gibbs Free Energy= 0.356093

Sum of electronic and zero-point Energies= -982.094686
Sum of electronic and thermal Energies= -982.074000
Sum of electronic and thermal Enthalpies= -982.073056
Sum of electronic and thermal Free Energies= -982.147556

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.58493500 | 2.85556500 | 1.42371300 |
| C | 2.07742800 | 3.02797100 | 1.08527800 |
| C | 2.04010000 | 3.39443000 | -0.37788600 |

| | | | |
|---|---|---|---|
| C | 0.85243500 | 3.15032900 | -0.92346600 |
| C | -0.11602000 | 2.55910700 | 0.08755300 |
| H | 0.19484000 | 3.80000400 | 1.81410500 |
| H | 2.63693000 | 2.09506400 | 1.21719200 |
| H | 2.56275200 | 3.78972100 | 1.70003100 |
| H | 2.90328800 | 3.77750500 | -0.91081400 |
| H | 0.59985100 | 3.30236500 | -1.96734200 |
| H | 0.37970900 | 2.07473200 | 2.15818800 |
| C | -1.55658300 | 3.05383400 | -0.05362900 |
| H | -2.07815200 | 2.90818300 | 0.89611900 |
| H | -1.58862300 | 4.11667300 | -0.29761400 |
| C | -2.17231700 | 2.15947300 | -1.15452800 |
| H | -3.16358600 | 1.80339300 | -0.87342400 |
| H | -2.26913900 | 2.68842700 | -2.10325200 |
| C | -1.17453600 | 0.97759900 | -1.31422600 |
| H | -0.53652900 | 1.15815500 | -2.18807600 |
| C | -1.79063200 | -0.37569100 | -1.47099300 |
| H | -1.64397700 | -0.87396100 | -2.42340400 |
| O | 0.87700200 | 0.42815000 | -0.29748200 |
| N | -0.34494200 | 1.10501300 | -0.09943400 |
| C | 0.98966100 | -0.63477600 | 0.64694400 |
| H | 1.04514100 | -0.22711600 | 1.66212500 |
| H | 0.10220200 | -1.27390300 | 0.57912300 |
| C | -2.61685300 | -1.03847900 | -0.52125900 |
| C | -3.19994900 | -2.28423900 | -0.86386100 |
| C | -2.89670600 | -0.51972300 | 0.76850600 |
| C | -4.01487000 | -2.96554800 | 0.02168700 |
| H | -2.99856900 | -2.70196500 | -1.84514800 |
| C | -3.71584300 | -1.21064800 | 1.64662500 |
| H | -2.44263700 | 0.41389700 | 1.07435900 |
| C | -4.28109900 | -2.43384700 | 1.28498900 |
| H | -4.44764400 | -3.91619600 | -0.26868500 |
| H | -3.91336900 | -0.79538700 | 2.62870100 |
| H | -4.91840100 | -2.96832600 | 1.97940600 |
| C | 2.23455800 | -1.40871400 | 0.31114500 |
| C | 3.31592700 | -1.45160100 | 1.18691800 |
| C | 2.31631900 | -2.09113800 | -0.90434700 |
| C | 4.46221000 | -2.17417200 | 0.86176900 |
| H | 3.26045500 | -0.91907800 | 2.13108400 |
| C | 3.45983400 | -2.80669700 | -1.23498700 |
| H | 1.47459000 | -2.05453800 | -1.58899800 |
| C | 4.53576600 | -2.85076600 | -0.35001400 |
| H | 5.29630100 | -2.20465300 | 1.55335900 |
| H | 3.51406600 | -3.33393900 | -2.18062400 |
| H | 5.42649900 | -3.41296000 | -0.60610600 |

**Vibrational frequencies**

16.11, 30.68, 34.76, 39.82, 50.94, 57.31, 72.11, 101.31, 112.83, 147.68, 165.98, 199.44, 222.47, 239.13, 256.46, 287.88, 304.29, 341.85, 367.73, 390.43, 414.26, 417.17, 434.96, 466.48, 480.81, 499.8, 518.75, 566.84, 580.7, 618.38, 632.68, 648.01, 661.02, 676.17, 689.99, 697.32, 717.57, 748.48, 757.6, 774.37, 776.35, 781.3, 820.27, 842.74, 854.57, 857.39, 870.68, 871.72, 927.41, 933.27, 940.79, 946.82, 956.41, 979.03, 995.94, 996.54, 998.21, 1001.68, 1005.37, 1010.57, 1012.66, 1021.9, 1027.09, 1028.01, 1040, 1052.87, 1064.75, 1085.36, 1094.59, 1109.49, 1110.57, 1119.93, 1124.64, 1140.64, 1160.43, 1163.49, 1180.46, 1186.12, 1193.25, 1203.63, 1216.81, 1223.62, 1236.68, 1250.63, 1253.12, 1257.46, 1278, 1302.9, 1308.28, 1319.14, 1329.36, 1329.66, 1343.58, 1344.85, 1350.62, 1356.61,

1393.39, 1407.18, 1415.84, 1434.59, 1468.31, 1485.72, 1490.22, 1492.14, 1499.39, 1505.15, 1508.62, 1508.97, 1547.59, 1613.11, 1634.93, 1669.9, 1687.15, 1699.01, 3040.78, 3042.19, 3048.19, 3070.08, 3076.78, 3087.34, 3092.11, 3093.6, 3123.62, 3130.95, 3138.89, 3171.65, 3174.66, 3175.9, 3176.46, 3181.06, 3187.92, 3191.36, 3195.2, 3197.73, 3200.05, 3200.98, 3209.37, 3216.6.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.404879
Thermal correction to Energy= 0.425900
Thermal correction to Enthalpy= 0.426845
Thermal correction to Gibbs Free Energy= 0.351755
Sum of electronic and zero-point Energies= -982.518812
Sum of electronic and thermal Energies= -982.497791
Sum of electronic and thermal Enthalpies= -982.496847
Sum of electronic and thermal Free Energies= -982.571936

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.72928800 | 2.82759000 | 1.41917000 |
| C | 2.20853500 | 3.15040500 | 1.10054600 |
| C | 2.19505400 | 3.39256300 | -0.38700000 |
| C | 1.03548100 | 3.05505700 | -0.94761200 |
| C | 0.03094300 | 2.52660500 | 0.06580300 |
| H | 0.25413900 | 3.70190800 | 1.87266400 |
| H | 2.87880900 | 2.31739300 | 1.34379500 |
| H | 2.57357300 | 4.01766300 | 1.66061300 |
| H | 3.05696300 | 3.77245600 | -0.92576900 |
| H | 0.82096100 | 3.11824400 | -2.00852600 |
| H | 0.60674200 | 1.99541200 | 2.11380500 |
| C | -1.38007100 | 3.12225200 | -0.09363600 |
| H | -1.90703400 | 3.05763800 | 0.86194400 |
| H | -1.33307800 | 4.17630800 | -0.37399000 |
| C | -2.07995800 | 2.24360700 | -1.15763700 |
| H | -3.09228000 | 1.97815100 | -0.85276000 |
| H | -2.15397900 | 2.74751400 | -2.12297600 |
| C | -1.17772800 | 0.97709700 | -1.29740600 |
| H | -0.55038800 | 1.08843800 | -2.19010400 |
| C | -1.90979500 | -0.32472200 | -1.43606600 |
| H | -1.81500900 | -0.81673900 | -2.39961900 |
| O | 0.89874000 | 0.32131900 | -0.32622700 |
| N | -0.30084000 | 1.07501100 | -0.09731300 |
| C | 0.95058500 | -0.81595700 | 0.55490000 |
| H | 0.91478000 | -0.48029700 | 1.59583500 |
| H | 0.08316800 | -1.45797000 | 0.37262000 |
| C | -2.77524000 | -0.94571800 | -0.50028200 |
| C | -3.46281300 | -2.13714100 | -0.87544600 |
| C | -3.01050700 | -0.45125500 | 0.81502200 |
| C | -4.32852400 | -2.77764300 | -0.00580200 |
| H | -3.29953800 | -2.54045300 | -1.86972000 |
| C | -3.88131400 | -1.10136800 | 1.67606000 |
| H | -2.47916000 | 0.42915600 | 1.14924100 |
| C | -4.54901600 | -2.26494500 | 1.27848800 |
| H | -4.83891300 | -3.68096700 | -0.32237600 |
| H | -4.04079900 | -0.70429400 | 2.67313500 |
| H | -5.22684200 | -2.76699900 | 1.95948400 |
| C | 2.23347700 | -1.55491000 | 0.27382900 |
| C | 3.29526000 | -1.51916000 | 1.18148900 |
| C | 2.38676900 | -2.27912900 | -0.91448000 |
| C | 4.48422100 | -2.19888800 | 0.91524100 |
| H | 3.18961800 | -0.95974800 | 2.10544700 |

| | | | |
|---|---|---|---|
| C | 3.57440900 | -2.95272600 | -1.18732600 |
| H | 1.56904600 | -2.31439800 | -1.62671500 |
| C | 4.62722800 | -2.91406900 | -0.27181600 |
| H | 5.29708000 | -2.16673900 | 1.63266000 |
| H | 3.67958500 | -3.51018600 | -2.11181800 |
| H | 5.55079900 | -3.44237400 | -0.48209500 |

**Vibrational frequencies**

21.56, 25.36, 40.44, 48.46, 49.25, 55.26, 70.18, 91.05, 100.68, 126.56, 153.51, 183.57, 213.26, 230.85, 244.2, 271.85, 309.4, 336.09, 354.65, 384.09, 413.77, 419.82, 429.21, 454.19, 477.42, 499.82, 515.54, 555.76, 583.49, 621.4, 635.91, 639.54, 663.97, 669.17, 689.64, 700.04, 712.45, 745.7, 752.09, 768.55, 770.51, 773.57, 812.44, 829.03, 833.96, 834.73, 854.2, 860.89, 906.62, 909.64, 919.42, 930.42, 937.28, 969.18, 980.17, 981.53, 983.05, 990.91, 992.21, 993.77, 995.02, 1000.41, 1008.91, 1014.15, 1018.26, 1032.6, 1035.71, 1046.62, 1049.94, 1081.83, 1097.48, 1104.75, 1107.75, 1112.78, 1135.39, 1169.94, 1175.27, 1177.93, 1183.17, 1197.57, 1200.05, 1211.18, 1228.57, 1235.37, 1238.14, 1248.54, 1265.28, 1301.31, 1305.59, 1314.75, 1322.14, 1326.38, 1338.38, 1340.46, 1347.51, 1354.91, 1382.09, 1392.6, 1401.21, 1436.61, 1473.67, 1479.61, 1480.7, 1485.54, 1491.76, 1498.3, 1506.22, 1515.21, 1526.99, 1576.19, 1597.97, 1625.18, 1645.53, 1674.1, 3000.97, 3017.63, 3028.24, 3038.91, 3045.83, 3054.33, 3065.91, 3068.45, 3089.96, 3098.93, 3110.52, 3149.71, 3157.46, 3160.7, 3163.4, 3163.83, 3165.41, 3173.4, 3173.68, 3181.54, 3188.68, 3189.51, 3190.5, 3208.94.

### mPWPW91/6-311+G(*d*,*p*)

Zero-point correction= 0.394411
Thermal correction to Energy= 0.416032
Thermal correction to Enthalpy= 0.416976
Thermal correction to Gibbs Free Energy= 0.340865
Sum of electronic and zero-point Energies= -982.378963
Sum of electronic and thermal Energies= -982.357342
Sum of electronic and thermal Enthalpies= -982.356398
Sum of electronic and thermal Free Energies= -982.432508

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.68387100 | 2.86591600 | 1.41633300 |
| C | 2.15942800 | 3.21526900 | 1.10096600 |
| C | 2.15221700 | 3.43812100 | -0.38996900 |
| C | 0.99222900 | 3.07635400 | -0.95553400 |
| C | -0.00413700 | 2.53938900 | 0.06146000 |
| H | 0.18515000 | 3.73879200 | 1.86333000 |
| H | 2.85083300 | 2.39584700 | 1.36135100 |
| H | 2.50715400 | 4.10171200 | 1.65533000 |
| H | 3.01733400 | 3.82489100 | -0.93243800 |
| H | 0.77969000 | 3.12345200 | -2.02455300 |
| H | 0.57212600 | 2.03131900 | 2.12051300 |
| C | -1.43191700 | 3.09636700 | -0.10974400 |
| H | -1.96657200 | 3.01645200 | 0.84819200 |
| H | -1.40941900 | 4.15793600 | -0.39066700 |
| C | -2.09848900 | 2.19923300 | -1.18180800 |
| H | -3.11577200 | 1.91051000 | -0.89035500 |
| H | -2.16820000 | 2.69963400 | -2.15657200 |
| C | -1.16742100 | 0.94712700 | -1.30500900 |
| H | -0.52494300 | 1.06618000 | -2.19521900 |
| C | -1.87592300 | -0.36734700 | -1.43748300 |
| H | -1.75618300 | -0.87970900 | -2.39578100 |
| O | 0.92912200 | 0.34527500 | -0.30321600 |
| N | -0.30650400 | 1.07136500 | -0.08379200 |
| C | 0.95447600 | -0.82803100 | 0.54567000 |
| H | 0.88390700 | -0.52639800 | 1.60321300 |
| H | 0.08915100 | -1.46942800 | 0.31141100 |
| C | -2.75455400 | -0.98007900 | -0.50339700 |

| | | | |
|---|---|---|---|
| C | -3.43349000 | -2.18582100 | -0.86858700 |
| C | -3.01088800 | -0.46125800 | 0.80476700 |
| C | -4.31241400 | -2.81661500 | 0.00345900 |
| H | -3.25261300 | -2.60782100 | -1.85981100 |
| C | -3.89378700 | -1.10248900 | 1.66850400 |
| H | -2.47962700 | 0.43166800 | 1.13061400 |
| C | -4.55404300 | -2.28016100 | 1.28038400 |
| H | -4.81800500 | -3.73319500 | -0.30608200 |
| H | -4.06932800 | -0.68652700 | 2.66266200 |
| H | -5.24355900 | -2.77640600 | 1.96470100 |
| C | 2.24895400 | -1.55250800 | 0.27498900 |
| C | 3.30365300 | -1.51300200 | 1.20012300 |
| C | 2.42603900 | -2.26520000 | -0.92378100 |
| C | 4.50727000 | -2.18001000 | 0.94150200 |
| H | 3.17742400 | -0.96031700 | 2.13368800 |
| C | 3.62919100 | -2.92573200 | -1.18896500 |
| H | 1.61182400 | -2.30222100 | -1.65029800 |
| C | 4.67346100 | -2.88455800 | -0.25583600 |
| H | 5.31560800 | -2.14688900 | 1.67409500 |
| H | 3.75326700 | -3.47643700 | -2.12308700 |
| H | 5.61095200 | -3.40459000 | -0.46022800 |

**Vibrational frequencies**

19.07, 25.44, 38, 50.81, 52.67, 58.46, 70.95, 88.44, 98.09, 126.78, 147.83, 178.68, 203.49, 219.7, 235.95, 263.42, 300.11, 326.04, 340.37, 370.31, 397.48, 402.9, 415.75, 439.41, 460.75, 484.08, 497.53, 537.24, 563.47, 600.78, 615.4, 617.85, 647.59, 648.01, 666.57, 679.19, 689.64, 725.16, 726.55, 743.72, 746.18, 749, 789.85, 803.78, 804.95, 811.71, 831.41, 832.44, 872.27, 879.98, 885.5, 899.05, 916.42, 925.07, 937.33, 943.68, 952.6, 953.4, 955.43, 964.98, 966.1, 967.93, 970.17, 983.82, 990.86, 995.5, 999.06, 1012.17, 1025.61, 1044.02, 1067.51, 1072.21, 1077.39, 1079.39, 1097.97, 1136.66, 1139.86, 1146.91, 1153.57, 1161.5, 1164.56, 1171.79, 1188.84, 1195.79, 1204.51, 1219.45, 1220.54, 1252.94, 1255.68, 1265.72, 1278.21, 1290.02, 1294.6, 1308.79, 1335.13, 1336.63, 1338.62, 1347.26, 1353.4, 1396.98, 1423.82, 1434.44, 1437.54, 1438.33, 1441.49, 1454.76, 1462.25, 1462.93, 1482.65, 1533.99, 1562.76, 1582.47, 1601.55, 1624.47, 2934.79, 2956.45, 2961.04, 2983.8, 2989.31, 2997.71, 2998.25, 3010.81, 3036.41, 3045.13, 3057.75, 3089.25, 3095.59, 3100.98, 3102.38, 3104.24, 3105.56, 3112.55, 3113.84, 3122.2, 3128.59, 3130.41, 3131.29, 3138.29.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.403884
Thermal correction to Energy= 0.425075
Thermal correction to Enthalpy= 0.426019
Thermal correction to Gibbs Free Energy= 0.350753

Sum of electronic and zero-point Energies= -982.585844
Sum of electronic and thermal Energies= -982.564653
Sum of electronic and thermal Enthalpies= -982.563709
Sum of electronic and thermal Free Energies= -982.638975

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.69679100 | 2.85925300 | 1.41291300 |
| C | 2.17888600 | 3.14243900 | 1.07776400 |
| C | 2.14788900 | 3.39971400 | -0.40656800 |
| C | 0.97324200 | 3.08000700 | -0.95362500 |
| C | -0.01076800 | 2.54589300 | 0.07179900 |
| H | 0.24367100 | 3.75779600 | 1.84377800 |
| H | 2.82664400 | 2.28496700 | 1.29971100 |
| H | 2.57628100 | 3.99340100 | 1.64218900 |
| H | 3.00770000 | 3.77331800 | -0.95499100 |
| H | 0.74078900 | 3.15248200 | -2.01134600 |
| H | 0.55763700 | 2.04450100 | 2.12667500 |
| C | -1.43731200 | 3.10045800 | -0.07675500 |

| | | | |
|---|---|---|---|
| H | -1.96011500 | 3.00581400 | 0.87981000 |
| H | -1.42329800 | 4.15858000 | -0.34848700 |
| C | -2.10811100 | 2.21014800 | -1.15042000 |
| H | -3.11284700 | 1.90891200 | -0.84946900 |
| H | -2.19186400 | 2.71982900 | -2.11280100 |
| C | -1.16825500 | 0.97340300 | -1.29643800 |
| H | -0.52928000 | 1.11112000 | -2.17785100 |
| C | -1.86079800 | -0.34782000 | -1.44335600 |
| H | -1.73826900 | -0.84859400 | -2.40085100 |
| O | 0.90984200 | 0.35812000 | -0.30133300 |
| N | -0.31583500 | 1.08520700 | -0.07754900 |
| C | 0.95879100 | -0.77558500 | 0.58976200 |
| H | 0.94159600 | -0.43011600 | 1.62898900 |
| H | 0.08045800 | -1.40683300 | 0.41763000 |
| C | -2.72724900 | -0.97619300 | -0.50830600 |
| C | -3.38540800 | -2.18605600 | -0.87507100 |
| C | -2.98448300 | -0.46571300 | 0.79666000 |
| C | -4.24806900 | -2.83242600 | -0.00372800 |
| H | -3.20270800 | -2.59889100 | -1.86331900 |
| C | -3.85120500 | -1.12173500 | 1.66003900 |
| H | -2.47146500 | 0.43182300 | 1.11991300 |
| C | -4.49140400 | -2.30541400 | 1.27197100 |
| H | -4.73739000 | -3.75103600 | -0.31245500 |
| H | -4.02906700 | -0.71355600 | 2.65043700 |
| H | -5.16627400 | -2.81201900 | 1.95405200 |
| C | 2.23156000 | -1.52421600 | 0.29067300 |
| C | 3.30115400 | -1.50998000 | 1.19152700 |
| C | 2.36730100 | -2.23497400 | -0.90927200 |
| C | 4.48137000 | -2.20017800 | 0.90757300 |
| H | 3.20722000 | -0.95970200 | 2.12354000 |
| C | 3.54652300 | -2.91840600 | -1.19959600 |
| H | 1.54276100 | -2.25149800 | -1.61573100 |
| C | 4.60722500 | -2.90281300 | -0.29060200 |
| H | 5.30081100 | -2.18586400 | 1.61940300 |
| H | 3.63906800 | -3.46565600 | -2.13253900 |
| H | 5.52402600 | -3.43903400 | -0.51444300 |

**Vibrational frequencies**

20.86, 25.85, 40.58, 48.25, 52.16, 60.22, 68.99, 94.03, 100.01, 132.18, 150.43, 184.79, 208.65, 223.77, 239.3, 266.59, 298.6, 329.24, 344.17, 376.2, 406.56, 413.86, 422.15, 446.41, 471.74, 491.57, 502.76, 546.58, 572.95, 609.87, 624.85, 629.56, 653.98, 661.47, 683.52, 690.02, 708.43, 739.32, 746.57, 763.35, 765.48, 769.21, 807.16, 824.09, 834.17, 836.31, 847.95, 862.06, 902.91, 905.15, 912.38, 928.98, 934.37, 962.4, 974.58, 977.16, 979.75, 987.29, 988.89, 989.38, 990.21, 996.59, 1004.57, 1010.42, 1012.82, 1028.22, 1033.42, 1034.68, 1047.63, 1076.31, 1093.47, 1098.2, 1106.14, 1108.12, 1130.78, 1168.86, 1172.78, 1177.86, 1181.82, 1196.08, 1197.39, 1209.02, 1223.2, 1232.55, 1233.32, 1245.89, 1261.01, 1293.43, 1300.11, 1310.3, 1321.88, 1328.21, 1334.03, 1350.87, 1353.74, 1356.35, 1383.13, 1384.41, 1390.67, 1430.27, 1478.07, 1479.58, 1481.14, 1490.98, 1496.97, 1499.44, 1511.31, 1520.11, 1526.98, 1576.95, 1597.69, 1624.71, 1644.1, 1666.43, 3001.19, 3017.43, 3024.19, 3038.23, 3044.43, 3052.9, 3065, 3067.76, 3091.79, 3097.96, 3112.37, 3148.08, 3154.24, 3157.58, 3160.14, 3161.58, 3162.31, 3171.6, 3171.91, 3179.59, 3186.47, 3187.32, 3189.83, 3197.29.

## 21a *cis*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.409112
Thermal correction to Energy= 0.429821
Thermal correction to Enthalpy= 0.430765
Thermal correction to Gibbs Free Energy= 0.355671

Sum of electronic and zero-point Energies= -982.091998
Sum of electronic and thermal Energies -982.071289
Sum of electronic and thermal Enthalpies= -982.070345
Sum of electronic and thermal Free Energies= -982.145439

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.43152200 | 3.23129200 | -0.18473800 |
| C | -2.21909200 | 2.85072200 | 1.08271800 |
| C | -1.12466500 | 2.43958500 | 2.03684000 |
| C | 0.03868300 | 2.25809800 | 1.41749700 |
| C | -0.08440300 | 2.49560100 | -0.07980300 |
| H | -1.23780300 | 4.30779200 | -0.17859100 |
| H | -2.89643500 | 2.00842600 | 0.90266100 |
| H | -2.82210700 | 3.67696500 | 1.46666300 |
| H | -1.29330300 | 2.29186900 | 3.09811400 |
| H | 0.96127400 | 1.93842100 | 1.89072400 |
| H | -1.94104200 | 2.98283500 | -1.11712700 |
| C | 1.11976500 | 3.17991700 | -0.71846700 |
| H | 0.81668600 | 3.59938000 | -1.68102700 |
| H | 1.50309300 | 3.98775100 | -0.09382200 |
| C | 2.14053300 | 2.04241600 | -0.91584000 |
| H | 2.71732500 | 2.17125100 | -1.83206800 |
| H | 2.84608400 | 2.00108500 | -0.08412600 |
| C | 1.29492500 | 0.73145000 | -0.94815700 |
| H | 1.41700100 | 0.23422300 | -1.91890000 |
| C | 1.64274400 | -0.24127000 | 0.13553200 |
| H | 0.89151800 | -0.46243000 | 0.88349100 |
| O | -0.98271000 | 0.32070000 | -0.30946900 |
| N | -0.09377300 | 1.24924600 | -0.88229000 |
| C | -1.78628400 | -0.26867400 | -1.31425900 |
| H | -2.28135400 | 0.51890000 | -1.89471800 |
| H | -1.16259300 | -0.85334500 | -2.00244100 |
| C | 2.87745700 | -0.93654800 | 0.18337600 |
| C | 3.12526600 | -1.87181700 | 1.22052700 |
| C | 3.89957100 | -0.74689600 | -0.78113300 |
| C | 4.31724400 | -2.56797100 | 1.28805100 |
| H | 2.35567500 | -2.03583500 | 1.96773700 |
| C | 5.09010800 | -1.45125500 | -0.70448700 |
| H | 3.75168500 | -0.04075200 | -1.59040600 |
| C | 5.31058100 | -2.36534800 | 0.32581700 |
| H | 4.47958300 | -3.27866300 | 2.09050900 |
| H | 5.85596400 | -1.29058100 | -1.45515700 |
| H | 6.24383100 | -2.91294000 | 0.37968400 |
| C | -2.80981200 | -1.16039400 | -0.65817400 |
| C | -3.61443200 | -1.97250100 | -1.46036100 |
| C | -2.98635300 | -1.18235100 | 0.72395100 |
| C | -4.58624000 | -2.78630400 | -0.89254900 |
| H | -3.47628800 | -1.96525500 | -2.53755300 |
| C | -3.95939100 | -2.00175600 | 1.29278700 |

| | | | |
|---|---|---|---|
| H | -2.35836200 | -0.55898900 | 1.34948500 |
| C | -4.76179600 | -2.80355900 | 0.48948300 |
| H | -5.20471200 | -3.41137500 | -1.52677400 |
| H | -4.08788200 | -2.01278800 | 2.36928800 |
| H | -5.51708000 | -3.44089100 | 0.93445100 |

**Vibrational frequencies**

10.21, 22.67, 32.53, 40.8, 56.62, 70.27, 71.24, 108.89, 128.96, 136.62, 178.55, 191.52, 215.4, 224.89, 235.12, 255.64, 315.84, 352.6, 370.31, 399.79, 412.47, 413.04, 457.66, 468.89, 479.29, 485.16, 521.96, 567.54, 584.05, 622.94, 629.84, 634.85, 658.97, 674.86, 694.85, 707.25, 712.35, 727.99, 751.69, 774.09, 776.51, 793.15, 832.58, 847.72, 849.29, 863.65, 866.15, 882.07, 902.05, 918.73, 932.02, 936.23, 950.87, 985.81, 990, 996.9, 1001.48, 1010.31, 1012.34, 1014.3, 1018.09, 1020.5, 1023.61, 1043.81, 1053.42, 1060.27, 1063.73, 1089.95, 1105.7, 1108.36, 1119.88, 1135.66, 1138.13, 1157.57, 1170.34, 1175.38, 1180.01, 1195.29, 1195.72, 1206.02, 1218.53, 1225.06, 1235.86, 1241.45, 1247.26, 1265.76, 1268.16, 1305.76, 1312.03, 1322.03, 1327.13, 1329.63, 1333.01, 1346.56, 1347.5, 1355.69, 1361.31, 1394.61, 1411.63, 1436.13, 1471.7, 1477.85, 1489.65, 1494.16, 1499.36, 1501.67, 1503.23, 1519.91, 1545.12, 1620.41, 1641.22, 1660.69, 1687.88, 1694.59, 3030.89, 3039.61, 3043.61, 3063.71, 3066.47, 3076.31, 3079.91, 3089.9, 3117.64, 3123.91, 3131.52, 3175.62, 3176.6, 3185.81, 3186.29, 3191.63, 3198.51, 3201.12, 3201.53, 3206.62, 3211.07, 3215.56, 3220.92, 3230.38.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.404604
Thermal correction to Energy= 0.425682
Thermal correction to Enthalpy= 0.426626
Thermal correction to Gibbs Free Energy= 0.350630

Sum of electronic and zero-point Energies= -982.518226
Sum of electronic and thermal Energies= -982.497148
Sum of electronic and thermal Enthalpies= -982.496204
Sum of electronic and thermal Free Energies= -982.572200

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -2.30815600 | 2.99153200 | -0.39592500 |
| C | -3.14054000 | 2.67951600 | 0.87007400 |
| C | -2.09242800 | 2.54418400 | 1.94535900 |
| C | -0.85583600 | 2.51884900 | 1.45102100 |
| C | -0.83445900 | 2.62723400 | -0.06746100 |
| H | -2.36403200 | 4.06141100 | -0.61532300 |
| H | -3.71251000 | 1.74880000 | 0.77482100 |
| H | -3.86541000 | 3.46889900 | 1.09457800 |
| H | -2.34193700 | 2.45450700 | 2.99764100 |
| H | 0.04575000 | 2.40435000 | 2.04215900 |
| H | -2.64943200 | 2.45843000 | -1.28425500 |
| C | 0.22002800 | 3.60470400 | -0.61082100 |
| H | -0.04963300 | 3.88568800 | -1.63297000 |
| H | 0.27316200 | 4.51567100 | -0.01155900 |
| C | 1.53517100 | 2.80324100 | -0.59407700 |
| H | 2.21829000 | 3.10332000 | -1.39050900 |
| H | 2.06135900 | 2.94166500 | 0.35277500 |
| C | 1.10550800 | 1.30536800 | -0.74223900 |
| H | 1.42478000 | 0.93030200 | -1.71890100 |
| C | 1.65253900 | 0.41529800 | 0.32899400 |
| H | 1.07139700 | 0.32289200 | 1.23891500 |
| O | -1.02323800 | 0.23342100 | -0.24810900 |
| N | -0.38903300 | 1.39775100 | -0.78146600 |
| C | -1.46433900 | -0.61024500 | -1.32833100 |
| H | -2.17518300 | -0.06016700 | -1.95314500 |
| H | -0.60546800 | -0.88719700 | -1.94983300 |
| C | 2.86820600 | -0.30265600 | 0.25782200 |
| C | 3.27699000 | -1.10531100 | 1.36517100 |
| C | 3.73862100 | -0.27490500 | -0.87181500 |

| | | | |
|---|---|---|---|
| C | 4.46116500 | -1.82010500 | 1.34252900 |
| H | 2.63497600 | -1.14885500 | 2.23886000 |
| C | 4.92216400 | -0.99638700 | -0.88194300 |
| H | 3.47741500 | 0.32134000 | -1.73799900 |
| C | 5.29753000 | -1.77421600 | 0.21924000 |
| H | 4.74204900 | -2.42079600 | 2.20118400 |
| H | 5.56496900 | -0.95492800 | -1.75499700 |
| H | 6.22564400 | -2.33386900 | 0.20339500 |
| C | -2.10060900 | -1.83739700 | -0.72990700 |
| C | -1.31091700 | -2.91613200 | -0.31684200 |
| C | -3.48620600 | -1.91210200 | -0.55968600 |
| C | -1.89402100 | -4.04618700 | 0.25213800 |
| H | -0.23423900 | -2.86845500 | -0.44320500 |
| C | -4.07401900 | -3.04211900 | 0.00731700 |
| H | -4.10841700 | -1.08143000 | -0.87704700 |
| C | -3.27807800 | -4.11159000 | 0.41468000 |
| H | -1.27013800 | -4.87617600 | 0.56561400 |
| H | -5.15079100 | -3.08800600 | 0.12902600 |
| H | -3.73335700 | -4.99246100 | 0.85411800 |

**Vibrational frequencies**

12.14, 26.13, 29.75, 37.4, 54.48, 55.17, 74.98, 89.36, 116.34, 123.1, 155.92, 180.43, 209.18, 225.79, 243.6, 273.35, 322.38, 344.43, 350.32, 384.9, 404.91, 416.16, 426.87, 444.89, 480.86, 496.19, 518.62, 556.13, 575.13, 612.41, 627.83, 636.4, 662.82, 675.88, 688.36, 691.03, 710.88, 719.26, 764.6, 766.73, 770.7, 780.25, 818.46, 830.35, 840.78, 852.66, 857.18, 860.79, 889.46, 897.63, 908.06, 930.16, 935.84, 968.22, 976.56, 980.17, 987.3, 990.79, 991.55, 993.22, 998.21, 1003.66, 1007.28, 1017.42, 1019.6, 1035.79, 1040.67, 1050.05, 1053.22, 1074.16, 1100.49, 1107.15, 1109.26, 1117.59, 1146.01, 1171.07, 1176.71, 1179.37, 1184.31, 1197.9, 1202.07, 1212.81, 1222.68, 1228.53, 1235.61, 1248.45, 1258.53, 1299.99, 1310.89, 1316.08, 1320.03, 1329.01, 1335.84, 1341.95, 1344.96, 1351.01, 1356.88, 1383.12, 1393, 1439.89, 1472.86, 1480.38, 1481.15, 1482.27, 1491.59, 1500.85, 1502, 1510.71, 1527.35, 1573.48, 1597.65, 1625.43, 1645.68, 1671.87, 3015.26, 3018.06, 3025.8, 3038.71, 3044.16, 3053.73, 3055.55, 3055.85, 3089.08, 3101.88, 3102.55, 3157.13, 3159.62, 3161.74, 3163.26, 3164.03, 3171.81, 3173.38, 3179.63, 3183.72, 3184, 3189.49, 3190.82, 3191.53.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction=0.394381
Thermal correction to Energy= 0.415949
Thermal correction to Enthalpy= 0.416893
Thermal correction to Gibbs Free Energy= 0.341188
Sum of electronic and zero-point Energies= -982.378489
Sum of electronic and thermal Energies= -982.356921
Sum of electronic and thermal Enthalpies= -982.355977
Sum of electronic and thermal Free Energies= -982.431683

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.15052300 | -2.11124100 | -0.51739400 |
| C | 3.88481800 | -1.46968700 | 0.68545200 |
| C | 2.94623800 | -1.72296800 | 1.83811400 |
| C | 1.75743900 | -2.19269100 | 1.43391500 |
| C | 1.67300000 | -2.32790500 | -0.07995100 |
| H | 3.59784600 | -3.09096000 | -0.74207200 |
| H | 4.04318200 | -0.38589900 | 0.55235100 |
| H | 4.88034200 | -1.91141100 | 0.85176000 |
| H | 3.21510500 | -1.51357800 | 2.87546700 |
| H | 0.91881700 | -2.41886900 | 2.09395000 |
| H | 3.19981300 | -1.51077700 | -1.43470600 |
| C | 1.02387100 | -3.63889200 | -0.55873800 |
| H | 1.27655500 | -3.80100500 | -1.61787200 |
| H | 1.38459900 | -4.50227900 | 0.01630400 |

| | | | |
|---|---|---|---|
| C | -0.48576800 | -3.39204900 | -0.38330600 |
| H | -1.10334600 | -3.99010100 | -1.06610000 |
| H | -0.79831300 | -3.64251500 | 0.64065800 |
| C | -0.68171600 | -1.86126200 | -0.62791200 |
| H | -1.14697800 | -1.69961000 | -1.61038300 |
| C | -1.48518800 | -1.19316200 | 0.43536500 |
| H | -1.04316100 | -1.16991500 | 1.43457100 |
| O | 0.92135900 | -0.03644100 | -0.20385100 |
| N | 0.74773900 | -1.36124500 | -0.75078300 |
| C | 0.90866400 | 0.92175700 | -1.29171100 |
| H | 1.67814800 | 0.64627000 | -2.03064800 |
| H | -0.07467500 | 0.90175800 | -1.79236800 |
| C | -2.75097500 | -0.57335000 | 0.28284100 |
| C | -3.37950600 | 0.02589000 | 1.42322300 |
| C | -3.46541900 | -0.50300400 | -0.95622000 |
| C | -4.61853600 | 0.64620800 | 1.32882400 |
| H | -2.85940000 | -0.01066900 | 2.38299700 |
| C | -4.70556800 | 0.12163600 | -1.03747500 |
| H | -3.03484300 | -0.94417500 | -1.85584900 |
| C | -5.29623400 | 0.70241500 | 0.09770300 |
| H | -5.06782000 | 1.09359300 | 2.21755800 |
| H | -5.22497200 | 0.15962400 | -1.99711500 |
| H | -6.26874200 | 1.19076500 | 0.02448000 |
| C | 1.17544500 | 2.28442800 | -0.70494600 |
| C | 0.13813800 | 3.01526500 | -0.10109300 |
| C | 2.46726400 | 2.83414300 | -0.72833100 |
| C | 0.38687300 | 4.26955200 | 0.46520400 |
| H | -0.87006800 | 2.59747400 | -0.07859400 |
| C | 2.71875000 | 4.09132900 | -0.16716600 |
| H | 3.27990100 | 2.27327300 | -1.19531700 |
| C | 1.67835600 | 4.81039100 | 0.43274900 |
| H | -0.42830700 | 4.82736200 | 0.92933600 |
| H | 3.72616800 | 4.50998500 | -0.19768100 |
| H | 1.87228100 | 5.79108900 | 0.87069000 |

**Vibrational frequencies**

22.3, 26.06, 32.92, 45.61, 55.76, 65.28, 77.83, 92.29, 114.67, 143.96, 146.52, 173.01, 197.05, 223.49, 242.19, 261.48, 308.01, 334.06, 335.31, 375.9, 393.23, 398.81, 406.16, 422.72, 467.81, 481.03, 502.44, 535.82, 556.35, 588.34, 606.9, 615.89, 626.73, 660.45, 663.47, 684.41, 688.47, 702.24, 736.84, 740.86, 748.02, 757.13, 793.36, 808.14, 814.81, 827.19, 830.05, 837.77, 853.5, 867.52, 885.71, 896.83, 915.4, 927.33, 942.75, 947.75, 951.22, 955.83, 957.56, 962.97, 964.31, 966.26, 971.68, 978.3, 988.42, 990.82, 999.44, 1014.32, 1025.57, 1039.5, 1066.3, 1069.5, 1079.41, 1081.45, 1122.75, 1132.95, 1142.34, 1146.52, 1159.19, 1162.23, 1165.01, 1173.25, 1184.55, 1186.07, 1203.51, 1212.64, 1221.71, 1254.49, 1265.88, 1271.32, 1284.38, 1286.16, 1301.29, 1301.79, 1309.51, 1335.54, 1338.21, 1339.46, 1346.1, 1406.43, 1419.86, 1430.19, 1437.28, 1437.64, 1439.96, 1449.3, 1462.62, 1469.48, 1482.8, 1531.47, 1562.55, 1581.97, 1601.62, 1622.38, 2946.41, 2962.09, 2983.84, 2986.48, 2991.34, 2992.2, 2995.94, 2997.95, 3037.83, 3047.1, 3047.84, 3097.9, 3098.23, 3099.52, 3104.45, 3104.55, 3104.71, 3113.08, 3115.24, 3121.12, 3123.59, 3128.87, 3129.55, 3132.43.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.403540
Thermal correction to Energy= 0.424817
Thermal correction to Enthalpy= 0.425761
Thermal correction to Gibbs Free Energy= 0.347755
Sum of electronic and zero-point Energies= -982.584963
Sum of electronic and thermal Energies= -982.563686
Sum of electronic and thermal Enthalpies= -982.562742
Sum of electronic and thermal Free Energies= -982.640748

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.99539400 | 3.12576100 | -0.29209300 |
| C | -2.80675400 | 2.80069500 | 0.98284000 |
| C | -1.73556500 | 2.55463100 | 2.01413900 |
| C | -0.51881700 | 2.46472700 | 1.47205600 |
| C | -0.55130600 | 2.62625500 | -0.03814300 |
| H | -1.96888100 | 4.20982300 | -0.44177100 |
| H | -3.42935200 | 1.90558100 | 0.86172400 |
| H | -3.47862100 | 3.61846600 | 1.26693600 |
| H | -1.95539100 | 2.43952600 | 3.07158000 |
| H | 0.39559500 | 2.26540200 | 2.02168400 |
| H | -2.40619000 | 2.67538900 | -1.19807000 |
| C | 0.57491600 | 3.50440800 | -0.59869100 |
| H | 0.31411600 | 3.81469200 | -1.61540200 |
| H | 0.72985000 | 4.40005400 | 0.00768400 |
| C | 1.80249100 | 2.57384200 | -0.60648000 |
| H | 2.51072200 | 2.82101700 | -1.40020500 |
| H | 2.33750500 | 2.63558300 | 0.34429000 |
| C | 1.22009400 | 1.13234100 | -0.78335000 |
| H | 1.49327200 | 0.74624200 | -1.77230100 |
| C | 1.66497500 | 0.15913100 | 0.26378000 |
| H | 0.99614300 | -0.01245600 | 1.10055500 |
| O | -1.00789100 | 0.28206500 | -0.26734400 |
| N | -0.25802300 | 1.38262700 | -0.80971400 |
| C | -1.50890200 | -0.51926800 | -1.35814600 |
| H | -2.09540900 | 0.11514400 | -2.03069200 |
| H | -0.66534000 | -0.93924800 | -1.91953000 |
| C | 2.88049300 | -0.56937000 | 0.22424600 |
| C | 3.17796000 | -1.50197700 | 1.26143600 |
| C | 3.84970100 | -0.42024600 | -0.81025900 |
| C | 4.35410400 | -2.23416100 | 1.25884900 |
| H | 2.45721700 | -1.63393800 | 2.06328600 |
| C | 5.02502900 | -1.15866700 | -0.80169600 |
| H | 3.67063700 | 0.28345600 | -1.61662500 |
| C | 5.28986800 | -2.07132300 | 0.22725900 |
| H | 4.55101500 | -2.93824400 | 2.06151800 |
| H | 5.74691500 | -1.02488400 | -1.60166500 |
| H | 6.21108000 | -2.64428500 | 0.22702200 |
| C | -2.35081800 | -1.61505800 | -0.75996500 |
| C | -1.75083100 | -2.77006900 | -0.24281600 |
| C | -3.74177500 | -1.48296700 | -0.68366800 |
| C | -2.52619100 | -3.77256600 | 0.33872700 |
| H | -0.67174500 | -2.88169000 | -0.29787700 |
| C | -4.52118400 | -2.48571500 | -0.10587700 |
| H | -4.21576900 | -0.59056900 | -1.08247000 |
| C | -3.91380300 | -3.63202900 | 0.40815900 |
| H | -2.04982900 | -4.66367700 | 0.73524800 |
| H | -5.59970700 | -2.37300000 | -0.05759600 |
| H | -4.51829900 | -4.41355300 | 0.85757600 |

**Vibrational frequencies**

1.69, 26.56, 34.99, 39.26, 50.32, 57.08, 70.55, 101.13, 110.12, 124.58, 152.16, 180.87, 206.7, 220.34, 237.82, 269.4, 317.07, 336.94, 341.74, 372.78, 396.28, 409.36, 421.07, 446.51, 470.97, 490.07, 504.64, 545.47, 567.09, 603.77, 618.32, 624.08, 650.33, 662.12, 680.23,

683.67, 706.66, 711.65, 756.66, 762.15, 765.08, 774.02, 815.93, 828.96, 837.16, 846.36, 853.02, 863.37, 882.27, 891.96, 900.86, 930.58, 934.76, 964.83, 974.84, 976.03, 984.14, 987.68, 988.93, 990.36, 994.23, 997, 1002.36, 1009.54, 1012.71, 1025.33, 1034.42, 1042.99, 1046.98, 1073.43, 1097.94, 1105.86, 1107.59, 1115.15, 1140.56, 1170.79, 1171.9, 1177.98, 1180.81, 1198.01, 1198.09, 1211.34, 1217.75, 1225.73, 1232.77, 1238.74, 1254.61, 1291.7, 1306.58, 1308.06, 1316.79, 1326.21, 1330.23, 1340.35, 1353.76, 1354.31, 1356.19, 1384.46, 1387.35, 1429.26, 1476, 1479.95, 1480.88, 1485.37, 1494.28, 1501.74, 1504.52, 1521, 1526.86, 1576.34, 1598.91, 1624.22, 1643.94, 1664.77, 3006.11, 3013.64, 3021.65, 3037.57, 3041.86, 3053.69, 3054.94, 3061.26, 3090.03, 3100.41, 3104.26, 3156.17, 3157.54, 3160.23, 3161.13, 3161.24, 3170.08, 3171.84, 3177.21, 3178.91, 3182.04, 3189.25, 3189.37, 3190.2.

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## **16**_*trans*_

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.423025
Thermal correction to Energy= 0.443443
Thermal correction to Enthalpy= 0.444387
Thermal correction to Gibbs Free Energy= 0.371587

Sum of electronic and zero-point Energies= -982.730744
Sum of electronic and thermal Energies= -982.710326
Sum of electronic and thermal Enthalpies= -982.709382
Sum of electronic and thermal Free Energies= -982.782182

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.26244400 | 2.38878200 | 1.50246400 |
| C | 1.73327800 | 2.75867400 | 1.23577300 |
| C | 1.68757300 | 3.25523900 | -0.18921700 |
| C | 0.55509100 | 2.91573200 | -0.79788100 |
| C | -0.35057200 | 2.11267800 | 0.12006500 |
| H | -0.24765700 | 3.25392100 | 1.93591500 |
| H | 2.39554900 | 1.88617000 | 1.29708400 |
| H | 2.11445200 | 3.50566400 | 1.93600000 |
| H | 2.51000600 | 3.78686800 | -0.65481400 |
| H | 0.31470800 | 3.12068300 | -1.83588000 |
| H | 0.12131400 | 1.54285600 | 2.17715200 |
| C | -1.83949600 | 2.40761000 | -0.04122400 |
| H | -2.37577600 | 2.01243500 | 0.82623400 |
| H | -2.03386400 | 3.47871500 | -0.11328300 |
| C | -2.22705400 | 1.62953800 | -1.31409300 |
| H | -3.24551100 | 1.24461800 | -1.25506700 |
| H | -2.16629500 | 2.27135900 | -2.19481500 |
| C | -1.18256100 | 0.49535200 | -1.41512700 |
| H | -0.53626000 | 0.65071100 | -2.28832200 |
| C | -1.74978500 | -0.92989900 | -1.50436800 |
| H | -2.15571600 | -1.07463700 | -2.50976400 |
| O | 0.94286700 | 0.19045200 | -0.46192200 |
| N | -0.36502600 | 0.66255200 | -0.20102100 |
| C | 1.32398800 | -0.77518700 | 0.51176300 |
| H | 1.23060900 | -0.35435300 | 1.51791100 |
| H | 0.66268200 | -1.64737500 | 0.44158300 |
| C | -2.82409200 | -1.24110100 | -0.48978200 |
| C | -4.15997400 | -1.34466400 | -0.88510200 |
| C | -2.52272900 | -1.40736100 | 0.86583000 |
| C | -5.16824500 | -1.60007300 | 0.04034300 |
| H | -4.41331900 | -1.22362400 | -1.93414100 |
| C | -3.52698400 | -1.66301300 | 1.79399300 |
| H | -1.49447100 | -1.32182700 | 1.19494600 |

| | | | |
|---|---|---|---|
| C | -4.85408900 | -1.75865500 | 1.38583800 |
| H | -6.19765000 | -1.67624700 | -0.29144600 |
| H | -3.27175000 | -1.78989200 | 2.84020100 |
| H | -5.63587400 | -1.95731200 | 2.10994400 |
| C | 2.75022700 | -1.16881400 | 0.23678100 |
| C | 3.72551600 | -1.05340500 | 1.22447200 |
| C | 3.11077500 | -1.65475500 | -1.02163700 |
| C | 5.04254500 | -1.42638200 | 0.96641600 |
| H | 3.45315800 | -0.67099800 | 2.20309500 |
| C | 4.42504200 | -2.01942700 | -1.28434300 |
| H | 2.35458900 | -1.73896800 | -1.79506600 |
| C | 5.39444600 | -1.90683500 | -0.28926000 |
| H | 5.79242200 | -1.33346000 | 1.74376200 |
| H | 4.69727600 | -2.39128900 | -2.26549100 |
| H | 6.41984800 | -2.19202900 | -0.49483300 |
| H | -0.91229400 | -1.62769700 | -1.39861600 |

**Vibrational frequencies**

13.03, 29.73, 43.17, 49.7, 58.18, 63.28, 90.92, 108.32, 127.68, 139.38, 174, 212.44, 229.75, 243.28, 263.69, 285.72, 318.44, 357.94, 375.76, 397.36, 412.69, 414.49, 430.14, 466.71, 470.57, 501.34, 512.65, 565.39, 586.73, 616.91, 630.48, 633.38, 669.85, 682.23, 715.87, 718.48, 733.67, 759.76, 770.48, 773.27, 781.39, 815.34, 836.14, 857.78, 867.71, 873.71, 876.29, 892.98, 926.12, 942.85, 944.88, 947.83, 965.08, 984.86, 994.35, 1001.89, 1005.92, 1009.71, 1018.62, 1019.26, 1021.52, 1023.31, 1026.06, 1032.96, 1047.95, 1062.87, 1064.85, 1085.61, 1090.84, 1111.54, 1113.61, 1121.88, 1127.24, 1140.21, 1162.57, 1173.74, 1174.68, 1187.32, 1200.04, 1203.52, 1211.06, 1220.12, 1234.97, 1238.13, 1243.51, 1247.25, 1252.23, 1274.14, 1310.82, 1320.34, 1327.07, 1335.72, 1336.68, 1344.67, 1346.6, 1353.26, 1358.44, 1366.06, 1394.99, 1399.73, 1409.87, 1472.44, 1474.53, 1481.55, 1490.57, 1494.72, 1496.42, 1503.65, 1526.06, 1540.44, 1544.07, 1661.01, 1665.49, 1680.26, 1685.35, 1693.33, 3029.21, 3040.79, 3043.5, 3053.62, 3057.86, 3060.09, 3082.77, 3099.2, 3101.93, 3106.6, 3117.6, 3118.94, 3131.85, 3165.45, 3173.08, 3179.68, 3183.68, 3189.04, 3189.82, 3195.65, 3203.64, 3203.8, 3212.47, 3213.12, 3215.86.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.418583
Thermal correction to Energy= 0.439489
Thermal correction to Enthalpy= 0.440433
Thermal correction to Gibbs Free Energy= 0.366149

Sum of electronic and zero-point Energies= -983.153226
Sum of electronic and thermal Energies= -983.132320
Sum of electronic and thermal Enthalpies= -983.131376
Sum of electronic and thermal Free Energies= -983.205660

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.38739200 | 2.68017100 | 1.39425400 |
| C | 1.77117500 | 3.31322300 | 1.10880700 |
| C | 1.76260000 | 3.51009000 | -0.38543200 |
| C | 0.71234800 | 2.93775000 | -0.97005700 |
| C | -0.20933800 | 2.25114500 | 0.02505400 |
| H | -0.27110800 | 3.42583800 | 1.84746400 |
| H | 2.60173600 | 2.66031100 | 1.40306300 |
| H | 1.91365700 | 4.25466300 | 1.64998100 |
| H | 2.55118900 | 4.04033500 | -0.90938500 |
| H | 0.52729000 | 2.93167100 | -2.03845200 |
| H | 0.43292400 | 1.83454700 | 2.08150500 |
| C | -1.69425200 | 2.60004600 | -0.17411600 |
| H | -2.23836300 | 2.38063500 | 0.74854500 |
| H | -1.82745400 | 3.66002100 | -0.39879300 |
| C | -2.16718200 | 1.67060600 | -1.31256300 |
| H | -3.18209200 | 1.31236700 | -1.13580200 |

| | | | |
|---|---|---|---|
| H | -2.16848100 | 2.18828900 | -2.27432200 |
| C | -1.13975300 | 0.51250600 | -1.33614400 |
| H | -0.50231000 | 0.60047300 | -2.22573400 |
| C | -1.72805500 | -0.91458100 | -1.36585400 |
| H | -2.08339900 | -1.09552600 | -2.38536400 |
| O | 1.00827800 | 0.20291300 | -0.38430300 |
| N | -0.29498700 | 0.76414000 | -0.14238000 |
| C | 1.34876000 | -0.75700700 | 0.63207600 |
| H | 1.34409000 | -0.27908400 | 1.61625300 |
| H | 0.60627400 | -1.56223600 | 0.64108800 |
| C | -2.85946900 | -1.22245400 | -0.40560000 |
| C | -4.14239600 | -1.49404300 | -0.89832000 |
| C | -2.66823500 | -1.26104800 | 0.98302300 |
| C | -5.20041800 | -1.79507100 | -0.04068900 |
| H | -4.31422100 | -1.47495400 | -1.97021900 |
| C | -3.72321000 | -1.55900400 | 1.84402700 |
| H | -1.68822800 | -1.04558400 | 1.38960600 |
| C | -4.99429500 | -1.82803400 | 1.33679500 |
| H | -6.18286600 | -2.00524700 | -0.44992600 |
| H | -3.55061100 | -1.58348100 | 2.91488400 |
| H | -5.81321400 | -2.06360700 | 2.00762500 |
| C | 2.71767600 | -1.30425400 | 0.31607200 |
| C | 3.83104600 | -0.93068700 | 1.07383000 |
| C | 2.89634000 | -2.19872100 | -0.74594500 |
| C | 5.09682500 | -1.43830400 | 0.78111400 |
| H | 3.70694200 | -0.23992600 | 1.90156400 |
| C | 4.15902200 | -2.70339900 | -1.04520900 |
| H | 2.04147400 | -2.50089100 | -1.34151800 |
| C | 5.26333300 | -2.32515600 | -0.28035900 |
| H | 5.95000400 | -1.14109000 | 1.38115600 |
| H | 4.28200200 | -3.39556300 | -1.87110500 |
| H | 6.24642500 | -2.72088100 | -0.51080100 |
| H | -0.90246500 | -1.61601000 | -1.20882300 |

**Vibrational frequencies**

23.52, 26.57, 28.13, 42.51, 55.62, 61.48, 75.91, 85.29, 106.66, 127.44, 161.82, 199.22, 216.73, 236.55, 243.65, 265.53, 322.89, 338.49, 357.89, 385.01, 412.96, 416.43, 424.07, 453.74, 469.51, 498.77, 513.16, 555.05, 588.99, 617.78, 634.87, 635.8, 659.28, 695.98, 709.07, 712.28, 733.3, 746.8, 764.77, 766.91, 770.49, 808.78, 819.46, 832.01, 854.09, 857.59, 857.65, 878.31, 903.1, 927.02, 929.2, 930.95, 945.96, 968.81, 981.17, 987.26, 987.98, 992.78, 998.77, 1002.17, 1004.93, 1006, 1009.44, 1015.85, 1018.27, 1040.57, 1048.55, 1049.13, 1057.15, 1080.6, 1098.34, 1106.88, 1107.75, 1115.97, 1139.83, 1174.75, 1175.36, 1177.49, 1196.45, 1197.55, 1201.64, 1214.22, 1218.13, 1229.59, 1230.48, 1233.73, 1240.25, 1263.1, 1301.9, 1311.41, 1317.66, 1328.09, 1337.19, 1340.45, 1342.72, 1352.44, 1356.56, 1363.48, 1384.08, 1393.18, 1411.01, 1474.8, 1477.95, 1481.29, 1484.25, 1484.99, 1494.09, 1507.38, 1515.83, 1522.62, 1526.45, 1619.01, 1624.98, 1640.64, 1645.32, 1675.65, 2986.58, 3014.1, 3020.66, 3033.8, 3037.2, 3047.52, 3054.52, 3058.86, 3062.14, 3065.8, 3089.57, 3102.47, 3104.32, 3153.33, 3159.49, 3162.49, 3163.78, 3163.98, 3171.36, 3172.27, 3180.08, 3184.43, 3189.51, 3189.60, 3197.48.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.407652
Thermal correction to Energy= 0.429183
Thermal correction to Enthalpy= 0.430128
Thermal correction to Gibbs Free Energy= 0.354774
Sum of electronic and zero-point Energies= -983.010579
Sum of electronic and thermal Energies= -982.989048
Sum of electronic and thermal Enthalpies= -982.988103
Sum of electronic and thermal Free Energies= -983.063457

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.37026300 | 2.69636800 | 1.38323400 |
| C | 1.75149300 | 3.33425200 | 1.08844200 |
| C | 1.74028800 | 3.51851900 | -0.40793400 |
| C | 0.68154600 | 2.93672000 | -0.98801400 |
| C | -0.22914900 | 2.25158800 | 0.01790200 |
| H | -0.29570500 | 3.44672700 | 1.83393200 |
| H | 2.59270600 | 2.68632400 | 1.38903100 |
| H | 1.89284600 | 4.28657700 | 1.62460000 |
| H | 2.53208800 | 4.04784700 | -0.94200400 |
| H | 0.49094300 | 2.92020800 | -2.06216900 |
| H | 0.41891600 | 1.85107700 | 2.08140300 |
| C | -1.72227400 | 2.57828100 | -0.17714200 |
| H | -2.26259400 | 2.34954800 | 0.75346900 |
| H | -1.87069800 | 3.64311400 | -0.40129400 |
| C | -2.18392200 | 1.64139600 | -1.31662200 |
| H | -3.20073700 | 1.26747000 | -1.13923300 |
| H | -2.19097400 | 2.16055800 | -2.28488300 |
| C | -1.14276700 | 0.49302400 | -1.33774600 |
| H | -0.49935100 | 0.58481900 | -2.23218000 |
| C | -1.71781300 | -0.94284000 | -1.35901500 |
| H | -2.06348500 | -1.14167300 | -2.38579100 |
| O | 1.02038100 | 0.20291700 | -0.38984100 |
| N | -0.30245200 | 0.75399900 | -0.13592100 |
| C | 1.37134500 | -0.74274200 | 0.64845000 |
| H | 1.37418200 | -0.24516800 | 1.63148600 |
| H | 0.62616400 | -1.55576400 | 0.67803100 |
| C | -2.85533900 | -1.24250200 | -0.40351000 |
| C | -4.13836800 | -1.53180300 | -0.90327300 |
| C | -2.67553700 | -1.24621900 | 0.99313600 |
| C | -5.20659800 | -1.81800900 | -0.04469300 |
| H | -4.30032700 | -1.53808000 | -1.98402500 |
| C | -3.74144100 | -1.52844600 | 1.85489000 |
| H | -1.69270200 | -1.01304100 | 1.40265000 |
| C | -5.01164600 | -1.81641400 | 1.34066200 |
| H | -6.19069800 | -2.04384800 | -0.45969700 |
| H | -3.57770200 | -1.52636000 | 2.93433600 |
| H | -5.84068900 | -2.04121400 | 2.01377700 |
| C | 2.74070700 | -1.28980400 | 0.32757600 |
| C | 3.86106000 | -0.91180300 | 1.08415000 |
| C | 2.91754100 | -2.18971900 | -0.73791300 |
| C | 5.13066200 | -1.42226600 | 0.78863200 |
| H | 3.73690700 | -0.21413800 | 1.91522600 |
| C | 4.18478000 | -2.69627600 | -1.04038300 |
| H | 2.05539100 | -2.49521500 | -1.33368700 |
| C | 5.29502900 | -2.31516700 | -0.27565600 |
| H | 5.99078900 | -1.12201200 | 1.38955500 |
| H | 4.30669700 | -3.39463400 | -1.87016600 |
| H | 6.28368400 | -2.71404900 | -0.50886700 |
| H | -0.88070600 | -1.63724000 | -1.18436600 |

**Vibrational frequencies**

21.21, 27.4, 33.61, 39.14, 54.69, 60.34, 73.68, 82.98, 105.53, 123.67, 157.31, 193.38, 210.2, 227.69, 233.88, 255.7, 310.49, 326.16, 344.04, 371.51, 396.73, 398.8, 409.24, 440.45, 452.12, 483.4, 495.32, 536.58, 568.1, 597.01, 614.44, 615.68, 637.19, 673.54, 685.1, 689.76, 710.61, 722.48, 739.5, 743.11, 745.25, 786.31, 794.65, 809.31, 825.93, 828.14, 831.11, 852.66, 875.29, 892.77, 895.23, 899.45, 915.37, 927.88, 939.28, 948.26, 948.73, 964.5, 965.11, 965.57, 966.76, 975.32, 980.32, 987.65, 990.87, 999.23, 1018.71, 1024.41, 1024.94, 1048.41, 1066.1, 1075.19, 1079.03, 1081.25, 1101.32, 1137.07, 1143.79, 1146.97, 1162.44, 1163.37, 1163.62, 1176.27, 1185.52, 1188.07, 1189.72, 1201.17, 1202.32, 1219.78, 1256.78, 1265.05, 1274.47, 1282.63, 1287.79, 1305.19, 1306.11, 1314.16, 1336.4, 1339.27, 1342.21, 1348.4, 1360.52, 1427.5, 1429.13, 1433.68, 1438.13, 1438.43, 1444.03, 1456.43, 1463.37, 1477.45, 1481.97, 1576.33, 1582.76, 1596.92, 1601.36, 1626.04, 2920.29, 2947.58, 2958.03, 2975.42, 2983.14, 2991.38, 2991.86, 2998.51, 3002.06, 3011.34, 3034.82, 3047.31, 3049.71, 3091.49, 3099.42, 3101.56, 3104.14, 3104.99, 3110.79, 3112.53, 3120.45, 3123.92, 3129.9, 3131.06, 3132.02.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.417405
Thermal correction to Energy= 0.438568
Thermal correction to Enthalpy= 0.439512
Thermal correction to Gibbs Free Energy= 0.364503

Sum of electronic and zero-point Energies= -983.218985
Sum of electronic and thermal Energies= -983.197823
Sum of electronic and thermal Enthalpies= -983.196878
Sum of electronic and thermal Free Energies= -983.271888

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.41975300 | 2.62473600 | 1.42968200 |
| C | 1.83946200 | 3.14873700 | 1.11271700 |
| C | 1.77453700 | 3.43273900 | -0.36585000 |
| C | 0.66680400 | 2.94563400 | -0.92877400 |
| C | -0.22752300 | 2.24250300 | 0.07573900 |
| H | -0.17039800 | 3.42776100 | 1.88221000 |
| H | 2.61801700 | 2.40353300 | 1.32099000 |
| H | 2.09212200 | 4.03890400 | 1.69964600 |
| H | 2.56777200 | 3.94873100 | -0.89893700 |
| H | 0.43068700 | 3.00234600 | -1.98680300 |
| H | 0.40845300 | 1.78047600 | 2.12215700 |
| C | -1.71828700 | 2.58359900 | -0.07041700 |
| H | -2.23909200 | 2.31376500 | 0.85324100 |
| H | -1.86859700 | 3.65107200 | -0.24760900 |
| C | -2.20161500 | 1.69786900 | -1.24041900 |
| H | -3.21097700 | 1.32043800 | -1.06358000 |
| H | -2.21835800 | 2.25594700 | -2.18018600 |
| C | -1.16558200 | 0.55105300 | -1.32606200 |
| H | -0.53307100 | 0.68139500 | -2.21469900 |
| C | -1.74151200 | -0.87866600 | -1.39772300 |
| H | -2.10815600 | -1.03317800 | -2.41858500 |
| O | 0.99216800 | 0.21278100 | -0.40291800 |
| N | -0.31910700 | 0.75807400 | -0.12450800 |
| C | 1.32512700 | -0.78388900 | 0.58214700 |
| H | 1.28807600 | -0.34853100 | 1.58594100 |
| H | 0.59530600 | -1.60193900 | 0.53562700 |
| C | -2.86151700 | -1.21068800 | -0.43314700 |
| C | -4.14357000 | -1.49745400 | -0.92283300 |
| C | -2.66211700 | -1.25053800 | 0.95558200 |
| C | -5.19438600 | -1.81663100 | -0.06098400 |
| H | -4.31859100 | -1.47578700 | -1.99539600 |
| C | -3.71050200 | -1.56643700 | 1.82037300 |
| H | -1.68125000 | -1.02128800 | 1.35627000 |

| | | | |
|---|---|---|---|
| C | -4.98101200 | -1.85167300 | 1.31681100 |
| H | -6.17659200 | -2.03918500 | -0.46663400 |
| H | -3.53319700 | -1.59259900 | 2.89136100 |
| H | -5.79416100 | -2.10158700 | 1.99093600 |
| C | 2.71295000 | -1.28674400 | 0.27564900 |
| C | 3.74788700 | -1.12591800 | 1.20251300 |
| C | 2.98599500 | -1.93282800 | -0.93764700 |
| C | 5.03079800 | -1.60479200 | 0.92954200 |
| H | 3.54829400 | -0.62293200 | 2.14465100 |
| C | 4.26724200 | -2.40448900 | -1.21640700 |
| H | 2.19254800 | -2.05950200 | -1.66738800 |
| C | 5.29308800 | -2.24408900 | -0.28147800 |
| H | 5.82304300 | -1.47542500 | 1.66019200 |
| H | 4.46633800 | -2.90153300 | -2.16072000 |
| H | 6.29013800 | -2.61432300 | -0.49804000 |
| H | -0.90806900 | -1.57753800 | -1.26383200 |

**Vibrational frequencies**

20.59, 23.44, 31.98, 40.72, 43.14, 63.9, 84.38, 86.52, 109.16, 119.05, 155.6, 194.17, 211, 228.91, 236.46, 261.88, 301.42, 328.61, 354.04, 373.51, 407.31, 410.38, 417.67, 445.35, 461.16, 489.69, 498.56, 546.78, 575.17, 609.34, 623.77, 624.26, 648.49, 677.72, 706.57, 709.08, 725.13, 739.33, 758.27, 761.66, 766.85, 801.24, 814.28, 831.82, 846.91, 859.01, 859.09, 872.08, 898.34, 925.48, 926.24, 927.86, 938.77, 960.29, 974.48, 985.06, 986.91, 987.76, 995.55, 999.48, 1000.09, 1001.39, 1006.1, 1010.36, 1013.28, 1037.02, 1045.89, 1047.13, 1052.3, 1073.27, 1093.76, 1104.29, 1105.92, 1110.76, 1135.32, 1172.45, 1174.16, 1176.62, 1196.25, 1196.99, 1197.97, 1209.7, 1215.07, 1222.57, 1224.22, 1235.48, 1237.56, 1258.62, 1302.11, 1306.57, 1314.64, 1324.85, 1329.96, 1346.65, 1348.11, 1352.72, 1355.07, 1360.88, 1385.27, 1390.23, 1398.87, 1474.95, 1477.81, 1480.43, 1486.81, 1487.49, 1495.03, 1508.29, 1519.94, 1521.57, 1526.78, 1618.13, 1623.66, 1638.83, 1644.16, 1666.69, 2987.61, 3009.57, 3016.37, 3027.89, 3038.5, 3046.82, 3053.06, 3055.09, 3056.74, 3062.92, 3089.2, 3098.85, 3104.07, 3149.48, 3157.28, 3159.9, 3162.01, 3163.33, 3169.73, 3172.96, 3181.9, 3183.19, 3188.03, 3190.34, 3192.27.

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## 16*cis*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.422604
Thermal correction to Energy= 0.443306
Thermal correction to Enthalpy= 0.444250
Thermal correction to Gibbs Free Energy= 0.370181
Sum of electronic and zero-point Energies= -982.728629
Sum of electronic and thermal Energies= -982.707927
Sum of electronic and thermal Enthalpies= -982.706983
Sum of electronic and thermal Free Energies= -982.781052

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.38163100 | 3.09429200 | -0.74642700 |
| C | -2.32382800 | 2.96813100 | 0.46531200 |
| C | -1.36288400 | 2.71374800 | 1.60092500 |
| C | -0.14820500 | 2.39195300 | 1.16469800 |
| C | -0.08850200 | 2.35650600 | -0.35452600 |
| H | -1.14109500 | 4.14930700 | -0.90564100 |
| H | -3.01334300 | 2.12225800 | 0.36204300 |
| H | -2.93036600 | 3.86352800 | 0.62137900 |
| H | -1.65544600 | 2.76532100 | 2.64419000 |
| H | 0.69781400 | 2.13927300 | 1.79505800 |
| H | -1.79236400 | 2.69594900 | -1.67538800 |
| C | 1.21205200 | 2.89176400 | -0.94545200 |
| H | 1.06247100 | 3.09664300 | -2.00925500 |

| | | | |
|---|---|---|---|
| H | 1.53169900 | 3.81228200 | -0.45493700 |
| C | 2.19208800 | 1.72720500 | -0.73897200 |
| H | 3.01191300 | 1.72677000 | -1.45718100 |
| H | 2.63685900 | 1.78939800 | 0.25818000 |
| C | 1.32539100 | 0.45227900 | -0.83896900 |
| H | 1.53002700 | -0.07230500 | -1.77789500 |
| C | 1.55498300 | -0.54079500 | 0.31125700 |
| H | 0.86819300 | -1.38297800 | 0.19683800 |
| O | -0.99683800 | 0.17511800 | -0.25530500 |
| N | -0.05952800 | 0.98757200 | -0.91997700 |
| C | -1.80436800 | -0.50635200 | -1.19548900 |
| H | -2.21688200 | 0.21395100 | -1.91181700 |
| H | -1.20263500 | -1.22999200 | -1.76132100 |
| C | 2.98020600 | -1.03460000 | 0.32206800 |
| C | 3.88384300 | -0.61180700 | 1.29802700 |
| C | 3.43592600 | -1.90842400 | -0.66960700 |
| C | 5.20683100 | -1.04564600 | 1.28618600 |
| H | 3.54481500 | 0.05871700 | 2.08156900 |
| C | 4.75612400 | -2.34395200 | -0.68656700 |
| H | 2.74407200 | -2.25821200 | -1.43013100 |
| C | 5.64795200 | -1.91156500 | 0.29195600 |
| H | 5.89153200 | -0.70757500 | 2.05587700 |
| H | 5.08989400 | -3.02519800 | -1.46121200 |
| H | 6.67679000 | -2.25229700 | 0.28136700 |
| C | -2.91600400 | -1.21490100 | -0.46435500 |
| C | -3.70540100 | -2.13342000 | -1.15851300 |
| C | -3.18979200 | -0.95991900 | 0.87834200 |
| C | -4.75791800 | -2.78248000 | -0.52510700 |
| H | -3.49197700 | -2.34033900 | -2.20321900 |
| C | -4.24331300 | -1.61467100 | 1.51366400 |
| H | -2.57187400 | -0.25443500 | 1.42157000 |
| C | -5.02950900 | -2.52482200 | 0.81680700 |
| H | -5.36314300 | -3.49306800 | -1.07637100 |
| H | -4.44734000 | -1.41185700 | 2.55909700 |
| H | -5.84739500 | -3.03306300 | 1.31446300 |
| H | 1.31494000 | -0.06118400 | 1.26346500 |

**Vibrational frequencies**

18.87, 25.48, 33.35, 37.43, 54.72, 58.69, 72.28, 95.73, 117.54, 142.07, 185.35, 196.57, 211.02, 229.57, 239.86, 264.35, 316.2, 354.63, 381.17, 395.15, 408.62, 412.02, 413.3, 456.61, 472.19, 508.9, 521.78, 561.89, 578.37, 611.38, 632.71, 632.94, 658.66, 691.95, 714.11, 719.85, 722.71, 751.57, 763.03, 774.15, 792.7, 828, 844.84, 851.64, 855.68, 875.75, 878.27, 885.4, 904.44, 937.48, 940.25, 946.16, 958.39, 987.66, 995.77, 1005.01, 1007.57, 1009.15, 1018.16, 1018.51, 1021.3, 1024.32, 1024.58, 1044.89, 1054.89, 1064.02, 1066.7, 1088.35, 1097.13, 1105.07, 1113, 1127.66, 1138.72, 1144.98, 1168.13, 1175.23, 1183.4, 1196.81, 1202.54, 1204.84, 1206.03, 1215.9, 1226.77, 1240.89, 1241.4, 1260.18, 1268.87, 1272.45, 1311.7, 1316.5, 1320.44, 1331.66, 1337.21, 1341.85, 1344.82, 1353.33, 1357.73, 1369.19, 1393.14, 1401.07, 1410.3, 1464.92, 1476.69, 1482.29, 1485.29, 1492.99, 1496.79, 1500.04, 1513.56, 1541.47, 1546.8, 1660.43, 1664.68, 1682.4, 1685.78, 1691.16, 3030.4, 3038.35, 3046.72, 3064.08, 3066.32, 3066.98, 3067.76, 3081.01, 3086.13, 3114.95, 3117.8, 3127, 3137.57, 3171.29, 3172.77, 3178.88, 3184.77, 3188.56, 3192.17, 3193.74, 3194.93, 3205.97, 3209.79, 3210.18, 3222.71.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.418162
Thermal correction to Energy= 0.439315
Thermal correction to Enthalpy= 0.440259
Thermal correction to Gibbs Free Energy= 0.364129
Sum of electronic and zero-point Energies= -983.151746
Sum of electronic and thermal Energies= -983.130593
Sum of electronic and thermal Enthalpies= -983.129649
Sum of electronic and thermal Free Energies= -983.205779

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.44919900 | 3.21562600 | -0.79618100 |
| C | -2.33817200 | 3.37675400 | 0.45971700 |
| C | -1.38518200 | 3.09309100 | 1.59300500 |
| C | -0.21620900 | 2.61521600 | 1.16893000 |
| C | -0.15596700 | 2.47999400 | -0.34612700 |
| H | -1.17500300 | 4.20263500 | -1.17892700 |
| H | -3.17491400 | 2.66814400 | 0.47320000 |
| H | -2.77857800 | 4.37681500 | 0.53022700 |
| H | -1.65065300 | 3.24795900 | 2.63389700 |
| H | 0.60318500 | 2.32381100 | 1.81618200 |
| H | -1.93995500 | 2.67724100 | -1.60768800 |
| C | 1.14430700 | 3.00599400 | -0.97479200 |
| H | 0.96715900 | 3.21029000 | -2.03459200 |
| H | 1.47296700 | 3.93409400 | -0.50304100 |
| C | 2.15261500 | 1.85452000 | -0.80096100 |
| H | 2.90025900 | 1.83515300 | -1.59536300 |
| H | 2.69391500 | 1.96305100 | 0.14202300 |
| C | 1.30089600 | 0.56017900 | -0.77064100 |
| H | 1.47598100 | -0.02892500 | -1.67629800 |
| C | 1.59493800 | -0.35786200 | 0.43883700 |
| H | 0.83334100 | -1.14037800 | 0.47180200 |
| O | -1.04305900 | 0.24694000 | -0.18521800 |
| N | -0.09829700 | 1.08053300 | -0.85442500 |
| C | -1.77797500 | -0.51455800 | -1.14161800 |
| H | -2.24214100 | 0.16218500 | -1.86915700 |
| H | -1.10052600 | -1.17456700 | -1.69921000 |
| C | 2.96747700 | -0.98982200 | 0.36353000 |
| C | 3.22669500 | -2.02382300 | -0.54739800 |
| C | 4.01521700 | -0.56148000 | 1.18716800 |
| C | 4.48903700 | -2.60632000 | -0.63525200 |
| H | 2.42698700 | -2.38478900 | -1.18687100 |
| C | 5.28106900 | -1.14264200 | 1.10462400 |
| H | 3.83648700 | 0.22833400 | 1.90990700 |
| C | 5.52368600 | -2.16592800 | 0.19069300 |
| H | 4.66385300 | -3.40892100 | -1.34390000 |
| H | 6.07580200 | -0.79699200 | 1.75716200 |
| H | 6.50582800 | -2.62115000 | 0.12655500 |
| C | -2.83348400 | -1.33834600 | -0.43975900 |
| C | -3.55699100 | -2.28058600 | -1.18171600 |
| C | -3.12349800 | -1.18172500 | 0.91778100 |
| C | -4.55308700 | -3.04586600 | -0.58196000 |
| H | -3.33856700 | -2.41485100 | -2.23728100 |
| C | -4.11962300 | -1.95285500 | 1.51975400 |
| H | -2.56745000 | -0.45911700 | 1.50087700 |
| C | -4.83770600 | -2.88513700 | 0.77506500 |
| H | -5.10430000 | -3.77059900 | -1.17136900 |
| H | -4.33222300 | -1.82238600 | 2.57550700 |
| H | -5.61066200 | -3.48287500 | 1.24544100 |
| H | 1.49868900 | 0.21004100 | 1.36744000 |

**Vibrational frequencies**

13.71, 17.92, 30.42, 40.84, 43.13, 55.5, 66.44, 78.24, 98.35, 125.1, 167.76, 187.58, 195.36, 218.34, 232.93, 252.66, 309.45, 348.69, 374.72, 380.52, 409.83, 411.3, 417.2, 450.84, 470.55, 507.21, 519.34, 558.56, 575.9, 605.11, 633.51, 635.02, 661.17, 692.88, 708.17, 712.02, 717, 741.68, 754.14, 762.82, 779.7, 817.32, 833.05, 834.54, 841.05, 858.35, 859.76, 863.91, 895.57, 918.38, 926.48, 931.59, 946.91, 967.62, 981.28, 987.66, 989.83, 995.76, 1004.72, 1005.09, 1010.02, 1014.99, 1015.75, 1023.41, 1036.95, 1047.72, 1048.96, 1056.68, 1073.36, 1082.96, 1090.56, 1108.55, 1110.71, 1117.21, 1129.15, 1175.49, 1176.62, 1179.15, 1194.25, 1197.39, 1198.61, 1203.95, 1219.81, 1220.8, 1223.98, 1249.71, 1252.13, 1261.35, 1303.08, 1308.53, 1318.66, 1323.95, 1330.82, 1335.46, 1340.55, 1351.34, 1354.3, 1356.56, 1385.43, 1390.28, 1398.11, 1471.23, 1478.55, 1478.83, 1484.62, 1488.58, 1491.82, 1501.69, 1504.97, 1523.15, 1525.69, 1619.58, 1621.81, 1640.85, 1645.61, 1671.48, 2993.51, 3013.63, 3019.9, 3024.06, 3037.58, 3043.98, 3052.94, 3054.2, 3056.01, 3089.47, 3094.83, 3102.32, 3104.16, 3151.89, 3154.21, 3156.87, 3163.19, 3164.13, 3167.76, 3173.99, 3175.04, 3187.19, 3187.29, 3190.85, 3206.52.

### mPWPW91/6-311+G(*d*,*p*)

Zero-point correction= 0.407230
Thermal correction to Energy= 0.429001
Thermal correction to Enthalpy= 0.429945
Thermal correction to Gibbs Free Energy= 0.352874

Sum of electronic and zero-point Energies= -983.009162
Sum of electronic and thermal Energies= -982.987392
Sum of electronic and thermal Enthalpies= -982.986448
Sum of electronic and thermal Free Energies= -983.063519

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.44984000 | 3.21504500 | -0.79887700 |
| C | -2.35372700 | 3.34640800 | 0.45145600 |
| C | -1.40522100 | 3.07108300 | 1.59150000 |
| C | -0.21643900 | 2.61604500 | 1.16888000 |
| C | -0.15194200 | 2.48531500 | -0.34644500 |
| H | -1.17847000 | 4.21703400 | -1.16351600 |
| H | -3.18191600 | 2.61719300 | 0.45133700 |
| H | -2.81985800 | 4.34169900 | 0.52818200 |
| H | -1.68308200 | 3.21260200 | 2.63814900 |
| H | 0.60968200 | 2.33232700 | 1.82239700 |
| H | -1.92648200 | 2.68254100 | -1.63158400 |
| C | 1.14934000 | 3.01290300 | -0.97769200 |
| H | 0.97062500 | 3.21226700 | -2.04506900 |
| H | 1.47322500 | 3.95079300 | -0.50695200 |
| C | 2.16334600 | 1.86529300 | -0.79420000 |
| H | 2.92103400 | 1.84640400 | -1.58810500 |
| H | 2.70172000 | 1.97861900 | 0.15799000 |
| C | 1.31689000 | 0.56574200 | -0.76146100 |
| H | 1.50064700 | -0.03417900 | -1.66752000 |
| C | 1.61007000 | -0.34348000 | 0.45884600 |
| H | 0.83398400 | -1.12148000 | 0.50418700 |
| O | -1.03697700 | 0.23893000 | -0.17722200 |
| N | -0.08950000 | 1.08037700 | -0.86184500 |
| C | -1.76739900 | -0.52990600 | -1.14261800 |
| H | -2.22009200 | 0.14744800 | -1.88813800 |
| H | -1.08449200 | -1.20550000 | -1.69032800 |
| C | 2.97698900 | -0.98590700 | 0.37561300 |
| C | 3.22507000 | -2.02189500 | -0.54557700 |
| C | 4.03861000 | -0.56301200 | 1.19487800 |
| C | 4.48902100 | -2.61159000 | -0.64676000 |
| H | 2.41249500 | -2.37927800 | -1.18272700 |
| C | 5.30567500 | -1.15200500 | 1.09900200 |
| H | 3.86688000 | 0.22987900 | 1.92655000 |

| | | | |
|---|---|---|---|
| C | 5.53671500 | -2.17693000 | 0.17507100 |
| H | 4.65533600 | -3.41745900 | -1.36415400 |
| H | 6.11258600 | -0.81070700 | 1.75024100 |
| H | 6.52233900 | -2.63916300 | 0.10030500 |
| C | -2.83750400 | -1.33894500 | -0.44336100 |
| C | -3.57911600 | -2.27189500 | -1.19020000 |
| C | -3.12395100 | -1.18176800 | 0.92122000 |
| C | -4.59009200 | -3.02592700 | -0.58824900 |
| H | -3.36307600 | -2.40700700 | -2.25313500 |
| C | -4.13456400 | -1.94212000 | 1.52460400 |
| H | -2.55176800 | -0.46462800 | 1.50861800 |
| C | -4.87111700 | -2.86455800 | 0.77506500 |
| H | -5.15717400 | -3.74433800 | -1.18286200 |
| H | -4.34451200 | -1.81093300 | 2.58778500 |
| H | -5.65739800 | -3.45545500 | 1.24766100 |
| H | 1.52518900 | 0.23985800 | 1.38720500 |

**Vibrational frequencies**

15.38, 17.85, 30.38, 42.08, 44.96, 54.94, 65.31, 74.2, 94.02, 120.6, 162.2, 182.4, 188.48, 209.66, 224.82, 243.26, 300.07, 335.69, 362.14, 367.36, 393.79, 395.83, 401.12, 437.34, 452.44, 490.71, 501.52, 540.06, 556.09, 585.83, 613.18, 614.85, 638.36, 670.06, 684.43, 689.48, 694.19, 712.89, 729.76, 739.64, 755.11, 793.68, 810.56, 813.77, 819.62, 827.47, 827.65, 839.65, 866.1, 882.21, 892.35, 913.83, 916.56, 930.83, 948.2, 948.56, 953.14, 963.55, 964.86, 970.49, 975.52, 985.85, 987.9, 988.12, 997.21, 1016.95, 1020.17, 1024.96, 1028.36, 1053.88, 1058.44, 1071.53, 1078.8, 1083.98, 1095.48, 1138.63, 1144.92, 1146.51, 1155.77, 1164.34, 1164.88, 1166.05, 1179.67, 1191.6, 1194.59, 1204.12, 1208.55, 1219.91, 1254.57, 1262.64, 1271.18, 1281.14, 1290.27, 1294.71, 1303.5, 1309.69, 1331.87, 1335.85, 1339.56, 1344.9, 1354.34, 1420.73, 1433.9, 1435.51, 1435.82, 1438.3, 1440.44, 1450.49, 1454.92, 1478.56, 1481.27, 1576.88, 1579.37, 1597.11, 1601.92, 1620.53, 2923.95, 2954.81, 2956.5, 2956.85, 2984.13, 2987.73, 2990.49, 2993.99, 2999, 3033.79, 3037.78, 3048.33, 3049.5, 3092.5, 3093.24, 3095.57, 3103.57, 3104.39, 3107.42, 3113.92, 3115.07, 3127.45, 3127.7, 3131, 3142.57.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.417342
Thermal correction to Energy= 0.438586
Thermal correction to Enthalpy= 0.439530
Thermal correction to Gibbs Free Energy= 0.364337
Sum of electronic and zero-point Energies= -983.217116
Sum of electronic and thermal Energies= -983.195873
Sum of electronic and thermal Enthalpies= -983.194929
Sum of electronic and thermal Free Energies= -983.270122

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.43317600 | 3.21902000 | -0.76997400 |
| C | -2.34357200 | 3.28737700 | 0.47664300 |
| C | -1.38337900 | 3.02391700 | 1.60848000 |
| C | -0.19413200 | 2.59595400 | 1.17698600 |
| C | -0.13834100 | 2.48477900 | -0.33696700 |
| H | -1.16730800 | 4.23461600 | -1.08018200 |
| H | -3.13213900 | 2.52439400 | 0.45806800 |
| H | -2.84520300 | 4.25680000 | 0.57178100 |
| H | -1.65731100 | 3.14913100 | 2.65220300 |
| H | 0.63717500 | 2.32206500 | 1.81874300 |
| H | -1.89597000 | 2.72222800 | -1.62504300 |
| C | 1.15904200 | 3.00717200 | -0.96960800 |
| H | 0.98214300 | 3.19955300 | -2.03254400 |
| H | 1.48892600 | 3.93841300 | -0.50311000 |
| C | 2.16287300 | 1.85431100 | -0.78097300 |
| H | 2.92615800 | 1.83462300 | -1.56137300 |
| H | 2.68279800 | 1.95840000 | 0.17629400 |

| | | | |
|---|---|---|---|
| C | 1.30799700 | 0.56350200 | -0.76815100 |
| H | 1.48919700 | -0.02579000 | -1.67340100 |
| C | 1.58277300 | -0.35399600 | 0.44536300 |
| H | 0.81221900 | -1.12936300 | 0.47410900 |
| O | -1.03785800 | 0.25600600 | -0.18793400 |
| N | -0.08914600 | 1.09046100 | -0.86769600 |
| C | -1.78790000 | -0.47950100 | -1.15745700 |
| H | -2.25694500 | 0.21918900 | -1.86169800 |
| H | -1.11867100 | -1.13122600 | -1.73542300 |
| C | 2.95083900 | -0.99313900 | 0.36451100 |
| C | 3.20216900 | -2.02053000 | -0.55798900 |
| C | 4.00419600 | -0.57262600 | 1.18702700 |
| C | 4.46361900 | -2.60594500 | -0.65691900 |
| H | 2.39681000 | -2.37314000 | -1.19696800 |
| C | 5.26913000 | -1.15701200 | 1.09297900 |
| H | 3.82923200 | 0.21284500 | 1.91719900 |
| C | 5.50436400 | -2.17422600 | 0.16815500 |
| H | 4.63322300 | -3.40356100 | -1.37377000 |
| H | 6.06895800 | -0.81875100 | 1.74464100 |
| H | 6.48580400 | -2.63174200 | 0.09518000 |
| C | -2.83666000 | -1.30876400 | -0.45263900 |
| C | -3.60382100 | -2.21125400 | -1.20230600 |
| C | -3.07371700 | -1.19661000 | 0.92084700 |
| C | -4.59257200 | -2.98105600 | -0.59302300 |
| H | -3.42627500 | -2.31013200 | -2.27029600 |
| C | -4.06285300 | -1.97180900 | 1.53136400 |
| H | -2.48139000 | -0.50497000 | 1.50795700 |
| C | -4.82537400 | -2.86438000 | 0.77955100 |
| H | -5.17897000 | -3.67436200 | -1.18789900 |
| H | -4.23487000 | -1.87632200 | 2.59909200 |
| H | -5.59307500 | -3.46541400 | 1.25632800 |
| H | 1.49333800 | 0.22012100 | 1.37205300 |

**Vibrational frequencies**

18.9, 30.58, 35.99, 40.76, 48.45, 60.09, 63.22, 91.33, 101.15, 121.9, 166.16, 183.69, 195.71, 215.32, 228.88, 245.24, 306.25, 337.64, 363.93, 371.59, 398.06, 406.55, 410.95, 444.11, 464.4, 499.89, 508, 548.4, 566.45, 596.54, 622.38, 623.82, 648.2, 681.91, 704.46, 705.26, 713.06, 739.43, 749.37, 762.2, 774.4, 813.36, 829.54, 835.34, 837, 858.73, 859.98, 863.04, 888.53, 917.9, 923.23, 932.54, 940.97, 965.17, 978.88, 985.26, 988.37, 994.29, 1000.59, 1000.97, 1002.52, 1009.8, 1010.21, 1015.85, 1031.82, 1045.47, 1046.85, 1051.26, 1059.42, 1079.78, 1086.46, 1105.07, 1106.01, 1113.62, 1124.55, 1174.54, 1174.86, 1176.42, 1191.01, 1196.17, 1197.12, 1199.16, 1217.15, 1219.08, 1222.4, 1241.7, 1246.12, 1258.38, 1293.14, 1307.47, 1316.05, 1324.61, 1330.62, 1332.21, 1347.18, 1352.15, 1354.36, 1356.08, 1382.77, 1386.02, 1392.46, 1477.95, 1478.18, 1480.69, 1488.6, 1494.52, 1498.73, 1506.55, 1509.18, 1522.57, 1524.93, 1619.11, 1621.29, 1639.44, 1643.98, 1662.6, 2994.28, 3017.51, 3019.91, 3026.92, 3039.84, 3043.89, 3045.59, 3050.02, 3055.76, 3090.85, 3094.32, 3102.1, 3102.53, 3150.57, 3151.06, 3153.58, 3159.47, 3162.37, 3166.11, 3172.8, 3174.3, 3186.59, 3187.01, 3187.6, 3202.54.

## 18b

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.454596
Thermal correction to Energy= 0.479607
Thermal correction to Enthalpy= 0.480551
Thermal correction to Gibbs Free Energy= 0.393767
Sum of electronic and zero-point Energies= -1135.627379
Sum of electronic and thermal Energies= -1135.602368
Sum of electronic and thermal Enthalpies= -1135.601424
Sum of electronic and thermal Free Energies= -1135.688208

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.38575400 | 1.52885700 | 2.03842200 |
| C | 0.42521500 | 2.73338300 | 1.99860700 |
| C | 0.62583000 | 3.58898200 | 0.77241700 |
| C | 0.24213700 | 3.18230400 | -0.48819400 |
| C | 1.09515000 | 0.50735500 | 0.97503300 |
| H | 1.28793700 | 1.04074400 | 3.01401400 |
| H | 0.59132500 | 3.34156500 | 2.89044600 |
| H | -0.60901000 | 2.37813800 | 2.03996200 |
| H | 2.41658200 | 1.87188100 | 1.92985400 |
| C | -0.19979200 | -0.26254700 | 1.01109500 |
| H | 0.03185900 | -1.31819600 | 0.84311600 |
| H | -0.64755900 | -0.17171300 | 2.00428000 |
| C | -1.22140300 | 0.19184000 | -0.05315800 |
| H | -1.60231800 | 1.18779100 | 0.18815400 |
| H | -0.70597400 | 0.26153600 | -1.01614700 |
| C | -2.35697300 | -0.78001200 | -0.15504700 |
| H | -2.08332700 | -1.79048900 | -0.45476500 |
| C | -3.63191500 | -0.47886000 | 0.09966600 |
| H | -3.87255800 | 0.54547000 | 0.38082100 |
| O | 1.63371100 | -0.60950600 | -0.86006400 |
| N | 1.99671500 | 0.34063900 | 0.08862000 |
| C | 2.76779700 | -0.91941200 | -1.66818300 |
| H | 2.35573900 | -1.46483900 | -2.51904800 |
| H | 3.21705600 | 0.01194900 | -2.02313900 |
| C | -4.78862200 | -1.39022600 | 0.02237100 |
| C | -6.07545600 | -0.85927100 | 0.16297300 |
| C | -4.66322700 | -2.77066100 | -0.18291800 |
| C | -7.20184600 | -1.67209700 | 0.09012800 |
| H | -6.19092900 | 0.20707500 | 0.32828500 |
| C | -5.78585700 | -3.58325900 | -0.25648800 |
| H | -3.68036200 | -3.21724400 | -0.27982500 |
| C | -7.06200000 | -3.03868600 | -0.12189700 |
| H | -8.18827700 | -1.23599900 | 0.19981900 |
| H | -5.66608600 | -4.64896500 | -0.41563700 |
| H | -7.93644800 | -3.67644200 | -0.17734200 |
| C | 3.77727100 | -1.76192100 | -0.93114700 |
| C | 4.89618500 | -1.18020900 | -0.33720400 |
| C | 3.57622000 | -3.13655600 | -0.79983600 |
| C | 5.80478800 | -1.96081400 | 0.37161200 |
| H | 5.04874200 | -0.10986700 | -0.42716900 |
| C | 4.47983700 | -3.91922100 | -0.09016300 |
| H | 2.70516700 | -3.59343400 | -1.25936100 |
| C | 5.59746600 | -3.33090100 | 0.49634600 |
| H | 6.67279200 | -1.49924900 | 0.82837300 |
| H | 4.31577400 | -4.98676200 | 0.00269400 |
| H | 6.30479500 | -3.93956100 | 1.04797800 |
| C | 1.25849700 | 4.83778400 | 0.83026500 |
| C | 1.46854900 | 5.59080400 | -0.32319900 |
| H | 1.95970800 | 6.55415700 | -0.24965000 |
| C | 1.05305500 | 5.11943000 | -1.56510800 |
| H | 1.22026300 | 5.70940700 | -2.45930200 |

| | | | |
|---|---|---|---|
| C | 0.41926000 | 3.87592400 | -1.65850200 |
| H | 1.58866100 | 5.21820900 | 1.79264500 |
| H | 0.08637600 | 3.48566100 | -2.61384200 |

**Vibrational frequencies**

16.58, 19.41, 24.35, 28.59, 39.92, 41.34, 43.92, 53.43, 63.66, 69.84, 94.96, 115.07, 126.63, 153.42, 171.03, 203.46, 215.23, 264.46, 274.26, 299.05, 309.77, 344.96, 359.24, 379.42, 398.86, 411.61, 412.62, 420.11, 428.72, 447.07, 484.75, 499.42, 502.62, 530.76, 564.47, 575.02, 614.28, 629.3, 630.99, 632.03, 636.21, 665.73, 706.02, 713.87, 719.34, 760.42, 763.78, 776.57, 781.35, 785.81, 840.53, 846.57, 864.25, 869.87, 875.63, 879.98, 882.01, 928.58, 946.31, 950.68, 953.97, 968.51, 971.61, 995.08, 1006.83, 1008.22, 1008.37, 1011.42, 1015.91, 1018.23, 1020.97, 1023.22, 1023.82, 1026.07, 1040.62, 1058.55, 1062.99, 1064.53, 1067.81, 1103.48, 1106.78, 1112.48, 1120.9, 1132.02, 1168.04, 1171.72, 1174.26, 1176.87, 1200.12, 1204.4, 1205.35, 1217.03, 1241.7, 1243.8, 1251.98, 1266.75, 1287.98, 1290.66, 1295.79, 1316.52, 1327.57, 1333.65, 1338.59, 1348.91, 1355.04, 1361.24, 1362.06, 1366.6, 1380.74, 1398.4, 1403.28, 1465.07, 1472.01, 1481.07, 1486.97, 1488.41, 1489.92, 1492.5, 1496.01, 1497.67, 1540.7, 1545.46, 1613.14, 1653.21, 1665.61, 1676.35, 1679.16, 1687.53, 1746.03, 1755.55, 3053.96, 3059.55, 3063.64, 3070.76, 3079.19, 3098.49, 3108.02, 3122, 3125.01, 3135.8, 3149.91, 3155.4, 3173.26, 3175.53, 3178.83, 3179.95, 3182.31, 3185.15, 3186.52, 3196.09, 3199.18, 3199.22, 3204.83, 3204.99, 3209.79, 3215.47.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.449539
Thermal correction to Energy= 0.474975
Thermal correction to Enthalpy= 0.475919
Thermal correction to Gibbs Free Energy= 0.387108

Sum of electronic and zero-point Energies= -1136.128254
Sum of electronic and thermal Energies= -1136.102818
Sum of electronic and thermal Enthalpies= -1136.101874
Sum of electronic and thermal Free Energies= -1136.190686

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.30738300 | 1.50171700 | 1.96328400 |
| C | 0.32017500 | 2.69505200 | 1.92484500 |
| C | 0.51752400 | 3.63034500 | 0.75144000 |
| C | 0.07332100 | 3.36190300 | -0.52660500 |
| C | 1.07512500 | 0.42879200 | 0.92751000 |
| H | 1.21756900 | 1.03013000 | 2.94989200 |
| H | 0.45132300 | 3.26444700 | 2.84894900 |
| H | -0.70853000 | 2.32323200 | 1.93238700 |
| H | 2.33225600 | 1.86684700 | 1.86800400 |
| C | -0.19235000 | -0.39403000 | 0.97217500 |
| H | 0.08908000 | -1.45091800 | 0.92347700 |
| H | -0.68839200 | -0.23211900 | 1.93313400 |
| C | -1.19104000 | -0.09514200 | -0.17464300 |
| H | -1.50096200 | 0.95296500 | -0.13900400 |
| H | -0.66683700 | -0.24064300 | -1.12447300 |
| C | -2.39531800 | -0.98848500 | -0.12649300 |
| H | -2.19054000 | -2.05688200 | -0.17215000 |
| C | -3.65984200 | -0.55369500 | -0.04533600 |
| H | -3.82488100 | 0.52194700 | -0.00453500 |
| O | 1.76692900 | -0.79246600 | -0.81580300 |
| N | 2.03294100 | 0.24655400 | 0.09626900 |
| C | 2.93493700 | -1.03750100 | -1.62328300 |
| H | 2.54729200 | -1.59162600 | -2.48080100 |
| H | 3.32837300 | -0.07929500 | -1.97174900 |
| C | -4.89002100 | -1.36164500 | -0.02133700 |
| C | -6.12967500 | -0.70309500 | 0.03048000 |
| C | -4.89608000 | -2.76755900 | -0.05366600 |
| C | -7.32770000 | -1.41388100 | 0.04904600 |
| H | -6.14963600 | 0.38196200 | 0.05450900 |

| | | | |
|---|---|---|---|
| C | -6.09075000 | -3.47793800 | -0.03405800 |
| H | -3.95991400 | -3.31231600 | -0.09562400 |
| C | -7.31453400 | -2.80638100 | 0.01665700 |
| H | -8.27046100 | -0.87893900 | 0.08849000 |
| H | -6.06942700 | -4.56227100 | -0.05923400 |
| H | -8.24427400 | -3.36408800 | 0.03110600 |
| C | 3.99804000 | -1.83704400 | -0.90907400 |
| C | 5.10147700 | -1.20706300 | -0.32534100 |
| C | 3.88225900 | -3.22806400 | -0.80447800 |
| C | 6.06939700 | -1.95073100 | 0.34915300 |
| H | 5.19862100 | -0.12918700 | -0.39678500 |
| C | 4.84573300 | -3.97398900 | -0.12952200 |
| H | 3.03187800 | -3.72834500 | -1.25726000 |
| C | 5.94272300 | -3.33536100 | 0.44962900 |
| H | 6.92125100 | -1.44959200 | 0.79591700 |
| H | 4.74477100 | -5.05167400 | -0.05949400 |
| H | 6.69590900 | -3.91476300 | 0.97242100 |
| C | 1.19491100 | 4.85655400 | 0.89070900 |
| C | 1.38223900 | 5.70857500 | -0.19830600 |
| H | 1.90571100 | 6.64771200 | -0.05706400 |
| C | 0.90270200 | 5.36627500 | -1.46234500 |
| H | 1.05018400 | 6.03163800 | -2.30658300 |
| C | 0.22363900 | 4.15136600 | -1.63976000 |
| H | 1.56992700 | 5.14192000 | 1.86977100 |
| H | -0.15816500 | 3.86076100 | -2.61278600 |

**Vibrational frequencies**

9.4, 17.08, 23.92, 25.29, 32.51, 35.07, 42.03, 48.83, 62.05, 72.78, 91.04, 109.3, 119.86, 153.48, 160.85, 199.17, 209.62, 257.36, 259, 285.52, 304.81, 330.9, 346.2, 367.99, 385, 410.08, 414.22, 416.41, 420.67, 440, 479.34, 494.17, 498.53, 528.71, 555.8, 568.99, 606.67, 626.97, 631.01, 634.54, 634.8, 655.7, 704.2, 707.35, 710.15, 745.16, 755.52, 767.48, 769.46, 777.47, 829.17, 833.89, 851.51, 852.86, 859.17, 859.38, 860.76, 885.35, 930.41, 935.7, 935.77, 945.84, 950.79, 987.84, 988.71, 989.32, 990.47, 994.12, 995.58, 1002.14, 1006.99, 1008.86, 1013.76, 1015.48, 1017.47, 1026.89, 1041.79, 1047.69, 1050.06, 1054.64, 1087.76, 1104.55, 1107.76, 1119.59, 1161.93, 1168.8, 1177.02, 1177.72, 1193.27, 1196.62, 1202.59, 1204.79, 1227.18, 1231.31, 1237.53, 1254.9, 1280.91, 1284.82, 1296.38, 1307.79, 1322.81, 1329.43, 1336.29, 1344.04, 1354.38, 1358.11, 1359.48, 1367.02, 1379.14, 1381.86, 1392.27, 1445.58, 1469.46, 1473.05, 1476, 1478.02, 1478.39, 1482.47, 1487.45, 1489.99, 1524.58, 1526.15, 1568.42, 1614.3, 1624.22, 1631.97, 1640.02, 1643.31, 1686.27, 1701.87, 3015.34, 3030.28, 3039.84, 3042.14, 3051.97, 3065.16, 3076.84, 3085.74, 3091.95, 3104.03, 3120.17, 3130.78, 3150.33, 3157.97, 3159.62, 3161.59, 3164.59, 3165.93, 3172.73, 3174.23, 3175.53, 3180.01, 3184.35, 3187.84, 3189.47, 3192.03.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.437311
Thermal correction to Energy= 0.463897
Thermal correction to Enthalpy= 0.464841
Thermal correction to Gibbs Free Energy= 0.372770

Sum of electronic and zero-point Energies= -1135.968409
Sum of electronic and thermal Energies= -1135.941823
Sum of electronic and thermal Enthalpies= -1135.940879
Sum of electronic and thermal Free Energies= -1136.032950

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.32457100 | 1.50115200 | 1.99339200 |
| C | 0.35314900 | 2.71080300 | 1.96545500 |
| C | 0.54362600 | 3.62127600 | 0.77111000 |
| C | 0.13326000 | 3.29838800 | -0.51104800 |
| C | 1.07254700 | 0.44077600 | 0.94899300 |
| H | 1.23151800 | 1.02188000 | 2.98366600 |
| H | 0.51225500 | 3.29412700 | 2.88442600 |

| | | | |
|---|---|---|---|
| H | -0.68684000 | 2.35080900 | 1.99798900 |
| H | 2.36070600 | 1.85476100 | 1.89567200 |
| C | -0.19708400 | -0.37830700 | 0.99296900 |
| H | 0.08360900 | -1.44210200 | 0.92513400 |
| H | -0.68973100 | -0.22996100 | 1.96552800 |
| C | -1.20546900 | -0.06242400 | -0.14607100 |
| H | -1.52154000 | 0.99019300 | -0.08827700 |
| H | -0.67766500 | -0.18495400 | -1.10562100 |
| C | -2.40184200 | -0.96617900 | -0.11478900 |
| H | -2.18815900 | -2.03900000 | -0.18442500 |
| C | -3.67881600 | -0.54194500 | -0.02118800 |
| H | -3.85309600 | 0.53847700 | 0.04379000 |
| O | 1.74988600 | -0.76868600 | -0.82465700 |
| N | 2.03453700 | 0.26522700 | 0.10204400 |
| C | 2.92733700 | -1.00822000 | -1.63985100 |
| H | 2.53302400 | -1.55690500 | -2.50665300 |
| H | 3.32266000 | -0.03956000 | -1.97969600 |
| C | -4.89986800 | -1.36109400 | -0.01403500 |
| C | -6.15265200 | -0.71368800 | 0.04984000 |
| C | -4.89292300 | -2.77256100 | -0.07604500 |
| C | -7.34763300 | -1.43925500 | 0.05156400 |
| H | -6.18214400 | 0.37743400 | 0.09635300 |
| C | -6.08502200 | -3.49735800 | -0.07319200 |
| H | -3.94471500 | -3.30981100 | -0.12834000 |
| C | -7.32049300 | -2.83653000 | -0.01062600 |
| H | -8.30176800 | -0.91150600 | 0.10078300 |
| H | -6.05280600 | -4.58745300 | -0.12143200 |
| H | -8.25050100 | -3.40703500 | -0.00990400 |
| C | 3.98703600 | -1.81547000 | -0.92793400 |
| C | 5.08030100 | -1.18472400 | -0.31169700 |
| C | 3.87774000 | -3.21445600 | -0.84669000 |
| C | 6.04388000 | -1.93572000 | 0.37140900 |
| H | 5.17111200 | -0.09841400 | -0.36687400 |
| C | 4.83770100 | -3.96742300 | -0.16348000 |
| H | 3.03318600 | -3.71530600 | -1.32563100 |
| C | 5.92367900 | -3.32817400 | 0.44816000 |
| H | 6.88993000 | -1.43359900 | 0.84391600 |
| H | 4.74257300 | -5.05351200 | -0.11202100 |
| H | 6.67579500 | -3.91462000 | 0.97870300 |
| C | 1.18934800 | 4.87444100 | 0.88444300 |
| C | 1.37867100 | 5.69722100 | -0.23296300 |
| H | 1.87850400 | 6.65966300 | -0.11220400 |
| C | 0.93359400 | 5.29957700 | -1.49927100 |
| H | 1.08332200 | 5.94317600 | -2.36860500 |
| C | 0.28700100 | 4.05625900 | -1.65052300 |
| H | 1.53910500 | 5.20099300 | 1.86800100 |
| H | -0.06812200 | 3.72328400 | -2.62794000 |

**Vibrational frequencies**

12.5, 13.96, 22.23, 28.22, 29.74, 34.46, 36.18, 41.84, 48.21, 64.32, 71.28, 92.52, 98.31, 133.14, 138.65, 163.5, 183.89, 219.26, 235.76, 275.35, 302.65, 308.8, 320.55, 340.03, 355.03, 357.86, 394.99, 397.07, 399.2, 408.55, 447.56, 476.02, 493.93, 509.38, 536.88, 574.59, 597.8, 610.71, 613.17, 614.1, 616.44, 662.54, 679.08, 679.77, 688.39, 713.07, 732.95, 741.88, 753.36, 756.93, 805.95, 807.87, 817.71, 820.58, 827.54, 827.73, 831.69, 860.21, 889.97, 894.13, 902.43, 906.44, 945.02, 949.17, 949.89, 954.31, 956.17, 961.22, 962.04, 967.71,

968.47, 974.43, 983.18, 986.53, 990.69, 995.72, 1006.29, 1018.56, 1024.4, 1026.02, 1057.72, 1074.49, 1081.66, 1091.95, 1131.8, 1139.59, 1146.99, 1149.9, 1151, 1164.04, 1166.21, 1186.24, 1195.05, 1201.67, 1205.93, 1219.76, 1228.71, 1238.18, 1256.48, 1271.84, 1273.2, 1286.12, 1295.52, 1306.04, 1311.78, 1317.7, 1325.03, 1326.15, 1345.91, 1348.22, 1348.66, 1402.65, 1419.64, 1427.45, 1432.08, 1436.13, 1439.54, 1440.18, 1443.22, 1461.9, 1479.33, 1484.02, 1523.18, 1570.29, 1583.1, 1593.11, 1595.71, 1602.34, 1614.79, 1649.18, 2964.43, 2966.58, 2967.55, 2983.66, 2990.17, 3009.36, 3010.53, 3020.25, 3039.33, 3040.96, 3053.73, 3067.8, 3088.44, 3098.63, 3100.3, 3100.41, 3103.22, 3104.35, 3112.29, 3112.67, 3113.76, 3120.47, 3120.71, 3126.01, 3130.6, 3130.97.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.447875
Thermal correction to Energy= 0.474011
Thermal correction to Enthalpy= 0.474955
Thermal correction to Gibbs Free Energy= 0.383720

Sum of electronic and zero-point Energies= -1136.202725
Sum of electronic and thermal Energies= -1136.176590
Sum of electronic and thermal Enthalpies= -1136.175645
Sum of electronic and thermal Free Energies= -1136.266880

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.32597000 | 1.50594600 | 1.99222600 |
| C | 0.35416400 | 2.71264000 | 1.95510800 |
| C | 0.55799700 | 3.61787700 | 0.76090800 |
| C | 0.15671700 | 3.29250400 | -0.52058200 |
| C | 1.07100700 | 0.44853500 | 0.94823300 |
| H | 1.22788100 | 1.03074400 | 2.97704600 |
| H | 0.50706000 | 3.29570700 | 2.86815800 |
| H | -0.67957500 | 2.35204700 | 1.97738100 |
| H | 2.35596200 | 1.85762400 | 1.89265300 |
| C | -0.19771800 | -0.36948000 | 0.99172300 |
| H | 0.08069300 | -1.42585000 | 0.90683900 |
| H | -0.68244800 | -0.22887100 | 1.96282100 |
| C | -1.20558000 | -0.03483600 | -0.13898400 |
| H | -1.53236300 | 1.00620200 | -0.05533100 |
| H | -0.68084700 | -0.13550400 | -1.09528600 |
| C | -2.39317000 | -0.95045500 | -0.11993800 |
| H | -2.17220100 | -2.01355600 | -0.21379500 |
| C | -3.66621000 | -0.53796500 | -0.00751600 |
| H | -3.85011800 | 0.53296700 | 0.07977200 |
| O | 1.72203500 | -0.74907300 | -0.82577900 |
| N | 2.02017800 | 0.27561700 | 0.09810500 |
| C | 2.89065000 | -0.99556800 | -1.64092400 |
| H | 2.49571200 | -1.54300900 | -2.49971600 |
| H | 3.28796500 | -0.03370500 | -1.97642100 |
| C | -4.87847800 | -1.36999100 | -0.00623700 |
| C | -6.13221300 | -0.73786100 | 0.06768000 |
| C | -4.85502700 | -2.77541400 | -0.08263500 |
| C | -7.31629900 | -1.47398600 | 0.06462500 |
| H | -6.17260200 | 0.34642600 | 0.12578000 |
| C | -6.03587200 | -3.51085500 | -0.08445000 |
| H | -3.90605000 | -3.29848200 | -0.14167300 |
| C | -7.27429000 | -2.86575300 | -0.01212100 |
| H | -8.27060900 | -0.95968300 | 0.12140500 |
| H | -5.99237800 | -4.59406700 | -0.14350700 |
| H | -8.19310000 | -3.44313400 | -0.01492800 |
| C | 3.94338200 | -1.80483100 | -0.92380400 |
| C | 5.02320600 | -1.17690100 | -0.29202400 |
| C | 3.83845500 | -3.20007900 | -0.85763700 |

| | | | |
|---|---|---|---|
| C | 5.97921500 | -1.92822800 | 0.39293100 |
| H | 5.10951500 | -0.09571600 | -0.33624400 |
| C | 4.79109900 | -3.95358600 | -0.17303500 |
| H | 3.00586600 | -3.69700200 | -1.34806000 |
| C | 5.86426200 | -3.31764700 | 0.45469800 |
| H | 6.81325300 | -1.42996700 | 0.87711600 |
| H | 4.70036900 | -5.03458900 | -0.13301300 |
| H | 6.60880000 | -3.90289400 | 0.98516000 |
| C | 1.20678700 | 4.86290900 | 0.87538900 |
| C | 1.41039100 | 5.67806300 | -0.24027600 |
| H | 1.91202700 | 6.63278200 | -0.11902200 |
| C | 0.97534300 | 5.28004000 | -1.50550000 |
| H | 1.13663100 | 5.91759900 | -2.36963800 |
| C | 0.32492400 | 4.04501200 | -1.65907000 |
| H | 1.54864400 | 5.19018400 | 1.85470200 |
| H | -0.02273700 | 3.71107700 | -2.63165300 |

**Vibrational frequencies**

12.09, 15.95, 22.91, 28.46, 29.49, 34.31, 36.29, 41.83, 48.96, 64.81, 71.76, 93.61, 98.65, 134.84, 138.68, 165.46, 186.76, 223.99, 240.49, 279.48, 306.05, 312.68, 320.18, 344.68, 357.45, 364.7, 405.62, 407.82, 408.03, 411.95, 452.56, 486.19, 503.6, 520.46, 545.39, 583.4, 606.88, 619.6, 622.12, 623.6, 625.53, 678.33, 696.38, 698.36, 708.7, 741.22, 753.77, 760.65, 771.58, 772.92, 822.62, 826.75, 839.01, 846.7, 852.15, 858.61, 860.09, 877.01, 922.45, 926.9, 937.69, 941.55, 979.63, 982.88, 985.4, 986.44, 987.02, 989.36, 993.02, 997.94, 1004.43, 1004.86, 1006.74, 1010.75, 1012.53, 1022.15, 1036.6, 1041.91, 1047.05, 1048.77, 1080.68, 1099.14, 1107.76, 1120.99, 1162.46, 1169, 1176.6, 1179.56, 1183.18, 1196.51, 1198.09, 1214.4, 1228.85, 1230.25, 1234.59, 1253.65, 1267.09, 1276.16, 1295.02, 1308.75, 1312.68, 1326.63, 1333.22, 1341.6, 1349.3, 1355.73, 1357.29, 1357.95, 1361.5, 1372.7, 1393.5, 1445.26, 1471.5, 1475.15, 1477.77, 1482.85, 1483.08, 1494.08, 1499.01, 1518.76, 1523.36, 1528.35, 1568.71, 1613.43, 1625.33, 1630.72, 1637.85, 1645.48, 1669.71, 1692.82, 3025.68, 3026.5, 3029.27, 3041, 3048.19, 3067.89, 3076.35, 3078.3, 3098.33, 3100.58, 3115.12, 3130.03, 3148.41, 3157.14, 3159.1, 3161.71, 3162.05, 3163.29, 3171.75, 3172.74, 3175.55, 3180.22, 3180.31, 3186.8, 3190.98, 3191.05.

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## 18b' TS1

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.452975
Thermal correction to Energy= 0.477451
Thermal correction to Enthalpy= 0.478395
Thermal correction to Gibbs Free Energy= 0.393056
Sum of electronic and zero-point Energies= -1135.616765
Sum of electronic and thermal Energies= -1135.592289
Sum of electronic and thermal Enthalpies= -1135.591345
Sum of electronic and thermal Free Energies= -1135.676684

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.31418400 | 0.16337500 | -1.32392900 |
| C | -0.24793900 | 1.01000200 | -0.17561300 |
| C | 0.66407100 | 0.84279300 | 1.01115900 |
| C | 1.97697500 | 0.51374600 | 0.75569000 |
| C | 1.80428900 | 0.36539300 | -1.50862200 |
| H | -0.18539900 | 0.41968600 | -2.26394400 |
| H | -1.27097900 | 0.70969400 | 0.06038100 |
| H | -0.28442600 | 2.06730100 | -0.46264200 |
| H | 0.14086500 | -0.89634900 | -1.12663200 |
| C | 2.29834700 | 1.72137000 | -1.98311700 |
| H | 2.68882200 | 1.56609200 | -2.99562200 |
| H | 1.44213000 | 2.39540300 | -2.07016600 |
| C | 3.38964800 | 2.40647200 | -1.14312600 |
| H | 2.97393700 | 2.73850400 | -0.18967200 |

| | | | |
|---|---|---|---|
| H | 4.17170900 | 1.67337900 | -0.92545800 |
| C | 3.98456100 | 3.57450700 | -1.87004700 |
| H | 4.47182300 | 3.35039000 | -2.81797100 |
| C | 3.93782800 | 4.83239600 | -1.42625600 |
| H | 3.41958500 | 5.02834200 | -0.48872900 |
| O | 3.79391300 | -0.46315500 | -2.04910700 |
| N | 2.48500600 | -0.73271400 | -1.68891100 |
| C | 4.48619600 | -1.68394700 | -2.24902400 |
| H | 5.54325100 | -1.40559100 | -2.26600500 |
| H | 4.31289400 | -2.34191100 | -1.39213400 |
| C | 4.51505800 | 6.02062100 | -2.08109300 |
| C | 4.13411000 | 7.29113400 | -1.63561400 |
| C | 5.43761100 | 5.93729100 | -3.13209200 |
| C | 4.64332200 | 8.44265000 | -2.22627200 |
| H | 3.42576700 | 7.37304900 | -0.81742000 |
| C | 5.94666500 | 7.08563300 | -3.72291800 |
| H | 5.77512100 | 4.96759500 | -3.47966600 |
| C | 5.55052000 | 8.34457100 | -3.27530100 |
| H | 4.33061400 | 9.41606200 | -1.86604000 |
| H | 6.66387900 | 6.99928600 | -4.53129700 |
| H | 5.95348500 | 9.23918100 | -3.73540900 |
| C | 4.11323400 | -2.38654500 | -3.53390200 |
| C | 4.47125700 | -3.72365600 | -3.70251300 |
| C | 3.45721800 | -1.72295200 | -4.56790300 |
| C | 4.18850300 | -4.38722100 | -4.89085600 |
| H | 4.97295500 | -4.24905800 | -2.89521700 |
| C | 3.16745200 | -2.38839000 | -5.75612000 |
| H | 3.16858700 | -0.68623700 | -4.43885600 |
| C | 3.53431500 | -3.71946000 | -5.92286200 |
| H | 4.47172700 | -5.42685900 | -5.00905900 |
| H | 2.65239700 | -1.86467800 | -6.55366300 |
| H | 3.30805900 | -4.23623500 | -6.84822600 |
| C | 0.30331700 | 0.99656800 | 2.35363500 |
| C | 1.25281200 | 0.81125700 | 3.35666900 |
| H | 0.96384000 | 0.92682200 | 4.39488500 |
| C | 2.56707900 | 0.46847600 | 3.04179000 |
| H | 3.29454900 | 0.31943100 | 3.83225500 |
| C | 2.95009600 | 0.31198900 | 1.70624800 |
| H | -0.71964400 | 1.25463800 | 2.61217700 |
| H | 3.96816100 | 0.04444000 | 1.44273200 |

**Vibrational frequencies**

477.72*i*, 8.76, 23.25, 25.24, 31.98, 35.18, 45.41, 54.01, 55.44, 81.5, 91.01, 93.04, 123.34, 155.43, 188.45, 208.05, 225.7, 243.6, 257.13, 262.9, 284.91, 303.58, 338.1, 385.46, 402.66, 413.72, 416.36, 417.58, 426.53, 445.43, 469.79, 480.29, 490.82, 511.15, 536.79, 559.94, 601.25, 612.87, 628.39, 629.7, 630.73, 661.02, 710.24, 711.09, 714.56, 754.9, 757.44, 760.58, 777.55, 789.74, 818.99, 835.42, 856.11, 870.08, 879.95, 882.35, 883.65, 906.54, 931.78, 950.05, 955.32, 966.73, 975.01, 990.48, 1001.14, 1010.47, 1013.51, 1015.01, 1015.8, 1017.54, 1019.17, 1026.62, 1028.78, 1049.16, 1053.46, 1060.81, 1061.7, 1066.54, 1068.05, 1105.69, 1107.13, 1115.12, 1125.87, 1134.66, 1166.24, 1171.47, 1174.68, 1177.65, 1194.6, 1197.2, 1205.62, 1210.71, 1228.72, 1239.52, 1243.47, 1253.71, 1280.32, 1286.96, 1309.2, 1315.12, 1321.01, 1330.06, 1332.47, 1339.18, 1351.75, 1354.45, 1359.53, 1365.38, 1377.3, 1388.98, 1411.73, 1460.55, 1465.31, 1474.76, 1479.97, 1480.17, 1486.4, 1491.97, 1492.92, 1497.74, 1542.56, 1542.86, 1554.97, 1621.53, 1655.27, 1664.87, 1667.74, 1682.61, 1687.01, 1742.13, 3050.79, 3053.54, 3057.65, 3064.35, 3072.12, 3101.14, 3110.78, 3123.34, 3127.3, 3130.35, 3137.92, 3144.59, 3179.07, 3179.51, 3180.01, 3187.91, 3188.45, 3190.15, 3195.07, 3196.43, 3198.14, 3203.03, 3208.21, 3209.28, 3214.62, 3219.77.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.448388
Thermal correction to Energy= 0.473040
Thermal correction to Enthalpy= 0.473985
Thermal correction to Gibbs Free Energy= 0.388736
Sum of electronic and zero-point Energies= -1136.120166
Sum of electronic and thermal Energies= -1136.095514
Sum of electronic and thermal Enthalpies= -1136.094570
Sum of electronic and thermal Free Energies= -1136.179818

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.73118000 | 0.01961300 | -1.03977000 |
| C | 0.18325800 | 0.84091400 | 0.14017600 |
| C | 1.14914500 | 0.73119800 | 1.29358000 |
| C | 2.47512800 | 0.49134200 | 0.99716800 |
| C | 2.20442800 | 0.26749400 | -1.32173000 |
| H | 0.16731400 | 0.25239600 | -1.95088600 |
| H | -0.81356600 | 0.48614300 | 0.41629500 |
| H | 0.06875800 | 1.89361600 | -0.14661000 |
| H | 0.60301100 | -1.04622900 | -0.83840900 |
| C | 2.60617900 | 1.62378100 | -1.88741900 |
| H | 2.84220400 | 1.45098200 | -2.94485300 |
| H | 1.72991300 | 2.27699500 | -1.86527000 |
| C | 3.79170400 | 2.37169600 | -1.23848400 |
| H | 3.54200200 | 2.63732700 | -0.20920000 |
| H | 4.65209000 | 1.69750400 | -1.20214400 |
| C | 4.15390900 | 3.60348000 | -2.01652500 |
| H | 4.44971500 | 3.43409500 | -3.05071600 |
| C | 4.13213900 | 4.85055400 | -1.52763800 |
| H | 3.83827200 | 4.98524000 | -0.48767300 |
| O | 4.17390200 | -0.56846500 | -2.00445600 |
| N | 2.89501000 | -0.83019300 | -1.51790000 |
| C | 4.85726100 | -1.80877400 | -2.29274000 |
| H | 5.91516500 | -1.54103500 | -2.26549100 |
| H | 4.64692400 | -2.51145100 | -1.48348000 |
| C | 4.47017600 | 6.09683100 | -2.23527600 |
| C | 4.45195100 | 7.30739900 | -1.52292200 |
| C | 4.81012400 | 6.14513100 | -3.59919900 |
| C | 4.75986600 | 8.51711200 | -2.14188200 |
| H | 4.19130000 | 7.29552600 | -0.46926200 |
| C | 5.11713000 | 7.35130200 | -4.21795900 |
| H | 4.83005100 | 5.23318300 | -4.18446100 |
| C | 5.09477500 | 8.54554700 | -3.49371100 |
| H | 4.73746000 | 9.43678900 | -1.56719200 |
| H | 5.37459600 | 7.36238200 | -5.27170700 |
| H | 5.33343400 | 9.48462200 | -3.98042500 |
| C | 4.48860100 | -2.38555600 | -3.63776600 |
| C | 3.41847600 | -3.27774400 | -3.76841500 |
| C | 5.20723600 | -2.02165000 | -4.78193800 |
| C | 3.06972500 | -3.78759700 | -5.01783900 |
| H | 2.85594000 | -3.56850600 | -2.88824100 |
| C | 4.86205000 | -2.53119500 | -6.03231200 |
| H | 6.04389500 | -1.33574700 | -4.69221900 |
| C | 3.79091200 | -3.41585000 | -6.15222900 |
| H | 2.23848700 | -4.47877600 | -5.10553600 |
| H | 5.43060700 | -2.24294400 | -6.90980500 |

| | | | |
|---|---|---|---|
| H | 3.52181200 | -3.81584500 | -7.12373300 |
| C | 0.81688600 | 0.85471900 | 2.65123900 |
| C | 1.80480300 | 0.72409300 | 3.62901000 |
| H | 1.53681100 | 0.81296300 | 4.67621900 |
| C | 3.13168500 | 0.47116100 | 3.27469800 |
| H | 3.89060600 | 0.36393300 | 4.04313000 |
| C | 3.48484600 | 0.34783900 | 1.92329400 |
| H | -0.21288600 | 1.04407600 | 2.94162300 |
| H | 4.51117500 | 0.14649200 | 1.63402100 |

**Vibrational frequencies**

291.57*i*, 10.23, 21.91, 26.08, 34.03, 38.9, 49.82, 59.48, 60.34, 80.52, 86.48, 104.54, 117.79, 150.95, 162.51, 201, 218.01, 245.52, 261.72, 266.91, 286.6, 314.93, 333.48, 361.81, 377.95, 414.98, 415.04, 417.36, 419.41, 438.05, 465.94, 490.83, 500.65, 512.93, 529.19, 557.06, 603.23, 612.73, 629.89, 633.44, 634.68, 642.47, 704.38, 706.64, 709.86, 744.62, 755.08, 768.04, 772.51, 783.19, 821.79, 833.56, 849.17, 853.26, 859.13, 859.44, 868.22, 900.39, 911.79, 932.41, 939.13, 943.46, 965, 968.13, 987.84, 990.17, 991.93, 993.1, 999.2, 1001.73, 1006.58, 1012.65, 1013.54, 1016.62, 1017.99, 1033.72, 1039.38, 1048.2, 1049.13, 1051.29, 1088.65, 1105.86, 1108.67, 1116.93, 1159.17, 1169.97, 1176.7, 1177.68, 1182.51, 1197.44, 1201.01, 1206.79, 1218.76, 1227.06, 1228.66, 1235.08, 1275.36, 1277.52, 1290.4, 1306.63, 1320.73, 1328.76, 1333.81, 1343.09, 1345.63, 1354.82, 1359.74, 1365.29, 1371.37, 1376.13, 1388.76, 1447.41, 1461.96, 1470.87, 1476.36, 1476.39, 1477.54, 1482.39, 1484.46, 1489.39, 1503.72, 1524.37, 1524.67, 1578.58, 1613.06, 1624.43, 1628.47, 1639.08, 1643.13, 1701.33, 3011.97, 3017.64, 3026.76, 3047.65, 3058.18, 3065.34, 3067.25, 3090.82, 3094.2, 3111.78, 3119.31, 3127.67, 3148.96, 3157.96, 3158.55, 3158.72, 3164.86, 3165.54, 3171.05, 3173.68, 3174.2, 3181.65, 3182.9, 3184.17, 3189.73, 3190.97.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.437063
Thermal correction to Energy= 0.462464
Thermal correction to Enthalpy= 0.463408
Thermal correction to Gibbs Free Energy= 0.376713
Sum of electronic and zero-point Energies= -1135.962612
Sum of electronic and thermal Energies= -1135.937211
Sum of electronic and thermal Enthalpies= -1135.936267
Sum of electronic and thermal Free Energies= -1136.022962

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.95386000 | -0.33084300 | -2.84953600 |
| C | 3.21736200 | 0.18807900 | -1.61845800 |
| H | 3.32598100 | -0.13013800 | -3.73028400 |
| H | 4.89043800 | 0.23374700 | -2.98179600 |
| C | 2.05378200 | 1.14289700 | -1.79014900 |
| H | 1.45823700 | 0.82403200 | -2.65790800 |
| H | 1.40410400 | 1.10595000 | -0.90632900 |
| C | 2.53851700 | 2.60542500 | -2.00452900 |
| H | 3.12719200 | 2.92805600 | -1.13365600 |
| H | 3.21385700 | 2.62583100 | -2.87823000 |
| C | 1.39672000 | 3.54942200 | -2.23915700 |
| H | 0.78303600 | 3.34427900 | -3.12377100 |
| O | 3.20197700 | 0.60182300 | 0.59884200 |
| N | 3.85753800 | 0.00310300 | -0.49120600 |
| C | 3.99323500 | 0.40143600 | 1.80228300 |
| H | 3.27456100 | 0.57599800 | 2.61474400 |
| H | 4.32313200 | -0.64708000 | 1.83268300 |
| C | 0.00081800 | 5.56302200 | -1.61004500 |
| C | -0.05163200 | 6.68695400 | -0.75761700 |
| C | -1.01699200 | 5.42642200 | -2.58032900 |
| C | -1.06592600 | 7.64192600 | -0.87508800 |
| H | 0.72145200 | 6.80879400 | 0.00456600 |
| C | -2.02936300 | 6.37920100 | -2.69855300 |

| | | | |
|---|---|---|---|
| H | -1.02058000 | 4.56224500 | -3.24640800 |
| C | -2.06047300 | 7.49368500 | -1.84781100 |
| H | -1.08071100 | 8.50212100 | -0.20339600 |
| H | -2.80486300 | 6.25065200 | -3.45590500 |
| H | -2.85511800 | 8.23543000 | -1.94156800 |
| C | 1.09689100 | 4.59671600 | -1.44376200 |
| H | 1.74223800 | 4.77856900 | -0.57634700 |
| C | 4.25920200 | -1.83729000 | -2.77407100 |
| H | 5.02281600 | -2.01966800 | -2.00001100 |
| H | 4.67986900 | -2.19211300 | -3.72718200 |
| C | 3.00122900 | -2.59610200 | -2.41666200 |
| C | 1.98212000 | -1.93822200 | -1.74864200 |
| C | 2.77919300 | -3.96054400 | -2.69575400 |
| C | 0.79771800 | -2.50014600 | -1.31697500 |
| C | 1.58943800 | -4.58216600 | -2.29295600 |
| H | 3.54262900 | -4.53509400 | -3.22794500 |
| C | 0.60028800 | -3.86538500 | -1.60686400 |
| H | 0.03691200 | -1.92704200 | -0.78220700 |
| H | 1.43239000 | -5.63843800 | -2.51794700 |
| H | -0.32405000 | -4.35791200 | -1.29717900 |
| C | 5.16148200 | 1.35354800 | 1.89576300 |
| C | 4.97715400 | 2.65911900 | 2.38228700 |
| C | 6.44006800 | 0.96597400 | 1.46184800 |
| C | 6.04656900 | 3.55903200 | 2.43350300 |
| H | 3.98774000 | 2.96953500 | 2.72608100 |
| C | 7.51219700 | 1.86391400 | 1.51269200 |
| H | 6.59096300 | -0.04594400 | 1.08192900 |
| C | 7.31684100 | 3.16285700 | 1.99642700 |
| H | 5.89105600 | 4.56884600 | 2.81732600 |
| H | 8.50117800 | 1.54951800 | 1.17467300 |
| H | 8.15228200 | 3.86388100 | 2.03753700 |

**Vibrational frequencies**

142.61*i*, 15.51, 19.29, 26.62, 30.4, 39.04, 43.56, 53.45, 57.62, 70.21, 84.48, 99.17, 111.17, 148.34, 160.81, 179.85, 192.89, 234.91, 248.48, 260.72, 292.16, 304.01, 335, 350.84, 361.56, 396.64, 398.02, 399.96, 414.27, 426.31, 442.62, 469.68, 473.79, 505.38, 536.78, 541.12, 593.42, 597.76, 607.05, 615.5, 616.21, 631.87, 674.4, 681.89, 687.77, 711.95, 731.01, 739.74, 746.09, 753.28, 801.69, 809.06, 821.26, 822.73, 824.99, 829.32, 845.43, 866.31, 881.95, 898.34, 900.89, 903.11, 931.01, 945.62, 947.84, 951.1, 952.83, 953.06, 960.03, 966.61, 967.67, 974.21, 974.89, 979.25, 985.88, 990.59, 1008.92, 1015.27, 1024.73, 1028.98, 1065.78, 1079.22, 1081.49, 1085.69, 1132.2, 1135.07, 1148.46, 1150.88, 1156.17, 1165.15, 1171.14, 1174.4, 1182.36, 1196.92, 1205.32, 1214.15, 1226.45, 1235.71, 1240.04, 1268.52, 1287.98, 1294.91, 1302.93, 1306.36, 1313.22, 1319.61, 1322.85, 1334.45, 1336.51, 1345.72, 1349.38, 1399.12, 1418.53, 1422.02, 1426.05, 1428.48, 1434.2, 1437.58, 1439.78, 1440.41, 1480.39, 1483.05, 1506.08, 1529.58, 1572.01, 1581.97, 1589.5, 1596.84, 1599.26, 1648.71, 2949.03, 2972.81, 2977.82, 2992.9, 2997.12, 3012.23, 3021.19, 3026.97, 3050.35, 3052.83, 3055.72, 3067.17, 3084.53, 3093.81, 3095.95, 3098.51, 3102.97, 3105.58, 3106.46, 3111.4, 3113.4, 3118.56, 3120.81, 3121.79, 3129.68, 3130.08.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.447607
Thermal correction to Energy= 0.472514
Thermal correction to Enthalpy= 0.473458
Thermal correction to Gibbs Free Energy= 0.387861
Sum of electronic and zero-point Energies= -1136.195845
Sum of electronic and thermal Energies= -1136.170939
Sum of electronic and thermal Enthalpies= -1136.169994
Sum of electronic and thermal Free Energies= -1136.255591

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.96528000 | -0.31847100 | -2.85306200 |
| C | 3.21260200 | 0.18329100 | -1.62655400 |
| H | 3.33869500 | -0.13747600 | -3.73174800 |
| H | 4.88607800 | 0.26140600 | -2.97849100 |
| C | 2.05091100 | 1.13795500 | -1.80023700 |
| H | 1.47536300 | 0.83568300 | -2.67993800 |
| H | 1.39380300 | 1.08832000 | -0.93038800 |
| C | 2.54508100 | 2.59860700 | -1.98119100 |
| H | 3.11133800 | 2.90235900 | -1.09652400 |
| H | 3.23129700 | 2.63167000 | -2.83813000 |
| C | 1.40731600 | 3.54602300 | -2.22039200 |
| H | 0.80912800 | 3.35434500 | -3.11100800 |
| O | 3.17238000 | 0.59446200 | 0.57848900 |
| N | 3.84403500 | 0.00269800 | -0.49846200 |
| C | 3.95135600 | 0.40224200 | 1.78376400 |
| H | 3.23635400 | 0.59494000 | 2.58625300 |
| H | 4.27130300 | -0.64220100 | 1.82434800 |
| C | 0.00483400 | 5.54344100 | -1.58842900 |
| C | -0.05479400 | 6.65929900 | -0.73507400 |
| C | -1.00062900 | 5.40760800 | -2.56407900 |
| C | -1.06707900 | 7.61035200 | -0.85672700 |
| H | 0.70795400 | 6.77888800 | 0.02940700 |
| C | -2.01100000 | 6.35605500 | -2.68658400 |
| H | -0.99673400 | 4.55016200 | -3.22913400 |
| C | -2.05053400 | 7.46397600 | -1.83466500 |
| H | -1.08844600 | 8.46355500 | -0.18594000 |
| H | -2.77617600 | 6.22936700 | -3.44619400 |
| H | -2.84156900 | 8.20050600 | -1.93151600 |
| C | 1.10057700 | 4.57762900 | -1.41720100 |
| H | 1.72959700 | 4.74931000 | -0.54366500 |
| C | 4.29248500 | -1.81723800 | -2.76269900 |
| H | 5.04844900 | -1.98174500 | -1.98608400 |
| H | 4.71362300 | -2.17541600 | -3.70736600 |
| C | 3.03436500 | -2.57107400 | -2.40196700 |
| C | 2.02418500 | -1.89378600 | -1.74639400 |
| C | 2.80066800 | -3.93054300 | -2.66585200 |
| C | 0.83536300 | -2.43770200 | -1.31051200 |
| C | 1.60621000 | -4.53200600 | -2.25966100 |
| H | 3.55371000 | -4.51732500 | -3.18674300 |
| C | 0.62649400 | -3.79885500 | -1.58556900 |
| H | 0.08532200 | -1.85306000 | -0.78632100 |
| H | 1.43817400 | -5.58312500 | -2.47186400 |
| H | -0.29778300 | -4.27716100 | -1.27463200 |
| C | 5.12658400 | 1.34469700 | 1.86459100 |
| C | 4.95650200 | 2.64942900 | 2.34470300 |
| C | 6.39424500 | 0.94447900 | 1.42584100 |
| C | 6.03097400 | 3.53749000 | 2.38517200 |
| H | 3.97722700 | 2.96830600 | 2.69108100 |
| C | 7.47144600 | 1.83040700 | 1.46565500 |
| H | 6.53267600 | -0.06486300 | 1.05145800 |
| C | 7.29107000 | 3.12923700 | 1.94339500 |
| H | 5.88764500 | 4.54495600 | 2.76306700 |

| | | | |
|---|---|---|---|
| H | 8.45014900 | 1.50770600 | 1.12462800 |
| H | 8.12845000 | 3.81911100 | 1.97609600 |

**Vibrational frequencies**

191.91*i*, 16.81, 18.88, 27.55, 32.19, 40.7, 44.78, 55.62, 60.2, 72.96, 85.13, 102.53, 114.03, 150.83, 164.19, 183.5, 196.02, 240.91, 253.3, 265.18, 297.01, 308.32, 338.04, 354.46, 364.59, 406.6, 408.27, 409.88, 414.3, 431.27, 447.02, 479.8, 483.54, 516.64, 542.86, 548.13, 601.48, 607.25, 618.88, 624.83, 625.77, 641.01, 692.68, 701.02, 707.56, 739.11, 751.01, 758.72, 765.87, 769.09, 820.02, 827.41, 840.24, 854.08, 856.87, 861.13, 868.52, 891.86, 904.5, 930.58, 934.31, 939.38, 957.23, 976.08, 982.79, 984.84, 985.16, 988.14, 994.96, 996.96, 1000.55, 1002.59, 1006.83, 1008.1, 1008.85, 1012.79, 1036.83, 1039.84, 1047.16, 1051.83, 1089.99, 1104.6, 1107.46, 1112.85, 1160.31, 1166.31, 1177.72, 1179.95, 1186.55, 1196.99, 1202.05, 1205.17, 1212.55, 1225.06, 1231.67, 1247.09, 1263.46, 1274.86, 1277.8, 1308.9, 1325.18, 1333.32, 1335.67, 1348.2, 1350.78, 1354.65, 1359.15, 1362.44, 1368.48, 1369.9, 1380.67, 1443.99, 1468.05, 1476.86, 1480.25, 1481.09, 1482.12, 1483.17, 1486.95, 1497.12, 1524.33, 1527.22, 1531.51, 1574.67, 1615.33, 1624.03, 1628.05, 1639.62, 1641.82, 1692.47, 3008.17, 3031.64, 3036.13, 3054.6, 3056.11, 3069.92, 3080.62, 3083.65, 3113.21, 3114.88, 3117.07, 3126.76, 3145.5, 3155.26, 3156.15, 3156.58, 3162.55, 3163.86, 3170.34, 3171.19, 3172.16, 3179.06, 3180.25, 3182.16, 3189.74, 3190.19.

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## 19b

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.456464
Thermal correction to Energy= 0.480536
Thermal correction to Enthalpy= 0.481480
Thermal correction to Gibbs Free Energy= 0.399340
Sum of electronic and zero-point Energies= -1135.676596
Sum of electronic and thermal Energies= -1135.652525
Sum of electronic and thermal Enthalpies= -1135.651581
Sum of electronic and thermal Free Energies= -1135.733721

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.31523600 | -2.64819900 | -1.65826700 |
| C | 0.89380300 | -1.34747900 | -0.90986300 |
| H | 0.51946800 | -3.38504200 | -1.52762600 |
| H | 1.42225600 | -2.45932800 | -2.72739900 |
| C | -0.63420100 | -1.28240600 | -0.77959800 |
| H | -1.03074100 | -1.30063100 | -1.80227400 |
| H | -0.98221700 | -2.19627400 | -0.29016400 |
| C | -1.21058900 | -0.06545500 | -0.04219500 |
| H | -1.06634300 | -0.17315200 | 1.03498200 |
| H | -0.67421500 | 0.83440000 | -0.36426200 |
| C | -2.67341300 | 0.09752100 | -0.32801900 |
| H | -2.93420100 | 0.28005200 | -1.36954400 |
| O | 2.60580900 | -0.21388400 | -1.88300700 |
| N | 1.28307500 | -0.13613700 | -1.63997100 |
| C | 3.12952100 | 1.07931900 | -2.22575900 |
| H | 4.12696200 | 0.87849700 | -2.61768800 |
| H | 2.50466000 | 1.51266000 | -3.01028100 |
| C | -5.08606400 | 0.14794900 | 0.36680200 |
| C | -5.97023400 | -0.25888500 | 1.37186600 |
| C | -5.62506200 | 0.68114000 | -0.81150900 |
| C | -7.34692800 | -0.15724500 | 1.20320000 |
| H | -5.56909700 | -0.66527500 | 2.29488100 |
| C | -6.99892300 | 0.78238400 | -0.98196600 |
| H | -4.96527700 | 1.03234700 | -1.59648200 |
| C | -7.86779000 | 0.36191800 | 0.02329400 |
| H | -8.01190900 | -0.48316300 | 1.99483500 |
| H | -7.39597800 | 1.19922500 | -1.90073400 |

| | | | |
|---|---|---|---|
| H | -8.93986700 | 0.44488400 | -0.11216600 |
| C | -3.63561400 | 0.00600400 | 0.59243700 |
| H | -3.34774100 | -0.21007500 | 1.62032500 |
| C | 2.61032600 | -3.15617800 | -1.00201300 |
| H | 3.48951700 | -2.86308600 | -1.58279200 |
| H | 2.62654800 | -4.24389100 | -0.90299600 |
| C | 2.63849700 | -2.45209600 | 0.33074200 |
| C | 1.69694400 | -1.42523300 | 0.38800000 |
| C | 3.51671700 | -2.66427600 | 1.38761000 |
| C | 1.67258700 | -0.55459100 | 1.47441800 |
| C | 3.46181800 | -1.82323400 | 2.49622900 |
| H | 4.24549100 | -3.46730500 | 1.34266400 |
| C | 2.55493500 | -0.76565700 | 2.53218000 |
| H | 1.00637700 | 0.29954000 | 1.49375600 |
| H | 4.14134600 | -1.98049000 | 3.32635200 |
| H | 2.54256100 | -0.09402100 | 3.38308500 |
| C | 3.17463400 | 1.95769700 | -1.00409900 |
| C | 4.14664600 | 1.74408200 | -0.02643000 |
| C | 2.19345800 | 2.92452800 | -0.79184100 |
| C | 4.14079000 | 2.49187000 | 1.14574000 |
| H | 4.90044900 | 0.97744400 | -0.17799000 |
| C | 2.18680300 | 3.67663800 | 0.37915800 |
| H | 1.42545000 | 3.07753900 | -1.54296700 |
| C | 3.16043500 | 3.46012300 | 1.34951700 |
| H | 4.89712600 | 2.31724300 | 1.90242800 |
| H | 1.42011600 | 4.42702000 | 0.53488700 |
| H | 3.15528000 | 4.04347000 | 2.26321900 |

**Vibrational frequencies**

20.55, 27.84, 28.72, 36.87, 47.86, 62.56, 66.15, 77.74, 86.02, 94.2, 109.04, 150.67, 165.6, 181.09, 201.05, 216.99, 243.97, 255.83, 276.13, 298.65, 325.41, 358.23, 378.82, 388.3, 398.68, 412.58, 412.94, 439, 448.19, 468.28, 493.9, 517.32, 530.73, 563.89, 585.06, 604.36, 630.62, 631.05, 634, 636.76, 674.69, 707.86, 722.46, 737.62, 743.07, 765.17, 774.64, 784.61, 795.54, 813.46, 841.01, 851.34, 855.64, 871.59, 878.77, 886.21, 896.93, 941.12, 947.98, 958.92, 974.25, 984.79, 999.55, 1008.73, 1009.69, 1016.18, 1016.44, 1017.02, 1018.16, 1018.92, 1022.89, 1025.77, 1030.73, 1037.66, 1061.15, 1064.85, 1065.9, 1069.08, 1101.72, 1105.29, 1111.01, 1126.82, 1136.94, 1155.98, 1161.92, 1173.06, 1175.57, 1186.15, 1191.02, 1207.15, 1211.11, 1212.8, 1221.09, 1245.31, 1249.31, 1251.91, 1275.59, 1282.22, 1294.52, 1302.73, 1321.37, 1325.57, 1338.68, 1346.57, 1347.07, 1353.47, 1359.39, 1360.45, 1367.49, 1372.03, 1399.12, 1401.48, 1465.08, 1474.52, 1484.85, 1488.5, 1493.39, 1495.66, 1501.23, 1503.2, 1526.58, 1543.58, 1547.32, 1653.43, 1662.15, 1664.49, 1680.79, 1681.06, 1685.07, 1744.23, 3034.44, 3047.23, 3072.68, 3081.27, 3084.47, 3089.18, 3111.89, 3112.27, 3135.52, 3146.1, 3150.56, 3151.84, 3171.33, 3179.96, 3186.36, 3189.67, 3192.32, 3194.17, 3198.3, 3199.82, 3202.16, 3204.51, 3212.69, 3213.45, 3217.6, 3221.85.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.451274
Thermal correction to Energy= 0.475786
Thermal correction to Enthalpy= 0.476730
Thermal correction to Gibbs Free Energy= 0.393015

Sum of electronic and zero-point Energies= -1136.172100
Sum of electronic and thermal Energies= -1136.147588
Sum of electronic and thermal Enthalpies= -1136.146643
Sum of electronic and thermal Free Energies= -1136.230359

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.36525400 | -2.60572600 | -1.76136600 |
| C | 0.97236700 | -1.40156200 | -0.83093600 |
| H | 0.51196700 | -3.28645200 | -1.81073600 |
| H | 1.56719500 | -2.26149400 | -2.77698500 |
| C | -0.57031500 | -1.28268800 | -0.77548600 |

| | | | |
|---|---|---|---|
| H | -0.91146100 | -1.19796400 | -1.81451600 |
| H | -0.97081500 | -2.22603800 | -0.39310900 |
| C | -1.16786800 | -0.11294400 | 0.03131300 |
| H | -1.03843500 | -0.28110700 | 1.10263200 |
| H | -0.62349700 | 0.80362900 | -0.22429800 |
| C | -2.62684300 | 0.08174000 | -0.26500000 |
| H | -2.86671400 | 0.32371200 | -1.29922200 |
| O | 2.80041200 | -0.14572700 | -1.44885100 |
| N | 1.43831000 | -0.12142100 | -1.39197400 |
| C | 3.32005400 | 1.09951000 | -1.98580300 |
| H | 4.35426600 | 0.85681800 | -2.23554900 |
| H | 2.77357900 | 1.32993600 | -2.90281000 |
| C | -5.05572200 | 0.14642700 | 0.41507300 |
| C | -5.94765300 | -0.21068500 | 1.43975400 |
| C | -5.59822900 | 0.66646300 | -0.77370400 |
| C | -7.32479900 | -0.07041200 | 1.28307100 |
| H | -5.55119200 | -0.60767300 | 2.36891200 |
| C | -6.97246000 | 0.80700700 | -0.93127700 |
| H | -4.94093100 | 0.97269300 | -1.57932300 |
| C | -7.84509300 | 0.43788800 | 0.09487100 |
| H | -7.99024400 | -0.35744600 | 2.09011000 |
| H | -7.36668600 | 1.21237800 | -1.85704500 |
| H | -8.91612900 | 0.55086900 | -0.03090800 |
| C | -3.61121200 | -0.03334300 | 0.63639000 |
| H | -3.33883000 | -0.30058400 | 1.65659800 |
| C | 2.56814600 | -3.32050300 | -1.11224800 |
| H | 3.51096800 | -3.02820500 | -1.58617100 |
| H | 2.49310700 | -4.40877200 | -1.19417300 |
| C | 2.54423300 | -2.84243100 | 0.31912100 |
| C | 1.67715000 | -1.75700800 | 0.48347100 |
| C | 3.29741700 | -3.31687700 | 1.39171100 |
| C | 1.59456000 | -1.11263100 | 1.71836600 |
| C | 3.19041400 | -2.69014500 | 2.63330700 |
| H | 3.96625200 | -4.16214600 | 1.26271700 |
| C | 2.34885200 | -1.58760000 | 2.79225200 |
| H | 0.96885100 | -0.23975300 | 1.85270000 |
| H | 3.76955900 | -3.05413800 | 3.47523200 |
| H | 2.28225200 | -1.09304100 | 3.75531300 |
| C | 3.24724000 | 2.23945200 | -1.00215100 |
| C | 4.13159900 | 2.29809200 | 0.08113700 |
| C | 2.28841400 | 3.24569400 | -1.14893700 |
| C | 4.05578900 | 3.34134800 | 1.00039700 |
| H | 4.87944700 | 1.52176300 | 0.20605700 |
| C | 2.21371200 | 4.29435100 | -0.23293300 |
| H | 1.59528600 | 3.20438100 | -1.98222700 |
| C | 3.09629200 | 4.34257700 | 0.84445600 |
| H | 4.74654600 | 3.37650200 | 1.83574800 |
| H | 1.46558600 | 5.06931000 | -0.35891500 |
| H | 3.03928600 | 5.15678100 | 1.55865500 |

**Vibrational frequencies**

17.11, 26.65, 30.23, 39.12, 45.56, 53.34, 54.9, 65.68, 75.7, 98.58, 105.84, 145.34, 156.3, 165.16, 183.51, 206.52, 239.72, 245.91, 257.69, 287.48, 318.47, 348.69, 377.34, 379.71, 395.48, 411.2, 414.21, 436.98, 445.04, 466.87, 484.07, 514.1, 526.39, 559.14, 582.5, 601.37,

629.83, 633.97, 635.36, 636.58, 671.67, 702.93, 708.95, 731.4, 736.12, 759.76, 766.39, 767.78, 788.2, 807.75, 833.63, 841.72, 849.58, 852.77, 857.6, 866.42, 883.31, 921.47, 929.14, 934.52, 957.44, 962.92, 964.07, 987.24, 988.7, 994.43, 998.39, 999.91, 1003.26, 1006.84, 1008.61, 1010.16, 1014.63, 1017.97, 1034.27, 1049.19, 1050.69, 1051.27, 1072.12, 1081.49, 1094.69, 1098.59, 1111.77, 1124.4, 1136, 1173.78, 1176.14, 1181.51, 1182.76, 1197.27, 1199.71, 1199.96, 1215.19, 1228.33, 1228.83, 1232.75, 1260.93, 1276.78, 1283.71, 1291.59, 1316.36, 1322.12, 1332.74, 1333.91, 1342.19, 1345.16, 1351.41, 1354.63, 1360.41, 1371.21, 1391.77, 1392.87, 1469.96, 1472.11, 1477.25, 1483.1, 1483.96, 1485.88, 1489.12, 1494.38, 1506.68, 1524.51, 1527.32, 1613.52, 1620.28, 1626.09, 1638.85, 1639.25, 1644.69, 1701.22, 3016.45, 3021.74, 3031.1, 3050.05, 3063.35, 3064.05, 3066.14, 3086.76, 3101.58, 3117.86, 3119.77, 3129.28, 3156.77, 3158.01, 3160.99, 3163.97, 3165.74, 3167.95, 3173.44, 3173.54, 3180.83, 3181.9, 3182.85, 3189.83, 3189.91, 3202.49.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.439688
Thermal correction to Energy= 0.464897
Thermal correction to Enthalpy= 0.465842
Thermal correction to Gibbs Free Energy= 0.380887
Sum of electronic and zero-point Energies= -1136.010521
Sum of electronic and thermal Energies= -1135.985311
Sum of electronic and thermal Enthalpies= -1135.984367
Sum of electronic and thermal Free Energies= -1136.069321

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.37215500 | -2.63278700 | -1.76808800 |
| C | 0.98422500 | -1.41877400 | -0.84135900 |
| H | 0.51331800 | -3.31880800 | -1.80100600 |
| H | 1.56019300 | -2.29260300 | -2.79493100 |
| C | -0.56110300 | -1.29967600 | -0.78074400 |
| H | -0.90791300 | -1.22095000 | -1.82568300 |
| H | -0.96232400 | -2.24669200 | -0.38914300 |
| C | -1.15079200 | -0.12067000 | 0.02283200 |
| H | -1.01849000 | -0.28462400 | 1.10160400 |
| H | -0.59179500 | 0.79341300 | -0.24279600 |
| C | -2.60786800 | 0.08486900 | -0.27233800 |
| H | -2.85018300 | 0.32682300 | -1.31365900 |
| O | 2.81762700 | -0.15670700 | -1.45456400 |
| N | 1.44171900 | -0.13659600 | -1.41090700 |
| C | 3.32524500 | 1.10637800 | -1.98983000 |
| H | 4.37143300 | 0.87484100 | -2.23076700 |
| H | 2.77825800 | 1.32947100 | -2.91702400 |
| C | -5.04095000 | 0.16410000 | 0.41859900 |
| C | -5.93637600 | -0.17401200 | 1.45626900 |
| C | -5.58788100 | 0.67497700 | -0.77975900 |
| C | -7.31784700 | -0.02456000 | 1.30288700 |
| H | -5.53503200 | -0.56454200 | 2.39424700 |
| C | -6.96677000 | 0.82458000 | -0.93352700 |
| H | -4.92680300 | 0.96720400 | -1.59701000 |
| C | -7.84141300 | 0.47443200 | 0.10527900 |
| H | -7.98633600 | -0.29734700 | 2.12144500 |
| H | -7.36446900 | 1.22363100 | -1.86852800 |
| H | -8.91874400 | 0.59522000 | -0.01817800 |
| C | -3.59869600 | -0.02360100 | 0.63664200 |
| H | -3.32225700 | -0.29290100 | 1.66306000 |
| C | 2.58546200 | -3.33832500 | -1.12541000 |
| H | 3.52915700 | -3.04094400 | -1.61034500 |
| H | 2.51798800 | -4.43399400 | -1.20451300 |
| C | 2.57188500 | -2.85548600 | 0.30573100 |
| C | 1.69607900 | -1.76847600 | 0.47258300 |

| | | | |
|---|---|---|---|
| C | 3.33875800 | -3.32148400 | 1.37976300 |
| C | 1.62005900 | -1.11404700 | 1.70878500 |
| C | 3.23601300 | -2.68625300 | 2.62381800 |
| H | 4.01561400 | -4.16900900 | 1.24979600 |
| C | 2.38690700 | -1.58266500 | 2.78377800 |
| H | 0.98937400 | -0.23575300 | 1.84210700 |
| H | 3.82642600 | -3.04530000 | 3.46882500 |
| H | 2.32442300 | -1.08052500 | 3.75090700 |
| C | 3.22255000 | 2.24051200 | -1.00116700 |
| C | 4.10139700 | 2.31242200 | 0.09332900 |
| C | 2.23348200 | 3.22618600 | -1.14638300 |
| C | 3.98962800 | 3.34762400 | 1.02612000 |
| H | 4.87330700 | 1.54983500 | 0.21637100 |
| C | 2.12296900 | 4.26616900 | -0.21626000 |
| H | 1.54415500 | 3.17327600 | -1.99117600 |
| C | 3.00000900 | 4.32726200 | 0.87235100 |
| H | 4.67781400 | 3.39365000 | 1.87184600 |
| H | 1.35048900 | 5.02697900 | -0.34018200 |
| H | 2.91515900 | 5.13706100 | 1.59900800 |

**Vibrational frequencies**

18.12, 27.24, 34.02, 34.89, 43.6, 49.38, 51.8, 64.76, 75.84, 95.55, 104.43, 140.89, 151.58, 158.02, 177.45, 200.2, 234.49, 238.97, 249.37, 277.94, 306.86, 338.95, 364.61, 365.54, 383.54, 395.16, 397.05, 424.76, 429.5, 453.42, 467.4, 497.69, 508.1, 542.27, 563.04, 582.65, 610.42, 613.48, 614.44, 617.57, 650.44, 678.79, 685.81, 709.87, 712.31, 734.44, 739.46, 743.27, 763.7, 783.09, 811.56, 818.87, 820.68, 827.58, 828.25, 835.22, 849.05, 887.77, 892.68, 900.57, 920.32, 921.4, 935.14, 947.84, 950.6, 957.21, 958.47, 966.33, 967.25, 969.12, 972.35, 984.81, 986.27, 990.98, 1009.87, 1020.3, 1024.8, 1027.57, 1028.57, 1038.4, 1059.21, 1069.98, 1085.42, 1092.8, 1104.75, 1141.21, 1145.59, 1150.64, 1152.57, 1159.87, 1165.66, 1168.33, 1175.49, 1192.22, 1199.78, 1205.9, 1218.8, 1232.21, 1242.35, 1249.59, 1280.55, 1285.72, 1286.8, 1296.34, 1297.66, 1316.25, 1319.95, 1335.27, 1339.85, 1346, 1348.98, 1351.15, 1419.48, 1422.49, 1433.45, 1434.66, 1439.51, 1441.23, 1443.27, 1443.73, 1461.78, 1479.64, 1484.13, 1569.87, 1578.13, 1584.53, 1594.15, 1595.37, 1601.45, 1649.62, 2952.71, 2961.89, 2973.23, 2991.89, 2998.13, 3009.48, 3010.5, 3028.3, 3046.81, 3056.08, 3058.68, 3065.56, 3096.7, 3097.25, 3101.03, 3103.24, 3105.41, 3107.9, 3112.64, 3113.19, 3120.79, 3120.93, 3121.67, 3129.21, 3130.02, 3137.91.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.450147
Thermal correction to Energy= 0.474969
Thermal correction to Enthalpy= 0.475913
Thermal correction to Gibbs Free Energy= 0.390762
Sum of electronic and zero-point Energies= -1136.246940
Sum of electronic and thermal Energies= -1136.222118
Sum of electronic and thermal Enthalpies= -1136.221174
Sum of electronic and thermal Free Energies= -1136.306325

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.34339900 | -2.66699900 | -1.68981100 |
| C | 0.95932700 | -1.44095300 | -0.79141800 |
| H | 0.49405900 | -3.35692400 | -1.69356300 |
| H | 1.51978800 | -2.35200100 | -2.72073600 |
| C | -0.58032600 | -1.30019500 | -0.75110700 |
| H | -0.91228900 | -1.24065300 | -1.79583200 |
| H | -0.99780600 | -2.22459900 | -0.33941200 |
| C | -1.15416400 | -0.09080600 | 0.01525500 |
| H | -1.04019700 | -0.23127500 | 1.09330500 |
| H | -0.58195700 | 0.80200100 | -0.26708100 |
| C | -2.60461700 | 0.12673000 | -0.30315500 |
| H | -2.82981800 | 0.35763600 | -1.34431000 |
| O | 2.80982700 | -0.23691600 | -1.43205600 |

| | | | |
|---|---|---|---|
| N | 1.44176100 | -0.17724700 | -1.37936700 |
| C | 3.34481200 | 1.00200600 | -1.98057500 |
| H | 4.38117900 | 0.74866900 | -2.21138800 |
| H | 2.80571800 | 1.22258400 | -2.90515100 |
| C | -5.03819700 | 0.23867200 | 0.35290600 |
| C | -5.94458100 | -0.05307100 | 1.38770700 |
| C | -5.56181300 | 0.71720100 | -0.86291400 |
| C | -7.31830800 | 0.11152400 | 1.21582700 |
| H | -5.56064100 | -0.41783800 | 2.33644700 |
| C | -6.93260400 | 0.88212700 | -1.03536200 |
| H | -4.89159300 | 0.97016300 | -1.67790300 |
| C | -7.82020100 | 0.57940100 | 0.00166900 |
| H | -7.99520700 | -0.12428400 | 2.03103100 |
| H | -7.31240000 | 1.25437900 | -1.98187300 |
| H | -8.88841300 | 0.71157400 | -0.13639600 |
| C | -3.60107800 | 0.03951500 | 0.59313000 |
| H | -3.34248500 | -0.21423400 | 1.62152200 |
| C | 2.56600600 | -3.34655500 | -1.04243100 |
| H | 3.49830200 | -3.03306500 | -1.52509400 |
| H | 2.51541800 | -4.43784900 | -1.11123300 |
| C | 2.53754300 | -2.84923900 | 0.38232200 |
| C | 1.65854300 | -1.76912700 | 0.52940200 |
| C | 3.29539300 | -3.29873800 | 1.46442700 |
| C | 1.56560300 | -1.10480000 | 1.75449300 |
| C | 3.17751800 | -2.65331600 | 2.69690800 |
| H | 3.97447900 | -4.13911400 | 1.35056400 |
| C | 2.32279200 | -1.55667400 | 2.83760400 |
| H | 0.93004200 | -0.23532200 | 1.87320600 |
| H | 3.75883200 | -2.99814000 | 3.54654300 |
| H | 2.24829100 | -1.04875500 | 3.79414800 |
| C | 3.25770700 | 2.14733300 | -1.00523400 |
| C | 4.13880800 | 2.22408200 | 0.08094000 |
| C | 2.28036400 | 3.13649900 | -1.15933900 |
| C | 4.04176300 | 3.27011500 | 0.99698600 |
| H | 4.89957900 | 1.45981800 | 0.21044700 |
| C | 2.18392800 | 4.18694100 | -0.24577100 |
| H | 1.59090600 | 3.07891500 | -1.99601900 |
| C | 3.06376400 | 4.25404400 | 0.83473700 |
| H | 4.73003000 | 3.32063400 | 1.83470200 |
| H | 1.42212900 | 4.94901400 | -0.37581200 |
| H | 2.99032200 | 5.06991800 | 1.54681900 |

**Vibrational frequencies**

10.99, 22.91, 25.51, 36.73, 41.89, 50.28, 54.2, 65.27, 76.28, 96.7, 102.64, 141.45, 151.76, 161.09, 178.68, 202.13, 235.23, 240.86, 252.78, 281.32, 311.31, 338.78, 365.54, 370.07, 386.08, 404.68, 406.7, 429.47, 439.03, 458.13, 477, 506.32, 517.78, 551.01, 571.6, 592.51, 618.92, 623.02, 625.69, 626.81, 660.9, 697.1, 705.34, 724.48, 729.46, 754.07, 762.34, 763.6, 782.64, 800.63, 828.51, 837.01, 844.76, 850.82, 859.12, 859.95, 881.28, 915.17, 924.43, 928.8, 953.34, 955.77, 962.33, 985.26, 986.78, 992.26, 995.25, 996.06, 999.06, 1003.84, 1005.76, 1007.24, 1009.8, 1012.87, 1030.1, 1047.05, 1048.96, 1050.79, 1059.98, 1068.98, 1087.95, 1094.83, 1111.86, 1121.74, 1133.11, 1171.82, 1175.92, 1181.33, 1181.37, 1192.83, 1198.67, 1200.12, 1210.68, 1225.92, 1227.78, 1232.09, 1257.6, 1271.04, 1278.9, 1289.88, 1320.46, 1322.51, 1328.98, 1333.31, 1338.61, 1357.88, 1359.3, 1359.55, 1361.78, 1366.32, 1384.73, 1385.3, 1473.73, 1476.34, 1476.82, 1483.67, 1485.39, 1491.31, 1495.45, 1499.47, 1505.84, 1523.95, 1528.51, 1612.36, 1619.48, 1627.1, 1636.07, 1637.63,

1644.44, 1692.91, 3014.26, 3019.33, 3031.29, 3044.84, 3062.17, 3064.62, 3067.1, 3086.85, 3100.17, 3117.54, 3123.47, 3126.25, 3154.81, 3156.3, 3159.56, 3162.65, 3164.39, 3166.52, 3171.78, 3172.25, 3180.51, 3180.9, 3180.98, 3189.65, 3190.28, 3197.42.

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## 19b' TS2*trans*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.455639
Thermal correction to Energy= 0.478533
Thermal correction to Enthalpy= 0.479477
Thermal correction to Gibbs Free Energy= 0.401079

Sum of electronic and zero-point Energies= -1135.655060
Sum of electronic and thermal Energies= -1135.632166
Sum of electronic and thermal Enthalpies= -1135.631221
Sum of electronic and thermal Free Energies= -1135.709620

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.79047000 | 0.63844300 | 0.23739300 |
| C | 3.90316900 | 1.23325000 | 1.65159200 |
| C | 3.27967300 | 0.15981700 | 2.50928300 |
| C | 2.52259500 | -0.71905200 | 1.73098400 |
| C | 2.53940600 | -0.27868200 | 0.27072300 |
| H | 4.66315500 | 0.01080500 | 0.03021000 |
| H | 3.32839500 | 2.16078100 | 1.72762600 |
| H | 4.93439700 | 1.45172500 | 1.93655100 |
| H | 3.70492900 | 1.38949100 | -0.55023700 |
| C | 2.56270500 | -1.39802100 | -0.76913700 |
| H | 2.94139400 | -0.97580300 | -1.70366300 |
| H | 3.25357700 | -2.18415700 | -0.45917200 |
| C | 1.12783700 | -1.93592900 | -0.98991400 |
| H | 0.92076000 | -2.03562300 | -2.05728000 |
| H | 1.02260000 | -2.93467800 | -0.55560800 |
| C | 0.09155400 | -1.03276500 | -0.35872100 |
| H | 0.02511400 | -1.08607500 | 0.72388300 |
| C | -1.04925000 | -0.64237500 | -1.02294800 |
| H | -1.08791000 | -0.76478600 | -2.10303800 |
| O | 0.92511500 | 1.29490200 | 0.86598200 |
| N | 1.37948700 | 0.52086700 | -0.16775500 |
| C | 0.27563300 | 2.46327600 | 0.33976600 |
| H | -0.39391900 | 2.15854700 | -0.46806000 |
| H | -0.31534900 | 2.85318600 | 1.16969100 |
| C | -2.20415000 | -0.01238300 | -0.40588700 |
| C | -3.32582900 | 0.29485300 | -1.19713700 |
| C | -2.25322100 | 0.32858400 | 0.96006700 |
| C | -4.44948800 | 0.89999900 | -0.65140100 |
| H | -3.30611900 | 0.04662100 | -2.25363700 |
| C | -3.37740900 | 0.93443500 | 1.50138000 |
| H | -1.39870500 | 0.13168700 | 1.59807500 |
| C | -4.48365100 | 1.22278500 | 0.70278900 |
| H | -5.30159100 | 1.12298300 | -1.28379800 |
| H | -3.39129700 | 1.18741800 | 2.55586000 |
| H | -5.35972700 | 1.69452300 | 1.13192100 |
| C | 1.28822000 | 3.47170800 | -0.13534300 |
| C | 1.83766900 | 4.39238400 | 0.75773700 |
| C | 1.73853600 | 3.45400000 | -1.45572300 |
| C | 2.82728600 | 5.27726700 | 0.34157800 |

| | | | |
|---|---|---|---|
| H | 1.48922800 | 4.41159200 | 1.78599000 |
| C | 2.72698600 | 4.33862100 | -1.87568100 |
| H | 1.31545500 | 2.73507300 | -2.14911400 |
| C | 3.27525200 | 5.24881500 | -0.97608900 |
| H | 3.24652700 | 5.98938500 | 1.04334200 |
| H | 3.07028400 | 4.31743500 | -2.90375700 |
| H | 4.04548900 | 5.93792100 | -1.30316500 |
| C | 1.91693100 | -1.82648200 | 2.31539100 |
| H | 1.36239500 | -2.54479200 | 1.72109800 |
| C | 2.04624800 | -2.02821100 | 3.68928100 |
| H | 1.58280800 | -2.89199400 | 4.15196500 |
| C | 2.77534200 | -1.13288900 | 4.46759400 |
| H | 2.87065600 | -1.30139500 | 5.53440200 |
| C | 3.40237100 | -0.03604300 | 3.87888700 |
| H | 3.99216000 | 0.64645900 | 4.48219100 |

**Vibrational frequencies**

600.07*i*, 23.99, 28.44, 31.41, 39.35, 47.05, 63.88, 76.53, 95.96, 113.56, 122.1, 155.41, 184.35, 194.61, 214.96, 231.67, 248.21, 287.56, 294.91, 318.22, 340.59, 367.76, 390.02, 402.32, 409.19, 414.5, 418.49, 440.37, 469.02, 488.77, 506.82, 519.49, 537.45, 559.12, 596.01, 607.15, 617.18, 629.82, 632.54, 638.13, 680.5, 708.8, 716.59, 736.49, 749.33, 764.24, 780.48, 782.36, 792.63, 817.21, 829.05, 844.5, 853.97, 870.59, 871.62, 879.25, 898.7, 925.71, 942.52, 953.56, 972.09, 975.69, 991.2, 992.82, 1003.05, 1009.04, 1010.4, 1011.45, 1017.91, 1020.07, 1022.68, 1026.46, 1031.53, 1039.95, 1048.61, 1062.52, 1064.56, 1065.69, 1070.37, 1097.37, 1107.65, 1113.95, 1120.92, 1127, 1149.9, 1172.21, 1173.64, 1179.71, 1184.26, 1200.3, 1204.07, 1206.7, 1210.21, 1229.88, 1240.3, 1251.26, 1254.09, 1290.07, 1294.13, 1304.37, 1307.77, 1316.62, 1324.75, 1325.9, 1345.75, 1348.02, 1349.39, 1356.58, 1361.81, 1365.02, 1377.03, 1406.71, 1473.16, 1478.43, 1484.09, 1489.82, 1491.36, 1498.98, 1499.17, 1504.8, 1522.67, 1528.58, 1544.38, 1560.05, 1638.96, 1662.61, 1662.81, 1665.28, 1682.25, 1685.2, 3059.75, 3065.61, 3070.58, 3074.77, 3086.55, 3104.95, 3115.74, 3125.07, 3131.1, 3146.42, 3154.08, 3173.42, 3176.9, 3181.42, 3181.85, 3182.14, 3186.36, 3188.22, 3193.33, 3193.8, 3199.72, 3202.4, 3204.38, 3210.67, 3212.68, 3219.4.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.450302
Thermal correction to Energy= 0.473756
Thermal correction to Enthalpy= 0.474701
Thermal correction to Gibbs Free Energy= 0.393810
Sum of electronic and zero-point Energies= -1136.145042
Sum of electronic and thermal Energies= -1136.121588
Sum of electronic and thermal Enthalpies= -1136.120644
Sum of electronic and thermal Free Energies= -1136.201534

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.89830800 | 0.46539800 | 0.20520300 |
| C | 4.21184500 | 1.00697700 | 1.61357000 |
| C | 3.52384100 | 0.01437300 | 2.51949600 |
| C | 2.60655000 | -0.76823900 | 1.80657300 |
| C | 2.57521400 | -0.35527300 | 0.32939000 |
| H | 4.69157800 | -0.22184300 | -0.10582300 |
| H | 3.79603100 | 2.00911400 | 1.75716900 |
| H | 5.28666400 | 1.07261900 | 1.80428800 |
| H | 3.80979100 | 1.24223300 | -0.55529200 |
| C | 2.49716800 | -1.50047300 | -0.69131600 |
| H | 2.87571700 | -1.12237200 | -1.64502800 |
| H | 3.14802600 | -2.32327600 | -0.38895300 |
| C | 1.02759800 | -1.95540400 | -0.86839300 |
| H | 0.80405000 | -2.09963800 | -1.92815100 |
| H | 0.86505000 | -2.92501600 | -0.38602000 |
| C | 0.05062500 | -0.95757500 | -0.27227400 |
| H | -0.06471300 | -1.01813000 | 0.80452800 |

| | | | |
|---|---|---|---|
| C | -1.07511700 | -0.55779400 | -0.98945400 |
| H | -1.04234100 | -0.66595700 | -2.07163300 |
| O | 1.08336500 | 1.35118800 | 0.94431500 |
| N | 1.43413500 | 0.49678500 | -0.09344500 |
| C | 0.39920000 | 2.52197700 | 0.42960200 |
| H | -0.30163600 | 2.20431500 | -0.34274300 |
| H | -0.16383500 | 2.89593100 | 1.28623100 |
| C | -2.29120000 | 0.01674200 | -0.45872500 |
| C | -3.32677100 | 0.38145000 | -1.35087000 |
| C | -2.52277400 | 0.22832800 | 0.92132800 |
| C | -4.52295500 | 0.91998300 | -0.89394900 |
| H | -3.17712700 | 0.23099100 | -2.41539500 |
| C | -3.71980600 | 0.76747400 | 1.37318600 |
| H | -1.75903100 | -0.03296800 | 1.64369700 |
| C | -4.72997000 | 1.11754700 | 0.47274900 |
| H | -5.29805200 | 1.18756300 | -1.60419000 |
| H | -3.86998500 | 0.91594400 | 2.43739000 |
| H | -5.66351000 | 1.53564400 | 0.83199100 |
| C | 1.34358700 | 3.57617700 | -0.09306700 |
| C | 1.91327000 | 4.51115200 | 0.77915900 |
| C | 1.67774600 | 3.63049600 | -1.45064200 |
| C | 2.79979800 | 5.47728000 | 0.30733500 |
| H | 1.65625200 | 4.48417700 | 1.83356200 |
| C | 2.56459800 | 4.59560100 | -1.92604800 |
| H | 1.24061900 | 2.91177200 | -2.13492800 |
| C | 3.12841600 | 5.52016800 | -1.04763000 |
| H | 3.22993700 | 6.19819400 | 0.99415000 |
| H | 2.81308800 | 4.62759700 | -2.98137400 |
| H | 3.81511900 | 6.27386400 | -1.41728900 |
| C | 1.90078700 | -1.77640000 | 2.46465000 |
| H | 1.21116100 | -2.42237000 | 1.93433400 |
| C | 2.09871600 | -1.97739200 | 3.83261800 |
| H | 1.55450400 | -2.76413000 | 4.34390700 |
| C | 2.99882900 | -1.18100000 | 4.54158800 |
| H | 3.14823800 | -1.34762800 | 5.60299900 |
| C | 3.71963700 | -0.18330300 | 3.88403200 |
| H | 4.43396200 | 0.42462900 | 4.43056100 |

**Vibrational frequencies**

524.5*i*, 19.58, 23.16, 25.27, 35.76, 38.33, 44.4, 64.47, 81.59, 100.7, 119.11, 141.44, 170.91, 181.99, 198.34, 216.58, 240.22, 275.5, 283.08, 325.09, 332.78, 350.02, 387.98, 390.38, 412.95, 413.5, 416.15, 438.42, 468.34, 479.69, 503.11, 513.7, 533.02, 555.23, 591.66, 606.21, 616.84, 629.12, 631.71, 635.39, 678.2, 693.8, 709.24, 725.69, 741.93, 750.39, 766.95, 769.91, 781.93, 806.11, 815.7, 831.8, 840.47, 842.99, 858.37, 859.88, 879.28, 908.03, 914.06, 930.45, 948.68, 955.72, 958.96, 980.36, 981.14, 982.82, 989.3, 995.03, 997.15, 1003.47, 1006.51, 1007.68, 1011.55, 1016.97, 1020.83, 1033.16, 1044.56, 1048.86, 1050.72, 1065.69, 1087.22, 1098.22, 1108.11, 1111.14, 1138.41, 1167.73, 1175.1, 1178.07, 1180.88, 1192.29, 1195.17, 1196.32, 1200.28, 1220.11, 1227.57, 1228.59, 1245.42, 1275.8, 1282.39, 1289.41, 1296.1, 1311.5, 1318.43, 1323.4, 1337.93, 1343.75, 1349.14, 1352.68, 1353.62, 1360.59, 1374.35, 1391.15, 1466.73, 1471.98, 1476.74, 1482.2, 1484.4, 1485.07, 1488.63, 1496.05, 1505.32, 1510.05, 1521.25, 1524.74, 1596.81, 1620.07, 1620.7, 1623.33, 1639.77, 1641.94, 3029.48, 3035.13, 3036.07, 3045.13, 3069.23, 3071.11, 3072.37, 3095.29, 3106, 3125.87, 3126.6, 3155.67, 3156.24, 3156.56, 3158.5, 3163.17, 3164.82, 3166.76, 3173.07, 3173.7, 3178.86, 3181.46, 3185.29, 3189.61, 3189.92, 3191.38.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.439033
Thermal correction to Energy= 0.463112
Thermal correction to Enthalpy= 0.464056
Thermal correction to Gibbs Free Energy= 0.382668
Sum of electronic and zero-point Energies= -1135.993063
Sum of electronic and thermal Energies= -1135.968983
Sum of electronic and thermal Enthalpies= -1135.968039
Sum of electronic and thermal Free Energies=-1136.049427

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.93983600 | 0.44729000 | 0.23092900 |
| C | 4.24416700 | 0.97744800 | 1.64726100 |
| C | 3.53766500 | -0.01388800 | 2.54222100 |
| C | 2.61685200 | -0.78738400 | 1.81034700 |
| C | 2.60157700 | -0.35789600 | 0.33746200 |
| H | 4.73027200 | -0.25439100 | -0.07885300 |
| H | 3.83309900 | 1.98843600 | 1.79487800 |
| H | 5.32382800 | 1.03528400 | 1.85070600 |
| H | 3.86715900 | 1.23327800 | -0.53181100 |
| C | 2.51072900 | -1.48845100 | -0.70238800 |
| H | 2.89441000 | -1.09507700 | -1.65572300 |
| H | 3.16298200 | -2.32281400 | -0.41071400 |
| C | 1.03723600 | -1.93557800 | -0.88766500 |
| H | 0.81469800 | -2.07063700 | -1.95598300 |
| H | 0.87130200 | -2.91730700 | -0.41458800 |
| C | 0.05376800 | -0.94848000 | -0.28495500 |
| H | -0.04800600 | -1.00198100 | 0.80192700 |
| C | -1.07835000 | -0.54773100 | -0.99596700 |
| H | -1.05095500 | -0.65587000 | -2.08586100 |
| O | 1.14327800 | 1.37226700 | 0.97015700 |
| N | 1.47622600 | 0.52152800 | -0.08384500 |
| C | 0.41609600 | 2.53424500 | 0.45709400 |
| H | -0.29794200 | 2.18659200 | -0.30024100 |
| H | -0.13641200 | 2.90330800 | 1.33112200 |
| C | -2.29516200 | 0.02106000 | -0.45827100 |
| C | -3.33763100 | 0.39534500 | -1.34898000 |
| C | -2.52760600 | 0.22174500 | 0.93004500 |
| C | -4.53716300 | 0.93287800 | -0.88427900 |
| H | -3.18754500 | 0.25238600 | -2.42169900 |
| C | -3.72801500 | 0.76009900 | 1.38937600 |
| H | -1.75929900 | -0.05134400 | 1.65423700 |
| C | -4.74344100 | 1.12076200 | 0.48987900 |
| H | -5.31775000 | 1.20853100 | -1.59593600 |
| H | -3.87813300 | 0.89927500 | 2.46187900 |
| H | -5.68192200 | 1.53930800 | 0.85612800 |
| C | 1.33508200 | 3.59528200 | -0.09511200 |
| C | 1.87617700 | 4.57886900 | 0.75085600 |
| C | 1.68426100 | 3.60511800 | -1.45657100 |
| C | 2.74957900 | 5.54978800 | 0.24940500 |
| H | 1.60598400 | 4.58505400 | 1.80942200 |
| C | 2.55978400 | 4.57383700 | -1.96004300 |
| H | 1.26578600 | 2.84682000 | -2.12043200 |
| C | 3.09454500 | 5.54755500 | -1.10781800 |
| H | 3.15770200 | 6.31126800 | 0.91634300 |
| H | 2.82129300 | 4.57186300 | -3.01970000 |

| | | | |
|---|---|---|---|
| H | 3.77311700 | 6.30654200 | -1.50092200 |
| C | 1.89115400 | -1.79785600 | 2.45488000 |
| H | 1.19949500 | -2.43854700 | 1.90635300 |
| C | 2.07282500 | -2.01041500 | 3.82903100 |
| H | 1.51369000 | -2.80160700 | 4.33173400 |
| C | 2.97467200 | -1.22317400 | 4.55690500 |
| H | 3.11091600 | -1.40001200 | 5.62536300 |
| C | 3.71529700 | -0.22312700 | 3.91322500 |
| H | 4.43298700 | 0.37800700 | 4.47615800 |

**Vibrational frequencies**

340.22*i*, 21.74, 23.66, 32.58, 40.02, 42.95, 48.49, 62.7, 82.6, 98.05, 115.48, 135.93, 164.85, 178.22, 191.46, 210.35, 230.77, 268.4, 272.75, 319.59, 321.3, 339.25, 373.79, 379.39, 397.21, 398.72, 401.86, 421.84, 455.54, 464.43, 486.81, 498.43, 515.99, 538.63, 573.18, 587.75, 597.53, 607.55, 611.22, 615.2, 659.89, 671.27, 687.34, 706.09, 716.19, 726.79, 742.25, 744.32, 758.01, 782.7, 791.33, 809.9, 812.19, 821.33, 829.96, 835.38, 845.68, 875.65, 882.31, 891.71, 914.57, 916.65, 926, 942.67, 952.03, 953.92, 956.72, 957.27, 962.54, 966.72, 968.55, 974.62, 978.74, 981.18, 989.7, 1006.41, 1019.78, 1024.46, 1025.11, 1031.31, 1055.66, 1068.6, 1080.41, 1082.85, 1106.95, 1136.44, 1144.32, 1147.82, 1150.07, 1159.74, 1160.7, 1163.59, 1166.97, 1188.03, 1198.08, 1199.3, 1210.08, 1232.41, 1245.05, 1247.51, 1255.58, 1273.93, 1283.29, 1285.45, 1298.67, 1303.25, 1312.79, 1324.16, 1334.65, 1345.21, 1346.16, 1348.13, 1421.23, 1426.9, 1427.41, 1431.73, 1437.44, 1439.7, 1442.19, 1446.23, 1460.18, 1466.89, 1480.54, 1489.81, 1552.69, 1578.27, 1581.1, 1581.94, 1595.44, 1597.94, 2968.41, 2978.3, 2979.91, 2988.88, 3010.66, 3013.89, 3015.29, 3042.17, 3051.44, 3059.88, 3068.57, 3079.82, 3093.92, 3096.56, 3098.74, 3100.86, 3105.45, 3106.76, 3111.83, 3114.23, 3117.6, 3120.93, 3121.93, 3127.97, 3129.83, 3130.35.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.449353
Thermal correction to Energy= 0.473000
Thermal correction to Enthalpy= 0.473945
Thermal correction to Gibbs Free Energy= 0.393193

Sum of electronic and zero-point Energies= -1136.226345
Sum of electronic and thermal Energies= -1136.202697
Sum of electronic and thermal Enthalpies= -1136.201753
Sum of electronic and thermal Free Energies= -1136.282504

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.90461800 | 0.48466500 | 0.23788900 |
| C | 4.14787600 | 1.04437000 | 1.65241000 |
| C | 3.45968100 | 0.03050500 | 2.53489700 |
| C | 2.58564400 | -0.77289900 | 1.78890000 |
| C | 2.58748800 | -0.34493500 | 0.32023200 |
| H | 4.71614900 | -0.20171500 | -0.02899900 |
| H | 3.68665300 | 2.03057600 | 1.77191800 |
| H | 5.21255000 | 1.14874300 | 1.88258100 |
| H | 3.83825900 | 1.25284100 | -0.53535800 |
| C | 2.52491800 | -1.46922400 | -0.72217500 |
| H | 2.90517300 | -1.06763400 | -1.66657100 |
| H | 3.17913900 | -2.29435600 | -0.43028200 |
| C | 1.05806500 | -1.92948400 | -0.91411200 |
| H | 0.83608600 | -2.04761100 | -1.97834400 |
| H | 0.90215300 | -2.91175700 | -0.45304900 |
| C | 0.07350900 | -0.95491200 | -0.29639600 |
| H | -0.01628700 | -1.01285800 | 0.78486100 |
| C | -1.06379900 | -0.55844000 | -0.99529300 |
| H | -1.05174800 | -0.66595500 | -2.07924600 |
| O | 1.09787900 | 1.35259100 | 0.94286500 |
| N | 1.45655000 | 0.51742700 | -0.11160000 |
| C | 0.39812300 | 2.51928100 | 0.42504800 |
| H | -0.30187700 | 2.18509700 | -0.34241300 |

| | | | |
|---|---|---|---|
| H | -0.15803500 | 2.89410100 | 1.28607000 |
| C | -2.26822500 | 0.01632800 | -0.43676800 |
| C | -3.32852300 | 0.37282500 | -1.30388400 |
| C | -2.46043400 | 0.23817100 | 0.94842100 |
| C | -4.51349300 | 0.91405500 | -0.81744600 |
| H | -3.20652400 | 0.21374300 | -2.37186200 |
| C | -3.64601700 | 0.78029200 | 1.42982700 |
| H | -1.67269700 | -0.01523300 | 1.64978700 |
| C | -4.68263500 | 1.12226100 | 0.55430300 |
| H | -5.30896000 | 1.17548800 | -1.50857300 |
| H | -3.76610300 | 0.93809500 | 2.49741200 |
| H | -5.60684100 | 1.54311600 | 0.93647000 |
| C | 1.34295400 | 3.56519200 | -0.10997300 |
| C | 1.88852600 | 4.53197400 | 0.74448100 |
| C | 1.70693600 | 3.57439000 | -1.46238900 |
| C | 2.78207600 | 5.48697300 | 0.25946400 |
| H | 1.60696200 | 4.53855300 | 1.79399300 |
| C | 2.60211200 | 4.52729400 | -1.94993100 |
| H | 1.28595200 | 2.82980800 | -2.13056200 |
| C | 3.14195300 | 5.48476400 | -1.08949000 |
| H | 3.19346000 | 6.23403400 | 0.93105000 |
| H | 2.87488700 | 4.52535300 | -3.00064700 |
| H | 3.83447700 | 6.22945700 | -1.46902400 |
| C | 1.88737700 | -1.80807800 | 2.41504100 |
| H | 1.23451800 | -2.46898800 | 1.85440400 |
| C | 2.04920800 | -2.01426800 | 3.78819200 |
| H | 1.51341500 | -2.82177900 | 4.27739500 |
| C | 2.90354200 | -1.19636000 | 4.53139600 |
| H | 3.02380600 | -1.36800400 | 5.59666100 |
| C | 3.61727700 | -0.17184000 | 3.90520100 |
| H | 4.29643900 | 0.45146800 | 4.48018600 |

**Vibrational frequencies**

445.91*i*, 21.93, 25.39, 32.34, 39.6, 42.42, 46.3, 62.48, 78.52, 98.28, 114.67, 137.08, 168.23, 179.14, 195.72, 210.42, 233.52, 272.35, 276.58, 320.39, 327.45, 341.28, 380.67, 383.52, 404, 409.12, 409.82, 431.55, 459.95, 472.79, 498.29, 506.13, 522.26, 545.8, 583.66, 596.54, 606.82, 617.65, 621.24, 624.56, 669.38, 691.75, 707.81, 719.05, 735.62, 748.06, 763.64, 765.4, 775.49, 800.54, 809.91, 827.08, 837.53, 841.88, 855.22, 862.58, 878.92, 901.9, 909.69, 927.36, 944.6, 950.81, 954.65, 978.22, 978.53, 979.94, 989.38, 989.87, 993.49, 996.88, 998.93, 1004.01, 1006.5, 1011.53, 1013.76, 1032.34, 1042.82, 1047.02, 1047.53, 1060.21, 1082.69, 1094.65, 1106.78, 1110.11, 1135.62, 1165.42, 1173.49, 1177.46, 1179.16, 1190.94, 1191.97, 1196, 1196.38, 1218.44, 1226.41, 1226.82, 1244.33, 1270.05, 1278.91, 1285.86, 1293.32, 1312.22, 1320.77, 1322.02, 1337.15, 1343.64, 1355.13, 1358.18, 1360.39, 1362.43, 1369.66, 1382.31, 1466.74, 1474.04, 1480.71, 1482.35, 1484.49, 1490.48, 1493.2, 1500.23, 1503.34, 1509.81, 1524.92, 1525.53, 1596.67, 1619.41, 1620.94, 1623.55, 1636.99, 1641, 3025.92, 3032.39, 3035.29, 3045.03, 3068.71, 3070.85, 3072.33, 3096.6, 3103.39, 3122.44, 3127.57, 3145.26, 3152.66, 3155.42, 3157.27, 3160.11, 3164.17, 3165.83, 3171.13, 3173.41, 3176.34, 3180.12, 3181.59, 3187.48, 3189.69, 3190.63.

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## 19b'' TS2$_{cis}$

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.455049
Thermal correction to Energy= 0.477997
Thermal correction to Enthalpy= 0.478942
Thermal correction to Gibbs Free Energy= 0.399013
Sum of electronic and zero-point Energies= -1135.658130
Sum of electronic and thermal Energies=-1135.635181
Sum of electronic and thermal Enthalpies= -1135.634237
Sum of electronic and thermal Free Energies= -1135.714165

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.64436700 | -0.46684200 | -0.40485900 |
| C | 1.31073700 | -1.23615100 | -0.22736600 |
| H | 2.96608800 | -0.45178800 | -1.44733800 |
| H | 2.48639300 | 0.56473700 | -0.07616700 |
| C | 1.20966000 | -2.45556600 | -1.15337700 |
| H | 1.43339900 | -2.13116500 | -2.17533000 |
| H | 1.92936300 | -3.22783200 | -0.87407300 |
| C | -0.23374500 | -2.94770800 | -1.07020100 |
| H | -0.43815200 | -3.68688700 | -1.84989000 |
| H | -0.41577500 | -3.42993000 | -0.10571000 |
| C | -1.15156700 | -1.75930300 | -1.23396500 |
| H | -1.16804000 | -1.34265700 | -2.23577700 |
| O | -0.22601200 | 0.36289300 | 0.40653000 |
| N | 0.19149900 | -0.39696400 | -0.65318500 |
| C | -0.73912700 | 1.61844600 | -0.05798100 |
| H | -1.44583300 | 1.43949600 | -0.87109900 |
| H | -1.27748000 | 2.02946000 | 0.79767300 |
| C | -3.37198900 | -0.68300900 | -0.71074100 |
| C | -4.35497300 | -0.48255000 | 0.27736400 |
| C | -3.48624500 | 0.05712900 | -1.90450400 |
| C | -5.39035700 | 0.42216200 | 0.09081300 |
| H | -4.28807800 | -1.04345300 | 1.20413000 |
| C | -4.52217400 | 0.95975000 | -2.08820500 |
| H | -2.75667400 | -0.07642900 | -2.69508600 |
| C | -5.48004200 | 1.15151200 | -1.09245900 |
| H | -6.13092000 | 0.56071600 | 0.87050000 |
| H | -4.58712200 | 1.51754900 | -3.01573100 |
| H | -6.28638900 | 1.86010500 | -1.23976500 |
| C | -2.29520600 | -1.61860900 | -0.46248000 |
| H | -2.36220200 | -2.18460900 | 0.46269100 |
| C | 3.62919100 | -1.16554200 | 0.54849800 |
| H | 4.41182800 | -0.49650600 | 0.91169400 |
| H | 4.12171900 | -2.01245000 | 0.05784500 |
| C | 2.72205300 | -1.65336400 | 1.65425400 |
| C | 1.38977100 | -1.65104100 | 1.23685000 |
| C | 3.05861200 | -2.06472900 | 2.93804200 |
| C | 0.37802900 | -2.02618000 | 2.11166800 |
| C | 2.04620300 | -2.45974000 | 3.81033600 |
| H | 4.09406400 | -2.06540600 | 3.26299500 |
| C | 0.71410200 | -2.43309900 | 3.40174100 |
| H | -0.66016100 | -1.97201800 | 1.80683400 |
| H | 2.29451000 | -2.77287300 | 4.81816100 |
| H | -0.06764500 | -2.71896400 | 4.09635400 |
| C | 0.37871900 | 2.52756900 | -0.49456300 |
| C | 0.74410600 | 2.61024700 | -1.83732100 |
| C | 1.11515900 | 3.23688300 | 0.45504400 |
| C | 1.82719000 | 3.39247500 | -2.22798100 |
| H | 0.17989400 | 2.05013800 | -2.57559600 |
| C | 2.19796800 | 4.01957600 | 0.06893300 |
| H | 0.83996700 | 3.16773200 | 1.50293600 |
| C | 2.55582000 | 4.09745200 | -1.27470900 |

| | | | |
|---|---|---|---|
| H | 2.10356800 | 3.45004600 | -3.27473700 |
| H | 2.76206700 | 4.56853300 | 0.81431200 |
| H | 3.39955600 | 4.70741800 | -1.57681700 |

**Vibrational frequencies**

609.13*i*, 11.1, 19.22, 32.06, 36.33, 41.76, 53.19, 71.14, 85.16, 103.12, 126.59, 159.08, 171.58, 192.23, 218.6, 241.44, 280.59, 288.47, 296.91, 329.33, 351.24, 359.58, 372.33, 402.2, 412.02, 418.3, 439.44, 447.06, 486.61, 501.96, 515.42, 520.92, 539.59, 556.79, 593.32, 603.29, 616, 624.53, 630.09, 632.24, 667.14, 701.98, 716, 734.6, 751.62, 758.55, 780.92, 784.99, 802.9, 815.61, 843.74, 850.57, 862.57, 864.82, 871.82, 873.34, 895.27, 921.03, 933.54, 947.88, 959.54, 973.33, 980.13, 987.6, 1001.15, 1005.62, 1007.08, 1008.83, 1014.56, 1015.72, 1019.34, 1020.1, 1027.25, 1039.13, 1056.8, 1060.99, 1062.08, 1068.46, 1077.27, 1097.58, 1101.69, 1113.68, 1115.55, 1120.52, 1146.44, 1171.06, 1174.78, 1177.75, 1180.98, 1195.76, 1196.4, 1205.95, 1210.38, 1224.63, 1240.16, 1244.8, 1248.31, 1279.42, 1282.55, 1291.03, 1296.64, 1317.64, 1326.98, 1331.89, 1339.45, 1343.7, 1351.29, 1355.54, 1360.57, 1361.44, 1383.61, 1398.68, 1474.01, 1475.52, 1481.5, 1483.75, 1489.64, 1491.98, 1495.93, 1502.24, 1520.88, 1531.85, 1539.77, 1541.91, 1639.48, 1659.25, 1663.74, 1664.03, 1680.84, 1687.04, 3050.76, 3056.38, 3064.64, 3065.88, 3086.6, 3106.19, 3108.97, 3115.63, 3135.21, 3144, 3155.6, 3167.08, 3175.88, 3177.99, 3178.03, 3178.3, 3184.43, 3187.57, 3192.41, 3197.33, 3201.55, 3204.14, 3208.48, 3213.89, 3214.21, 3217.18.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.450589
Thermal correction to Energy= 0.473837
Thermal correction to Enthalpy= 0.474782
Thermal correction to Gibbs Free Energy= 0.394324
Sum of electronic and zero-point Energies= -1136.148342
Sum of electronic and thermal Energies= -1136.125094
Sum of electronic and thermal Enthalpies= -1136.124150
Sum of electronic and thermal Free Energies= -1136.204607

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.72166900 | -0.65181200 | -0.45234200 |
| C | 1.33814900 | -1.33163500 | -0.21590800 |
| H | 3.03562900 | -0.72920800 | -1.49460600 |
| H | 2.62901500 | 0.40765200 | -0.20470800 |
| C | 1.13795100 | -2.56666800 | -1.12003800 |
| H | 1.39731800 | -2.28740300 | -2.14704400 |
| H | 1.79188300 | -3.38969100 | -0.82432400 |
| C | -0.34249000 | -2.94545400 | -1.04194700 |
| H | -0.60305300 | -3.65818200 | -1.83182400 |
| H | -0.56190300 | -3.43393100 | -0.08886100 |
| C | -1.17924100 | -1.69031300 | -1.18648400 |
| H | -1.20818000 | -1.29804200 | -2.19747300 |
| O | -0.07629300 | 0.42096700 | 0.38927500 |
| N | 0.25630300 | -0.43467100 | -0.65379400 |
| C | -0.58128900 | 1.68151100 | -0.11211000 |
| H | -1.26007100 | 1.48808500 | -0.94396400 |
| H | -1.15876200 | 2.08293000 | 0.72294500 |
| C | -3.45269200 | -0.65518200 | -0.70342600 |
| C | -4.47783800 | -0.50232000 | 0.26160400 |
| C | -3.60214100 | 0.05141700 | -1.92182200 |
| C | -5.58221300 | 0.30500100 | 0.02535900 |
| H | -4.39008700 | -1.03181500 | 1.20504500 |
| C | -4.70889000 | 0.85667100 | -2.15339200 |
| H | -2.84947000 | -0.04276700 | -2.69589700 |
| C | -5.70724500 | 0.99273800 | -1.18413700 |
| H | -6.35018300 | 0.40091100 | 0.78557300 |
| H | -4.79881300 | 1.38246500 | -3.09815000 |
| H | -6.56979200 | 1.62216700 | -1.37135500 |
| C | -2.33666900 | -1.51984900 | -0.41463700 |

| | | | |
|---|---|---|---|
| H | -2.38846000 | -2.04871600 | 0.53358100 |
| C | 3.68763700 | -1.33002100 | 0.54024400 |
| H | 4.48915000 | -0.66224300 | 0.86777900 |
| H | 4.16748300 | -2.20831000 | 0.09102900 |
| C | 2.77331000 | -1.74552000 | 1.67043800 |
| C | 1.43259100 | -1.71472700 | 1.26677900 |
| C | 3.11712200 | -2.12878500 | 2.96455600 |
| C | 0.42671700 | -2.04710800 | 2.17155900 |
| C | 2.10818600 | -2.47341900 | 3.86537600 |
| H | 4.15732700 | -2.15022100 | 3.27454400 |
| C | 0.77005200 | -2.42692400 | 3.47084600 |
| H | -0.61596600 | -1.98941300 | 1.88772400 |
| H | 2.36346800 | -2.76531900 | 4.87846000 |
| H | -0.01066700 | -2.67743600 | 4.18120100 |
| C | 0.51779000 | 2.63362500 | -0.51363100 |
| C | 0.87620700 | 2.79305800 | -1.85563300 |
| C | 1.21487100 | 3.35824400 | 0.46078400 |
| C | 1.90975600 | 3.65612600 | -2.21900500 |
| H | 0.34242300 | 2.23716200 | -2.61882400 |
| C | 2.24894900 | 4.21982800 | 0.10209000 |
| H | 0.94490900 | 3.24507300 | 1.50604000 |
| C | 2.59920500 | 4.37014400 | -1.24031600 |
| H | 2.17592800 | 3.77056800 | -3.26427100 |
| H | 2.77881600 | 4.77660700 | 0.86740500 |
| H | 3.40228900 | 5.04281500 | -1.52112900 |

**Vibrational frequencies**

495.87*i*, 16.67, 19.86, 27.67, 29.58, 39.35, 64.6, 72.33, 76.5, 103.79, 118.83, 151.88, 167.85, 184.18, 204.98, 231.11, 267.99, 283.87, 291.46, 319.19, 344.81, 353.92, 374.29, 397.83, 411.97, 412.47, 436.03, 446.86, 480.39, 502.64, 511.56, 519.02, 538.97, 550.22, 590.79, 601.26, 613.01, 619.88, 630.3, 634.66, 663.11, 697.19, 709.18, 722.77, 742.64, 752.43, 766.64, 773.37, 795.55, 806.57, 830.87, 840.07, 846.88, 852.28, 856.62, 859.42, 879.54, 911.04, 918.04, 926.34, 942.43, 957.5, 965, 974.81, 977.16, 987.24, 989.56, 995.02, 998.76, 999.87, 1002.78, 1007.2, 1015.3, 1018.25, 1032.53, 1043.79, 1048.06, 1048.57, 1056.31, 1062.46, 1093.61, 1101.28, 1101.66, 1108.08, 1127.42, 1164.18, 1175.86, 1176.81, 1176.94, 1188.14, 1195.7, 1196.27, 1200.35, 1213.82, 1223.66, 1226.25, 1236.26, 1269.62, 1274.63, 1284.92, 1290.24, 1311.77, 1321.92, 1327.73, 1335, 1343.03, 1350.08, 1352.25, 1355.87, 1357.76, 1378.59, 1383.41, 1463.99, 1476.28, 1477.94, 1479.34, 1481.59, 1484.2, 1488.46, 1492, 1502.77, 1507.48, 1517.68, 1524.58, 1594.25, 1617.08, 1619.88, 1623.52, 1641.12, 1642.44, 3011.7, 3028.1, 3033.25, 3055.77, 3065.9, 3066.17, 3073.69, 3093.77, 3106.67, 3117.37, 3139.46, 3154.18, 3157.14, 3158.73, 3159.18, 3164.48, 3164.65, 3166.44, 3173.23, 3174.36, 3180.2, 3182.18, 3182.39, 3189.78, 3191.09, 3202.33.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.439280
Thermal correction to Energy= 0.463184
Thermal correction to Enthalpy= 0.464128
Thermal correction to Gibbs Free Energy= 0.383048
Sum of electronic and zero-point Energies= -1135.996456
Sum of electronic and thermal Energies= -1135.972552
Sum of electronic and thermal Enthalpies= -1135.971608
Sum of electronic and thermal Free Energies= -1136.052688

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.75194600 | -0.65955300 | -0.43240000 |
| C | 1.35982400 | -1.33177600 | -0.20226600 |
| H | 3.06150000 | -0.72094200 | -1.48390500 |
| H | 2.66634800 | 0.40258400 | -0.16328100 |
| C | 1.14550400 | -2.55659200 | -1.12161800 |
| H | 1.39982200 | -2.26280600 | -2.15321600 |

| | | | |
|---|---|---|---|
| H | 1.80317500 | -3.38989100 | -0.83865200 |
| C | -0.33829100 | -2.92670500 | -1.03171700 |
| H | -0.61037500 | -3.64566600 | -1.82156100 |
| H | -0.55393600 | -3.41482600 | -0.06934000 |
| C | -1.17145500 | -1.66780500 | -1.17340400 |
| H | -1.19215000 | -1.26444100 | -2.18877400 |
| O | -0.02918500 | 0.42737700 | 0.43485100 |
| N | 0.28397300 | -0.41829200 | -0.62897500 |
| C | -0.58092300 | 1.68715000 | -0.05808300 |
| H | -1.28675700 | 1.47068600 | -0.87089800 |
| H | -1.13988100 | 2.07856500 | 0.80261100 |
| C | -3.45467600 | -0.63818200 | -0.70695200 |
| C | -4.49765200 | -0.48600800 | 0.24941300 |
| C | -3.59341800 | 0.07208900 | -1.93270300 |
| C | -5.60504500 | 0.32108900 | -0.00168900 |
| H | -4.41846800 | -1.01873800 | 1.19994200 |
| C | -4.70352600 | 0.87710500 | -2.17857100 |
| H | -2.82689000 | -0.02274700 | -2.70343600 |
| C | -5.71828100 | 1.01180000 | -1.21773400 |
| H | -6.38716900 | 0.41556100 | 0.75409500 |
| H | -4.78412200 | 1.40530400 | -3.13073400 |
| H | -6.58570700 | 1.64258800 | -1.41664800 |
| C | -2.33810400 | -1.49812700 | -0.40636500 |
| H | -2.39599500 | -2.03183200 | 0.54769100 |
| C | 3.71468800 | -1.36627200 | 0.54615900 |
| H | 4.53229600 | -0.71109900 | 0.88145500 |
| H | 4.18442000 | -2.24882600 | 0.07831000 |
| C | 2.80105800 | -1.78945400 | 1.67566400 |
| C | 1.45308900 | -1.73620900 | 1.27532200 |
| C | 3.14371000 | -2.20139500 | 2.96725400 |
| C | 0.43988300 | -2.07032700 | 2.17964500 |
| C | 2.12732000 | -2.54931100 | 3.86743700 |
| H | 4.19056400 | -2.24203700 | 3.27680300 |
| C | 0.78342500 | -2.47749000 | 3.47666400 |
| H | -0.60904700 | -1.99113700 | 1.89549500 |
| H | 2.38254200 | -2.86290700 | 4.88133000 |
| H | -0.00322000 | -2.73003800 | 4.19014400 |
| C | 0.49350600 | 2.65072500 | -0.49607300 |
| C | 0.86776000 | 2.74668400 | -1.84672200 |
| C | 1.16359700 | 3.44484700 | 0.45103200 |
| C | 1.89054500 | 3.61599400 | -2.24349300 |
| H | 0.35230500 | 2.13457500 | -2.58894600 |
| C | 2.18596600 | 4.31414100 | 0.05767500 |
| H | 0.88038400 | 3.37885200 | 1.50400700 |
| C | 2.55216200 | 4.40063900 | -1.29166200 |
| H | 2.16975900 | 3.68267600 | -3.29655700 |
| H | 2.69524300 | 4.92794700 | 0.80275100 |
| H | 3.34765200 | 5.08111300 | -1.60019100 |

**Vibrational frequencies**

332.57*i*, 21.28, 24.98, 28.24, 34.38, 40.34, 61.67, 68.56, 73.34, 100.86, 114.35, 146.63, 164.17, 179.4, 197.28, 223.48, 259.85, 279.21, 282.89, 313.29, 331.15, 343.46, 363.9, 383.15, 396.66, 396.9, 421.06, 432.77, 465.41, 486.38, 495.47, 503.47, 519.01, 536.49, 573.34, 581.45, 592.99, 599.86, 610.64, 615.74, 641.83, 673.51, 686.08, 704.58, 716.28, 727.37, 742, 747.07, 772.56, 780.3, 809.11, 815.13,

820.94, 826.36, 827.39, 832.96, 846.16, 879.38, 886.02, 891.27, 911.46, 918.7, 923.42, 943, 948.15, 949.65, 953.4, 958.46, 958.94, 965.95, 966.94, 974.84, 983.27, 990.33, 1002.88, 1017.67, 1024.15, 1025.39, 1025.74, 1030.79, 1061.41, 1065.24, 1073.05, 1081.13, 1095.5, 1132.77, 1145.53, 1145.83, 1149, 1152.45, 1162.31, 1164.27, 1164.93, 1183.32, 1194.24, 1197.63, 1202.58, 1229.48, 1240.51, 1247.78, 1249.57, 1276.26, 1279.74, 1286.33, 1297.97, 1304.62, 1313.72, 1327.89, 1331.77, 1346, 1347.76, 1349.5, 1424.47, 1424.92, 1426.18, 1427.03, 1436.31, 1439.39, 1440.72, 1442.88, 1458.63, 1464.32, 1480.54, 1484.34, 1549.58, 1578.06, 1578.27, 1581.39, 1597.09, 1598.47, 2956.61, 2970.49, 2974.04, 2999.05, 3003.37, 3011.8, 3015.27, 3039.6, 3053.14, 3059.44, 3070.17, 3084.43, 3096.9, 3097.8, 3099.43, 3101.68, 3104.87, 3106.74, 3112.77, 3113.29, 3117.93, 3120.53, 3122.23, 3130.01, 3131.12, 3133.56.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.449580
Thermal correction to Energy= 0.473032
Thermal correction to Enthalpy= 0.473976
Thermal correction to Gibbs Free Energy= 0.393530
Sum of electronic and zero-point Energies= -1136.229565
Sum of electronic and thermal Energies= -1136.206114
Sum of electronic and thermal Enthalpies= -1136.205170
Sum of electronic and thermal Free Energies= -1136.285616

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.73098300 | -0.62000700 | -0.41690600 |
| C | 1.35307100 | -1.31227200 | -0.20435000 |
| H | 3.04308200 | -0.65531500 | -1.46307300 |
| H | 2.63229100 | 0.42809800 | -0.12156500 |
| C | 1.16053800 | -2.52959600 | -1.13078200 |
| H | 1.40354300 | -2.22427900 | -2.15550000 |
| H | 1.82664800 | -3.35110500 | -0.85494300 |
| C | -0.31572400 | -2.92034000 | -1.03678300 |
| H | -0.57971300 | -3.64026000 | -1.82011000 |
| H | -0.52072600 | -3.39995400 | -0.07457700 |
| C | -1.16087700 | -1.67195600 | -1.18175200 |
| H | -1.18267600 | -1.26765500 | -2.18952600 |
| O | -0.06183600 | 0.41402600 | 0.43924200 |
| N | 0.27072500 | -0.41159800 | -0.63129700 |
| C | -0.60222700 | 1.67222400 | -0.04701200 |
| H | -1.30720700 | 1.46207400 | -0.85367400 |
| H | -1.14791000 | 2.06809700 | 0.81191700 |
| C | -3.43338600 | -0.63926700 | -0.70522500 |
| C | -4.46387000 | -0.48131200 | 0.25429200 |
| C | -3.57090200 | 0.06768300 | -1.92590800 |
| C | -5.56280300 | 0.33389400 | 0.01100900 |
| H | -4.38368200 | -1.01245800 | 1.19878900 |
| C | -4.67168700 | 0.88114300 | -2.16445300 |
| H | -2.81261300 | -0.03308900 | -2.69569400 |
| C | -5.67584400 | 1.02385500 | -1.20009100 |
| H | -6.33548500 | 0.43453800 | 0.76709100 |
| H | -4.75256700 | 1.40766800 | -3.11062800 |
| H | -6.53386400 | 1.65945800 | -1.39241000 |
| C | -2.32075600 | -1.50795000 | -0.41104100 |
| H | -2.37632600 | -2.04015900 | 0.53680400 |
| C | 3.69534900 | -1.33893200 | 0.54716500 |
| H | 4.50923600 | -0.69155800 | 0.88704800 |
| H | 4.15557500 | -2.21329100 | 0.06869700 |
| C | 2.78029500 | -1.77098300 | 1.67071300 |
| C | 1.43906100 | -1.72111100 | 1.26703000 |
| C | 3.11844800 | -2.18413300 | 2.95877600 |
| C | 0.42502800 | -2.05979000 | 2.16227400 |

| | | | |
|---|---|---|---|
| C | 2.10206600 | -2.53605800 | 3.85056800 |
| H | 4.15815300 | -2.22214300 | 3.27180800 |
| C | 0.76340500 | -2.46769000 | 3.45551100 |
| H | -0.61668200 | -1.98282600 | 1.87355900 |
| H | 2.35217000 | -2.84966000 | 4.85942800 |
| H | -0.02086300 | -2.72299100 | 4.16162200 |
| C | 0.48002700 | 2.62267800 | -0.49158800 |
| C | 0.84066100 | 2.71824200 | -1.84083900 |
| C | 1.16594100 | 3.40233300 | 0.44903600 |
| C | 1.86726800 | 3.57375900 | -2.24343100 |
| H | 0.31394600 | 2.11784200 | -2.57607900 |
| C | 2.19204200 | 4.25811200 | 0.05023700 |
| H | 0.89328200 | 3.33637700 | 1.49865400 |
| C | 2.54541500 | 4.34451000 | -1.29814100 |
| H | 2.13636100 | 3.63982300 | -3.29306400 |
| H | 2.71313900 | 4.85960200 | 0.78852100 |
| H | 3.34217000 | 5.01236300 | -1.61016900 |

**Vibrational frequencies**

432.82*i*, 19.73, 23.04, 28.96, 31.7, 42.91, 63.14, 69.54, 76.1, 101.33, 116.09, 149.37, 165.11, 181.82, 203.9, 226, 264.09, 281.44, 286.16, 317.13, 332.38, 348.25, 365.43, 387.97, 405.44, 407.09, 430.79, 438.05, 473.85, 495.2, 505.28, 511.61, 525.29, 542.47, 583.01, 590.28, 602.7, 610.39, 619.5, 624.92, 651.94, 693.11, 705.79, 717.05, 736.02, 749.08, 763.59, 769.61, 789.14, 799.93, 826.11, 835.02, 844.12, 850.74, 851.34, 858.79, 878.29, 905.03, 912.82, 922.53, 936.97, 953.55, 956.93, 968.26, 972.19, 984.3, 986.27, 990.73, 994.3, 994.85, 997.8, 1002.23, 1010.06, 1012.83, 1026.9, 1040.47, 1045.66, 1048.16, 1051.7, 1059.47, 1088.61, 1096, 1097.89, 1107.65, 1124.3, 1162.17, 1174.86, 1175.16, 1178.6, 1183.53, 1193.06, 1196.77, 1196.9, 1213.02, 1221.55, 1225.5, 1233.44, 1265.99, 1271.95, 1283.65, 1288.45, 1312.56, 1318.88, 1326.65, 1335.53, 1346.47, 1355.4, 1358.89, 1359.75, 1362.95, 1375.26, 1376.95, 1464.13, 1479.29, 1481.43, 1481.81, 1483.89, 1485.32, 1492.27, 1496.34, 1502.27, 1507.27, 1519.83, 1524.95, 1594.17, 1616.89, 1619.13, 1623.68, 1638.78, 1641.13, 3012.41, 3025.26, 3030.13, 3052.48, 3063.81, 3067.53, 3071.72, 3092.98, 3106.44, 3120.57, 3133.44, 3149.26, 3155.6, 3156.05, 3157.23, 3161.09, 3162.58, 3165.06, 3171.43, 3172.14, 3178.52, 3179.25, 3181.36, 3189.21, 3190.7, 3194.67.

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## 21b *trans*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.457161
Thermal correction to Energy= 0.480207
Thermal correction to Enthalpy= 0.481151
Thermal correction to Gibbs Free Energy= 0.401902

Sum of electronic and zero-point Energies= -1135.685869
Sum of electronic and thermal Energies= -1135.662823
Sum of electronic and thermal Enthalpies= -1135.661879
Sum of electronic and thermal Free Energies= -1135.741128

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.29143500 | -1.41845400 | 2.17784300 |
| C | -0.85716600 | -1.81721300 | 0.75630600 |
| H | -1.59919300 | -2.32389800 | 2.70982600 |
| H | -0.46237900 | -0.96548700 | 2.72491400 |
| C | -0.08989800 | -3.13525000 | 0.62524000 |
| H | 0.53426000 | -3.27251500 | 1.51206300 |
| H | -0.77314000 | -3.98294400 | 0.56051600 |
| C | 0.79562700 | -2.97049400 | -0.63392400 |
| H | 1.82922300 | -3.25056500 | -0.43000900 |
| H | 0.44937100 | -3.58401500 | -1.46634100 |
| C | 0.69210800 | -1.46745700 | -1.00514800 |
| O | -0.39451700 | 0.38235700 | -0.04266800 |

| | | | |
|---|---|---|---|
| N | 0.17045800 | -0.87853300 | 0.24170100 |
| C | 0.28930900 | 1.38694900 | 0.70187400 |
| H | 0.13187300 | 1.23102200 | 1.77533800 |
| H | 1.36382400 | 1.31331800 | 0.49984100 |
| C | -2.51349200 | -0.49659700 | 2.00022500 |
| H | -2.21247200 | 0.55138900 | 1.90432100 |
| H | -3.22108400 | -0.56741700 | 2.82860700 |
| C | -3.10114200 | -0.98155800 | 0.69556100 |
| C | -2.17388700 | -1.75350700 | -0.00597100 |
| C | -4.37239100 | -0.76622300 | 0.17894000 |
| C | -2.51562900 | -2.33579500 | -1.22114700 |
| C | -4.71229500 | -1.34001200 | -1.04512800 |
| H | -5.09582800 | -0.16761400 | 0.72265300 |
| C | -3.79326300 | -2.12425600 | -1.73845700 |
| H | -1.81171600 | -2.96246100 | -1.75984100 |
| H | -5.70347600 | -1.18576300 | -1.45665900 |
| H | -4.07542400 | -2.57782900 | -2.68168000 |
| C | -0.24454600 | 2.72699100 | 0.27478600 |
| C | -0.69873000 | 3.64809100 | 1.21532500 |
| C | -0.26896300 | 3.06807500 | -1.07918800 |
| C | -1.16251300 | 4.89907200 | 0.81406200 |
| H | -0.68945700 | 3.38673000 | 2.26891100 |
| C | -0.73939500 | 4.31123600 | -1.48235800 |
| H | 0.07891100 | 2.34808900 | -1.81251900 |
| C | -1.18484200 | 5.23152700 | -0.53516400 |
| H | -1.51287700 | 5.60880100 | 1.55486300 |
| H | -0.75748800 | 4.56616800 | -2.53600700 |
| H | -1.54903100 | 6.20237800 | -0.85102100 |
| C | 1.95794100 | -0.82090700 | -1.47064700 |
| H | 1.98533100 | -0.48290700 | -2.50094200 |
| C | 3.14790400 | -0.65443800 | -0.70913300 |
| C | 3.27353000 | -1.05486000 | 0.64567200 |
| C | 4.27803500 | -0.05360700 | -1.31882400 |
| C | 4.46157000 | -0.86528600 | 1.33247000 |
| H | 2.42135300 | -1.49088100 | 1.15073700 |
| C | 5.45751200 | 0.13434200 | -0.62201900 |
| H | 4.20425600 | 0.26349000 | -2.35407600 |
| C | 5.56040500 | -0.27177200 | 0.70995700 |
| H | 4.53410700 | -1.17828500 | 2.36822700 |
| H | 6.30458100 | 0.59938800 | -1.11352300 |
| H | 6.48453400 | -0.12349900 | 1.25586100 |
| H | -0.06124900 | -1.33541100 | -1.79154600 |

**Vibrational frequencies**

18.36, 26.19, 31.07, 32.83, 44.26, 69.49, 84.73, 92.77, 101.89, 117.38, 153.64, 180.14, 192.38, 216.88, 220.73, 243.95, 267.03, 269.05, 301.02, 314.37, 353.69, 408.8, 415.25, 415.93, 429.66, 435.85, 460.7, 482.26, 487.4, 497.88, 527.81, 554.83, 568.02, 603.07, 616.41, 624.51, 631.23, 649.86, 660.96, 679.6, 690.98, 698.4, 717.72, 743.01, 746.43, 769.68, 773.66, 777.87, 787.13, 814.27, 830.74, 856.88, 857.71, 873.54, 879.7, 900.55, 926.75, 928.97, 944.93, 947.41, 974.99, 986.64, 990.7, 999.47, 1005.92, 1012.07, 1015.33, 1015.37, 1015.87, 1021.1, 1026.97, 1029.19, 1040.45, 1057.27, 1058.29, 1059.82, 1079.27, 1088.83, 1103.3, 1112.27, 1117.32, 1122.7, 1141.74, 1156.82, 1166.64, 1170.97, 1173.73, 1175.45, 1183.15, 1192.66, 1197.5, 1200.36, 1210.89, 1228.81, 1244.14, 1249.99, 1258, 1261.22, 1284.41, 1302.44, 1310.49, 1319.15, 1325.87, 1327.97, 1334.03, 1342.73, 1349.83, 1353.87, 1360.07, 1364.1, 1414.04, 1421.58, 1443.69, 1463.06, 1478.62, 1481.47, 1495.41, 1496.86, 1500.02, 1505.69, 1513.71, 1516.35, 1518.84, 1541.74, 1618.32, 1640.39, 1662.29, 1663.98, 1680.45, 1685.42, 3041.99, 3052.8, 3053.19, 3059.14, 3061.87, 3086.69, 3090.92, 3108.35, 3119.83, 3123.44,

3140.08, 3171.84, 3177.73, 3177.83, 3183.28, 3185.23, 3187.47, 3189.68, 3196.36, 3197.09, 3197.44, 3205.79, 3206.22, 3210.51, 3215.22, 3220.13.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.452658
Thermal correction to Energy= 0.476007
Thermal correction to Enthalpy= 0.476952
Thermal correction to Gibbs Free Energy= 0.397356
Sum of electronic and zero-point Energies= -1136.166581
Sum of electronic and thermal Energies= -1136.143232
Sum of electronic and thermal Enthalpies= -1136.142288
Sum of electronic and thermal Free Energies= -1136.221884

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.30681100 | -1.49508800 | 2.19496900 |
| C | -0.88317200 | -1.82622400 | 0.74176100 |
| H | -1.54422800 | -2.43426800 | 2.70476500 |
| H | -0.49207800 | -1.01745000 | 2.74205800 |
| C | -0.12761500 | -3.15769300 | 0.57623000 |
| H | 0.46481800 | -3.34647500 | 1.47490200 |
| H | -0.82267100 | -3.99079300 | 0.46187800 |
| C | 0.80300800 | -2.97413200 | -0.64829000 |
| H | 1.82207900 | -3.28542100 | -0.41919400 |
| H | 0.47417700 | -3.55745300 | -1.50996200 |
| C | 0.74272500 | -1.45437500 | -0.98668900 |
| O | -0.40837400 | 0.40267000 | -0.04653300 |
| N | 0.16875400 | -0.87558800 | 0.25596300 |
| C | 0.29446200 | 1.44280800 | 0.65382200 |
| H | 0.17520600 | 1.31589200 | 1.73496300 |
| H | 1.36221900 | 1.37391400 | 0.42342300 |
| C | -2.58692400 | -0.63795300 | 2.09695600 |
| H | -2.35540700 | 0.43231100 | 2.09221600 |
| H | -3.27529500 | -0.81557000 | 2.92762000 |
| C | -3.16666300 | -1.05134300 | 0.76430600 |
| C | -2.21764900 | -1.73477400 | -0.00476500 |
| C | -4.45385300 | -0.83820100 | 0.27806200 |
| C | -2.56411800 | -2.22525400 | -1.26399600 |
| C | -4.79435000 | -1.31954900 | -0.98705300 |
| H | -5.18907900 | -0.30920000 | 0.87643700 |
| C | -3.85549500 | -2.01352800 | -1.75200500 |
| H | -1.85408500 | -2.78061200 | -1.86660800 |
| H | -5.79559900 | -1.16267900 | -1.37377700 |
| H | -4.13169300 | -2.39549800 | -2.72888400 |
| C | -0.25994400 | 2.77427300 | 0.21305300 |
| C | -0.73164200 | 3.69439500 | 1.15277700 |
| C | -0.28419400 | 3.12298400 | -1.14300200 |
| C | -1.21004400 | 4.94244700 | 0.75160400 |
| H | -0.72349800 | 3.43518800 | 2.20674700 |
| C | -0.77050800 | 4.36322800 | -1.54686000 |
| H | 0.07414000 | 2.41532000 | -1.88201300 |
| C | -1.23244400 | 5.27880500 | -0.59970300 |
| H | -1.57005200 | 5.64664700 | 1.49386700 |
| H | -0.78713600 | 4.61856800 | -2.60098100 |
| H | -1.60799000 | 6.24613900 | -0.91508600 |
| C | 2.04025600 | -0.83728000 | -1.42096900 |
| H | 2.08468100 | -0.52362000 | -2.45965200 |

| | | | |
|---|---|---|---|
| C | 3.23087500 | -0.67434400 | -0.66854100 |
| C | 3.36071700 | -1.03020400 | 0.70528000 |
| C | 4.38036600 | -0.11663700 | -1.30207300 |
| C | 4.55800700 | -0.84669300 | 1.37975300 |
| H | 2.50222500 | -1.42444000 | 1.23107700 |
| C | 5.56872400 | 0.06589500 | -0.61619200 |
| H | 4.31131700 | 0.16823100 | -2.34711600 |
| C | 5.67082500 | -0.29934500 | 0.73178800 |
| H | 4.62874300 | -1.12558500 | 2.42603600 |
| H | 6.42450100 | 0.49415100 | -1.12712000 |
| H | 6.60155900 | -0.15591900 | 1.26885400 |
| H | 0.02533100 | -1.29897700 | -1.80140400 |

**Vibrational frequencies**

24.09, 30.27, 32.6, 35.6, 45, 62.74, 83.7, 91.58, 97.2, 102.26, 135.32, 169.13, 185.44, 207.98, 221.79, 239.11, 261.38, 263.51, 296.12, 311.89, 349.08, 402.08, 410.35, 415.84, 423.54, 436.17, 462.72, 480.48, 483.97, 496.4, 524.96, 549.1, 562.87, 597.95, 614.47, 624.77, 634.32, 642.78, 664.25, 678.32, 682.38, 693.9, 710.5, 735.64, 741.17, 754.74, 761.43, 772.77, 778.52, 811.73, 821.13, 838.99, 846.35, 859.59, 864.82, 882.03, 907.73, 909.42, 922.35, 927.26, 953.76, 969.76, 974.06, 985.79, 990.06, 990.35, 993.44, 995.91, 997.23, 1007.48, 1010.73, 1013.37, 1018.05, 1033.45, 1038.62, 1048.06, 1048.91, 1052.39, 1077.57, 1083.29, 1098.01, 1102.67, 1108.4, 1129.29, 1156.72, 1166.02, 1174.23, 1177.38, 1179.06, 1187.1, 1188.66, 1197.92, 1198.16, 1222.15, 1228.13, 1241.18, 1245.52, 1251.98, 1280.83, 1293.44, 1306.12, 1309.74, 1323.88, 1327.6, 1335.02, 1340.91, 1343.13, 1349.86, 1353.31, 1354.48, 1399, 1404.16, 1439.53, 1472.83, 1481.35, 1481.75, 1483.19, 1488.3, 1488.92, 1500.1, 1504.88, 1507.72, 1512.64, 1527.02, 1576.98, 1598.8, 1621.02, 1624.51, 1640.28, 1645.54, 3004.54, 3022, 3035.74, 3037.51, 3051.43, 3060.08, 3068.05, 3069.5, 3093.91, 3095.33, 3113.28, 3154.22, 3156.46, 3158.79, 3160.04, 3165.49, 3165.74, 3165.76, 3174.56, 3174.64, 3175.99, 3183.12, 3185.57, 3190.52, 3190.81, 3215.56.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.440910
Thermal correction to Energy= 0.465035
Thermal correction to Enthalpy= 0.465979
Thermal correction to Gibbs Free Energy= 0.384683

Sum of electronic and zero-point Energies= -1136.008970
Sum of electronic and thermal Energies= -1135.984845
Sum of electronic and thermal Enthalpies= -1135.983901
Sum of electronic and thermal Free Energies= -1136.065197

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.32224700 | -1.50565000 | 2.20880400 |
| C | -0.88761300 | -1.84054700 | 0.75811900 |
| H | -1.57053900 | -2.44943700 | 2.71940100 |
| H | -0.50294500 | -1.03097800 | 2.76514900 |
| C | -0.12201600 | -3.16813200 | 0.59263100 |
| H | 0.47550500 | -3.35415700 | 1.49661800 |
| H | -0.81825800 | -4.00917900 | 0.47895700 |
| C | 0.80509300 | -2.97903900 | -0.63633100 |
| H | 1.83462800 | -3.28150800 | -0.40958000 |
| H | 0.47761900 | -3.56866000 | -1.50258300 |
| C | 0.73227200 | -1.45719300 | -0.97884900 |
| O | -0.42718600 | 0.40474400 | -0.02280900 |
| N | 0.17065700 | -0.88080400 | 0.28033600 |
| C | 0.31184600 | 1.44750400 | 0.65404400 |
| H | 0.22527100 | 1.32777800 | 1.74689700 |
| H | 1.37866300 | 1.36650700 | 0.38848000 |
| C | -2.59684600 | -0.63853200 | 2.09738200 |
| H | -2.35507700 | 0.43635600 | 2.09038600 |
| H | -3.29875700 | -0.80693800 | 2.92733400 |
| C | -3.16951800 | -1.04999000 | 0.75967900 |

| | | | |
|---|---|---|---|
| C | -2.21499100 | -1.75019400 | -0.00040200 |
| C | -4.45431700 | -0.82654000 | 0.25615800 |
| C | -2.55440300 | -2.24852600 | -1.26485000 |
| C | -4.78694400 | -1.31484200 | -1.01472000 |
| H | -5.19593200 | -0.28437500 | 0.84721800 |
| C | -3.84413500 | -2.02646900 | -1.76857700 |
| H | -1.84015900 | -2.82247700 | -1.85792400 |
| H | -5.78896600 | -1.15026300 | -1.41514000 |
| H | -4.11705200 | -2.41610800 | -2.75089800 |
| C | -0.24673600 | 2.77970300 | 0.21764500 |
| C | -0.72117200 | 3.70084300 | 1.16416100 |
| C | -0.27756500 | 3.13082700 | -1.14369000 |
| C | -1.20635800 | 4.95234500 | 0.76430600 |
| H | -0.70773800 | 3.43744500 | 2.22422500 |
| C | -0.77223400 | 4.37444400 | -1.54604600 |
| H | 0.08417800 | 2.42032400 | -1.88853400 |
| C | -1.23505500 | 5.29096700 | -0.59237000 |
| H | -1.56782500 | 5.65951400 | 1.51296500 |
| H | -0.79366600 | 4.63256900 | -2.60638400 |
| H | -1.61709200 | 6.26351800 | -0.90731600 |
| C | 2.02313000 | -0.83589500 | -1.42415400 |
| H | 2.06068200 | -0.51757600 | -2.46918700 |
| C | 3.22060100 | -0.67297100 | -0.67642900 |
| C | 3.35470300 | -1.02920500 | 0.70288900 |
| C | 4.37218900 | -0.11331200 | -1.31657300 |
| C | 4.55841300 | -0.84408100 | 1.37619700 |
| H | 2.48856000 | -1.42175900 | 1.23305000 |
| C | 5.56702500 | 0.07059500 | -0.63168000 |
| H | 4.29828200 | 0.17201000 | -2.36848900 |
| C | 5.67360300 | -0.29491900 | 0.72175200 |
| H | 4.63272400 | -1.12300300 | 2.42932500 |
| H | 6.42659200 | 0.50143100 | -1.14852700 |
| H | 6.61172800 | -0.14971100 | 1.25919600 |
| H | -0.00351300 | -1.30475200 | -1.78855800 |

**Vibrational frequencies**

21.55, 28.44, 30.16, 36.19, 43.93, 59.74, 74.83, 88.23, 90.31, 99.72, 129.41, 161.68, 178.23, 199.38, 212.3, 229.83, 252.26, 254.45, 285.27, 301.39, 336.28, 389.64, 395.01, 398.99, 409.34, 419.6, 448.38, 462.43, 466.6, 480.14, 507.73, 531.76, 545.36, 580.12, 594.12, 604.73, 614.16, 620.33, 644.31, 657.63, 661.21, 672.4, 687.29, 715.14, 716.04, 728.08, 736.58, 746.8, 753.17, 788.63, 799.45, 809.34, 823.46, 829.34, 837.93, 849.91, 873.6, 878.79, 887.9, 892.22, 915.38, 929.84, 944.97, 947.98, 951.2, 955.63, 957.68, 961.2, 967.87, 969.07, 971.41, 986.55, 990.39, 997, 1003.11, 1015.41, 1023.99, 1024.41, 1043.02, 1046.34, 1065.9, 1073.4, 1080.62, 1094.13, 1124.5, 1130.43, 1144.73, 1146.38, 1146.99, 1150.88, 1157.13, 1160.41, 1165.73, 1187.87, 1191.04, 1204.31, 1205.69, 1221.82, 1235.61, 1251.89, 1259.96, 1267.31, 1284.05, 1293.11, 1296.32, 1298.66, 1305.28, 1336.86, 1337.8, 1349.26, 1351.86, 1356.71, 1400.03, 1422.36, 1435.54, 1437.58, 1438.76, 1440.35, 1442.2, 1453.72, 1458.78, 1459.76, 1464.04, 1482.72, 1535, 1563.63, 1578.67, 1582.22, 1595.35, 1601.58, 2932.06, 2950.73, 2979.91, 2981.56, 2989.33, 2994.89, 3011.68, 3016.07, 3039.29, 3040.45, 3059.03, 3093.73, 3096.14, 3098.59, 3098.65, 3103.46, 3105.39, 3105.98, 3112.58, 3114.81, 3115.65, 3123.16, 3124.61, 3130.86, 3131.22, 3144.6.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.451352
Thermal correction to Energy= 0.474992
Thermal correction to Enthalpy= 0.475937
Thermal correction to Gibbs Free Energy= 0.395462
Sum of electronic and zero-point Energies= -1136.246484
Sum of electronic and thermal Energies= -1136.222843
Sum of electronic and thermal Enthalpies= -1136.221899
Sum of electronic and thermal Free Energies= -1136.302373

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.33320000 | -1.48600400 | 2.20273400 |
| C | -0.88710600 | -1.83218600 | 0.76336200 |
| H | -1.59835400 | -2.41930900 | 2.71181900 |
| H | -0.52138500 | -1.01591400 | 2.76283900 |
| C | -0.11552000 | -3.15381700 | 0.61235300 |
| H | 0.48473800 | -3.32188000 | 1.51108300 |
| H | -0.80098700 | -3.99733300 | 0.50714300 |
| C | 0.80511200 | -2.96701500 | -0.62007100 |
| H | 1.83257300 | -3.25577100 | -0.39351400 |
| H | 0.47887100 | -3.56327500 | -1.47500700 |
| C | 0.71604000 | -1.45286200 | -0.97100500 |
| O | -0.42487300 | 0.40231800 | -0.01197600 |
| N | 0.16836800 | -0.87837700 | 0.28781300 |
| C | 0.30825600 | 1.43442600 | 0.67560200 |
| H | 0.20345300 | 1.31081600 | 1.75954700 |
| H | 1.37030400 | 1.34588500 | 0.42225900 |
| C | -2.59550400 | -0.60828700 | 2.06770300 |
| H | -2.34190800 | 0.45714900 | 2.04152500 |
| H | -3.30093200 | -0.75742900 | 2.89060800 |
| C | -3.15945000 | -1.04055300 | 0.73396700 |
| C | -2.20418100 | -1.75037000 | -0.00547300 |
| C | -4.43766200 | -0.82699000 | 0.22041600 |
| C | -2.53301900 | -2.27077800 | -1.25907100 |
| C | -4.76058000 | -1.33705900 | -1.03962500 |
| H | -5.17975300 | -0.27783600 | 0.79315500 |
| C | -3.81573400 | -2.05939200 | -1.77280900 |
| H | -1.81737700 | -2.85112600 | -1.83347800 |
| H | -5.75478000 | -1.18182000 | -1.44719800 |
| H | -4.08148700 | -2.46477900 | -2.74412800 |
| C | -0.24000300 | 2.76841400 | 0.23615200 |
| C | -0.68665200 | 3.69826200 | 1.18040600 |
| C | -0.28772700 | 3.10739900 | -1.12288100 |
| C | -1.16245100 | 4.94873300 | 0.78004000 |
| H | -0.65975700 | 3.44354200 | 2.23631900 |
| C | -0.77187400 | 4.35047700 | -1.52539400 |
| H | 0.05014200 | 2.38998400 | -1.86364900 |
| C | -1.20783200 | 5.27654600 | -0.57435800 |
| H | -1.50272800 | 5.66147700 | 1.52473900 |
| H | -0.80694400 | 4.59989000 | -2.58138300 |
| H | -1.58152300 | 6.24582100 | -0.88904000 |
| C | 1.99673200 | -0.81909400 | -1.42652800 |
| H | 2.02357300 | -0.49097300 | -2.46277000 |
| C | 3.19797100 | -0.66081600 | -0.68354700 |
| C | 3.33750200 | -1.03178100 | 0.68514200 |
| C | 4.33888900 | -0.09311000 | -1.32237400 |
| C | 4.54099300 | -0.85171200 | 1.35307900 |
| H | 2.48043900 | -1.43332500 | 1.21149900 |
| C | 5.53406300 | 0.08553800 | -0.64366100 |
| H | 4.25848400 | 0.20190600 | -2.36495800 |
| C | 5.64779200 | -0.29404900 | 0.70075100 |
| H | 4.62105900 | -1.14105700 | 2.39673900 |

| | | | |
|---|---|---|---|
| H | 6.38535000 | 0.52159300 | -1.15729800 |
| H | 6.58330100 | -0.15361200 | 1.23221000 |
| H | -0.02562200 | -1.30878300 | -1.76710700 |

**Vibrational frequencies**

21.44, 27.86, 28.97, 36.43, 44.71, 61.91, 79.32, 89.35, 91.38, 103.94, 131.24, 164.66, 180.86, 204.42, 214.87, 233.03, 254.45, 258.86, 289.1, 303.46, 341.35, 395.71, 403.89, 409.57, 417.36, 429.1, 453.53, 471.77, 476.41, 487.43, 515.5, 538.66, 554.09, 591.17, 604.62, 613.72, 623.23, 630.44, 651.53, 668.34, 675.01, 689.86, 706.79, 728.26, 733.79, 750.31, 756.72, 766.07, 773.59, 803.83, 814.89, 839.07, 840.63, 860.21, 861.27, 880.76, 901.23, 905.25, 914.22, 924.99, 951.61, 965.58, 968.45, 982.47, 983.24, 988.26, 989.41, 991.63, 992.38, 1003.19, 1003.72, 1009.69, 1013.14, 1028.57, 1036.46, 1039.92, 1044.54, 1046.55, 1068.64, 1077.73, 1093.17, 1098.46, 1106.46, 1121.82, 1153.17, 1161.45, 1172.85, 1175.36, 1176.85, 1182.29, 1185.56, 1195.03, 1197.45, 1219.9, 1223.19, 1236.97, 1238.69, 1249.62, 1275.73, 1291.69, 1303.67, 1305.34, 1323.52, 1329.9, 1335.91, 1339.11, 1344.56, 1355.35, 1356.13, 1364.01, 1389.7, 1395.16, 1434.3, 1477.13, 1480.25, 1480.63, 1481.89, 1491.32, 1492.82, 1501.56, 1502.25, 1509.23, 1518.06, 1526.69, 1577.99, 1598.81, 1619.79, 1624.32, 1636.53, 1643.77, 3001.52, 3016.9, 3033.73, 3039.71, 3048.12, 3057.31, 3066.51, 3072.98, 3093.51, 3094.75, 3113.7, 3151.05, 3154.14, 3156.49, 3156.76, 3160.84, 3163.59, 3164.43, 3171.17, 3173.69, 3174.35, 3182.57, 3183.76, 3189.38, 3191.05, 3203.43.

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## 21b *cis*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.457137
Thermal correction to Energy= 0.480278
Thermal correction to Enthalpy= 0.481222
Thermal correction to Gibbs Free Energy= 0.400785

Sum of electronic and zero-point Energies= -1135.680677
Sum of electronic and thermal Energies= -1135.657536
Sum of electronic and thermal Enthalpies= -1135.656592
Sum of electronic and thermal Free Energies= -1135.737029

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.16159300 | -1.78767800 | -1.93745800 |
| C | 0.87013000 | -1.75976800 | -1.10055900 |
| H | 1.97111400 | -2.08350300 | -2.97025200 |
| H | 2.57702400 | -0.77529200 | -1.93676800 |
| C | -0.15777200 | -2.83681600 | -1.47666100 |
| H | -0.24101000 | -2.88469300 | -2.56636700 |
| H | 0.12322200 | -3.82191100 | -1.10232900 |
| C | -1.45525900 | -2.30768900 | -0.86286800 |
| H | -2.34853500 | -2.73248500 | -1.32122100 |
| H | -1.49018900 | -2.52783600 | 0.20635500 |
| C | -1.36259000 | -0.77502500 | -1.08309900 |
| H | -1.88996400 | -0.52757700 | -2.01320000 |
| O | 0.64172400 | 0.52286700 | -0.60978700 |
| N | 0.09383800 | -0.53657900 | -1.35122900 |
| C | 0.66606400 | 1.70238000 | -1.39636800 |
| H | 1.14806000 | 1.48039700 | -2.35575600 |
| H | -0.35752500 | 2.04114300 | -1.60178100 |
| C | -3.33260300 | 0.18449300 | 0.24243500 |
| C | -3.79536000 | 0.97049100 | 1.32879200 |
| C | -4.31003400 | -0.43416200 | -0.57691600 |
| C | -5.14585400 | 1.12335100 | 1.57949600 |
| H | -3.06478400 | 1.45612200 | 1.96733000 |
| C | -5.66129800 | -0.27199800 | -0.31803600 |
| H | -4.00110600 | -1.04059700 | -1.42027200 |
| C | -6.09166800 | 0.50313300 | 0.75886300 |

| | | | |
|---|---|---|---|
| H | -5.47140300 | 1.72919900 | 2.41747900 |
| H | -6.38981400 | -0.75391100 | -0.96033400 |
| H | -7.14996000 | 0.62397800 | 0.95653100 |
| C | -1.93758800 | 0.04743600 | 0.01993700 |
| H | -1.25623300 | 0.57012600 | 0.67900100 |
| C | 3.11482500 | -2.72617300 | -1.18022100 |
| H | 4.16817500 | -2.48885700 | -1.33944600 |
| H | 2.96284900 | -3.76798600 | -1.48385100 |
| C | 2.68175200 | -2.53627400 | 0.25532200 |
| C | 1.40912100 | -1.96488700 | 0.31456000 |
| C | 3.37133200 | -2.85215800 | 1.41953400 |
| C | 0.81971200 | -1.69201600 | 1.54368100 |
| C | 2.77923700 | -2.58211200 | 2.65185300 |
| H | 4.36185200 | -3.29278700 | 1.37117200 |
| C | 1.51337800 | -2.00284200 | 2.71252100 |
| H | -0.15626400 | -1.22458700 | 1.60392300 |
| H | 3.30985800 | -2.81376500 | 3.56843000 |
| H | 1.06743900 | -1.78344100 | 3.67588800 |
| C | 1.42702900 | 2.76432600 | -0.64583800 |
| C | 2.41178400 | 2.42606700 | 0.28270400 |
| C | 1.17042700 | 4.11027300 | -0.90739900 |
| C | 3.13146200 | 3.42424000 | 0.93339600 |
| H | 2.60336900 | 1.38158000 | 0.50004100 |
| C | 1.89596100 | 5.10660200 | -0.26339100 |
| H | 0.39555600 | 4.37902500 | -1.61865400 |
| C | 2.87923500 | 4.76517300 | 0.66083500 |
| H | 3.89115700 | 3.15162400 | 1.65708900 |
| H | 1.68735000 | 6.14883200 | -0.47615600 |
| H | 3.44101100 | 5.54011100 | 1.16934300 |

**Vibrational frequencies**

13.62, 18.26, 24.15, 32.38, 47.12, 55.07, 74.64, 97.11, 109.86, 124.69, 143.60, 182.38, 197.52, 204.92, 228.69, 243.39, 249.82, 278.58, 298.10, 330.00, 365.01, 382.92, 409.22, 412.07, 433.04, 446.20, 470.07, 477.50, 487.82, 516.78, 530.04, 549.94, 563.41, 593.45, 608.24, 616.74, 627.59, 630.97, 669.84, 671.42, 679.39, 695.87, 713.45, 731.73, 750.14, 756.57, 774.07, 782.40, 799.71, 837.73, 847.46, 853.51, 866.04, 867.20, 878.02, 895.27, 907.48, 919.07, 937.62, 948.23, 971.66, 976.10, 991.06, 997.00, 999.21, 1010.67, 1011.14, 1017.03, 1017.18, 1018.12, 1024.68, 1035.39, 1044.59, 1053.18, 1059.32, 1060.48, 1076.91, 1097.54, 1105.64, 1109.19, 1115.75, 1129.85, 1147.67, 1160.09, 1165.87, 1168.18, 1172.19, 1174.14, 1183.04, 1187.85, 1197.76, 1204.71, 1218.25, 1225.44, 1241.23, 1242.56, 1248.40, 1261.18, 1292.77, 1295.79, 1313.67, 1318.66, 1321.70, 1329.18, 1333.73, 1336.28, 1344.32, 1348.11, 1349.52, 1354.88, 1356.08, 1412.74, 1438.05, 1476.20, 1480.08, 1491.49, 1492.12, 1493.07, 1498.70, 1501.30, 1512.08, 1512.44, 1517.65, 1540.18, 1614.49, 1631.82, 1656.00, 1657.65, 1677.17, 1680.36, 3017.53, 3031.49, 3056.10, 3071.17, 3071.82, 3074.65, 3091.10, 3119.32, 3135.72, 3138.59, 3145.98, 3189.06, 3192.97, 3194.56, 3199.46, 3201.48, 3203.34, 3209.30, 3210.84, 3214.78, 3217.76, 3219.20, 3222.45, 3224.11, 3224.25, 3227.24

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.452234
Thermal correction to Energy= 0.475655
Thermal correction to Enthalpy= 0.476600
Thermal correction to Gibbs Free Energy= 0.395929
Sum of electronic and zero-point Energies= -1136.164686
Sum of electronic and thermal Energies= -1136.141265
Sum of electronic and thermal Enthalpies= -1136.140321
Sum of electronic and thermal Free Energies= -1136.220992

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.09414000 | -1.96607400 | -1.92712300 |
| C | 0.83781500 | -1.91650000 | -1.01960600 |
| H | 1.85037100 | -2.29636400 | -2.93890600 |
| H | 2.50235700 | -0.95457700 | -1.99468000 |

| | | | |
|---|---|---|---|
| C | -0.22629200 | -2.98360200 | -1.36550900 |
| H | -0.32127800 | -3.05422600 | -2.45343100 |
| H | 0.03883200 | -3.97003700 | -0.98203200 |
| C | -1.51578700 | -2.42883100 | -0.75057900 |
| H | -2.41849900 | -2.84179400 | -1.20472500 |
| H | -1.55549300 | -2.64723800 | 0.31876300 |
| C | -1.40887800 | -0.89374200 | -0.97746900 |
| H | -1.92613800 | -0.64743500 | -1.91075800 |
| O | 0.62470800 | 0.41914700 | -0.54115700 |
| N | 0.06070300 | -0.67856500 | -1.25148000 |
| C | 0.74613800 | 1.55519100 | -1.41311300 |
| H | 1.33353000 | 1.26416500 | -2.29206300 |
| H | -0.24318700 | 1.87175400 | -1.76058600 |
| C | -3.31778900 | 0.37193000 | 0.21553800 |
| C | -3.72865300 | 1.14181800 | 1.34452500 |
| C | -4.31139100 | 0.09158800 | -0.76770000 |
| C | -5.02961400 | 1.59316400 | 1.47756200 |
| H | -2.99442600 | 1.37456400 | 2.10883600 |
| C | -5.61126800 | 0.55084700 | -0.62321300 |
| H | -4.05299200 | -0.49054300 | -1.64421500 |
| C | -5.98562900 | 1.30376000 | 0.49531900 |
| H | -5.30853300 | 2.17706800 | 2.34824800 |
| H | -6.34596000 | 0.32194700 | -1.38801200 |
| H | -7.00461400 | 1.65807300 | 0.60058600 |
| C | -1.97569700 | -0.06603500 | 0.12679000 |
| H | -1.30560100 | 0.21423500 | 0.92996400 |
| C | 3.10580100 | -2.87486100 | -1.20200600 |
| H | 4.14474300 | -2.60149300 | -1.40436800 |
| H | 2.98721200 | -3.92219000 | -1.50625700 |
| C | 2.72489200 | -2.70496100 | 0.25174900 |
| C | 1.44681900 | -2.14539700 | 0.37276300 |
| C | 3.46530900 | -3.04078600 | 1.38272400 |
| C | 0.90592300 | -1.91852000 | 1.63726800 |
| C | 2.92183800 | -2.80978300 | 2.64740800 |
| H | 4.45726900 | -3.47091000 | 1.28388900 |
| C | 1.64909200 | -2.25035500 | 2.77206900 |
| H | -0.07456000 | -1.47514900 | 1.75506100 |
| H | 3.49257200 | -3.05757400 | 3.53595500 |
| H | 1.23610900 | -2.06429700 | 3.75768800 |
| C | 1.41370600 | 2.67367400 | -0.65343500 |
| C | 2.61360000 | 2.45601500 | 0.03478100 |
| C | 0.85393000 | 3.95401800 | -0.64559100 |
| C | 3.24044300 | 3.50031600 | 0.70973200 |
| H | 3.04866200 | 1.46330300 | 0.04967600 |
| C | 1.48582200 | 5.00397700 | 0.02150000 |
| H | -0.08245300 | 4.13163900 | -1.16486600 |
| C | 2.68018000 | 4.77873300 | 0.70219600 |
| H | 4.16692500 | 3.31733000 | 1.24333700 |
| H | 1.03980400 | 5.99262200 | 0.01631900 |
| H | 3.17050000 | 5.59152200 | 1.22677700 |

**Vibrational frequencies**

13.71, 21.22, 30.87, 38.61, 41.7, 60.52, 69.82, 87.32, 98.8, 120.85, 143.74, 175.34, 189.3, 192.13, 230.97, 238.96, 249.24, 269.74, 298.77, 321.71, 359.61, 376.42, 402.2, 416.57, 425.63, 445.93, 458.63, 480.31, 482.28, 507.79, 521.6, 545.02, 559.05, 587.51, 602.67, 609.07, 627.33, 634.74, 660.13, 670.96, 677.1, 690.99, 710.24, 717.37, 742.97, 757.62, 769.63, 770.26, 791.89, 830.12, 833.43, 843.58, 853.87, 859.73, 863.21, 875.95, 887.39, 898.91, 916.89, 930.08, 954.96, 959.54, 977.81, 981.85, 992.3, 992.58, 993.02, 995.63, 997.58, 1008.69, 1011.55, 1017.69, 1024.66, 1036.95, 1041.87, 1047.94, 1049.66, 1057.98, 1072.96, 1093.11, 1095.5, 1105.76, 1109.43, 1133.1, 1156.22, 1156.94, 1171.18, 1176.26, 1179.03, 1185.34, 1192.78, 1199.79, 1204.47, 1213.77, 1229.18, 1229.91, 1239.46, 1244.6, 1277.78, 1291.19, 1313.72, 1320.3, 1320.37, 1326.78, 1331.59, 1334.73, 1336.18, 1344.46, 1350.7, 1352.64, 1353.61, 1403.92, 1438.63, 1476.99, 1480.2, 1482.14, 1482.36, 1485.8, 1492.23, 1498.99, 1502.25, 1504.73, 1511.61, 1527.85, 1574.45, 1598.05, 1620.22, 1624.27, 1641.31, 1645.51, 3008.16, 3010.08, 3013.6, 3039.2, 3047.73, 3052.02, 3058.77, 3068.78, 3097.64, 3098.39, 3106.75, 3154.75, 3158.71, 3159.75, 3163.76, 3164.72, 3166.53, 3174.65, 3175.88, 3181.01, 3184.44, 3185.41, 3190.5, 3192.03, 3192.32, 3197.78.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.440687
Thermal correction to Energy= 0.464816
Thermal correction to Enthalpy= 0.465760
Thermal correction to Gibbs Free Energy= 0.383882
Sum of electronic and zero-point Energies= -1136.006895
Sum of electronic and thermal Energies= -1135.982767
Sum of electronic and thermal Enthalpies= -1135.981822
Sum of electronic and thermal Free Energies= -1136.063701

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.08060700 | -1.98498800 | -1.94789800 |
| C | 0.84434800 | -1.95991400 | -1.00770500 |
| H | 1.81590600 | -2.31977600 | -2.96000400 |
| H | 2.46707500 | -0.95803800 | -2.02273200 |
| C | -0.20767700 | -3.05363700 | -1.31897300 |
| H | -0.33596300 | -3.12962800 | -2.41001600 |
| H | 0.09481700 | -4.03819500 | -0.93948300 |
| C | -1.48836300 | -2.52324800 | -0.66154200 |
| H | -2.40380300 | -2.97085600 | -1.07141800 |
| H | -1.47817400 | -2.71984100 | 0.41983100 |
| C | -1.43267100 | -0.99034700 | -0.92619700 |
| H | -1.96929200 | -0.78349200 | -1.86643500 |
| O | 0.59067200 | 0.37285600 | -0.50151400 |
| N | 0.03587000 | -0.73463100 | -1.23255400 |
| C | 0.65286900 | 1.52724700 | -1.37039700 |
| H | 1.21928100 | 1.25695200 | -2.27890700 |
| H | -0.36172900 | 1.82698300 | -1.68205400 |
| C | -3.31458500 | 0.38782500 | 0.19924100 |
| C | -3.71565100 | 1.17439700 | 1.32735800 |
| C | -4.28955100 | 0.19339900 | -0.83047500 |
| C | -4.98818600 | 1.72361000 | 1.41504800 |
| H | -2.99260700 | 1.34210400 | 2.12844700 |
| C | -5.56106100 | 0.74933200 | -0.73088000 |
| H | -4.03672200 | -0.39834900 | -1.71115200 |
| C | -5.92604100 | 1.51770500 | 0.38749000 |
| H | -5.25968300 | 2.31986300 | 2.28822000 |
| H | -6.28343000 | 0.58382800 | -1.53257300 |
| H | -6.92507800 | 1.94973500 | 0.45714500 |
| C | -2.00351400 | -0.15150400 | 0.16334200 |
| H | -1.35249400 | 0.06950400 | 1.01042900 |
| C | 3.12855700 | -2.87454900 | -1.24774200 |
| H | 4.16366200 | -2.58497300 | -1.48035000 |
| H | 3.01870300 | -3.93124100 | -1.54753800 |

| | | | |
|---|---|---|---|
| C | 2.78419500 | -2.70889300 | 0.21671400 |
| C | 1.49244100 | -2.17184600 | 0.37101700 |
| C | 3.56079000 | -3.03341400 | 1.33351900 |
| C | 0.97786000 | -1.95203400 | 1.65377400 |
| C | 3.04233000 | -2.81074700 | 2.61624900 |
| H | 4.56375000 | -3.44857200 | 1.20937500 |
| C | 1.75852500 | -2.27158400 | 2.77367700 |
| H | -0.01275100 | -1.52142500 | 1.79659600 |
| H | 3.64291200 | -3.04973100 | 3.49582700 |
| H | 1.36562000 | -2.09026400 | 3.77574700 |
| C | 1.32130500 | 2.65241300 | -0.61928000 |
| C | 2.54443800 | 2.44930600 | 0.04381700 |
| C | 0.73929300 | 3.92943900 | -0.59268500 |
| C | 3.17244300 | 3.50490900 | 0.71164900 |
| H | 2.99657200 | 1.45659100 | 0.04449900 |
| C | 1.37349500 | 4.99039000 | 0.06512600 |
| H | -0.21852500 | 4.09349300 | -1.09162200 |
| C | 2.59136400 | 4.77976200 | 0.72057000 |
| H | 4.11884100 | 3.33292000 | 1.22752900 |
| H | 0.90984500 | 5.97837700 | 0.07399600 |
| H | 3.08417600 | 5.60333900 | 1.24003800 |

**Vibrational frequencies**

13.73, 21.56, 29.76, 37.91, 39.09, 68.3, 69.38, 85.96, 95.32, 119.36, 136.08, 164.96, 183.04, 184.97, 222.77, 232.45, 240.38, 260.15, 288.66, 312.34, 349.5, 365.5, 385.78, 400.12, 408.32, 431.16, 441.12, 462.8, 466.9, 490.24, 505.14, 527.3, 539.96, 570.5, 581.9, 589.15, 607.6, 615, 635.64, 648.37, 659.43, 673.68, 687.16, 696.24, 718.43, 731.12, 744.03, 747.33, 769.79, 803.31, 806.64, 820, 828.71, 832.11, 836.01, 843.79, 854.07, 865.16, 889.81, 895.36, 917.51, 930.21, 945.36, 953.53, 954.16, 956.9, 958.5, 966.91, 967.95, 968.92, 977.34, 989.09, 991.63, 993.54, 1002.91, 1015.42, 1025.07, 1025.81, 1039.49, 1060.56, 1063.23, 1071.96, 1081.41, 1097.57, 1123.08, 1127.66, 1143.22, 1145.84, 1149, 1154.76, 1160.21, 1166.29, 1166.76, 1180.56, 1191.35, 1191.8, 1198.45, 1211.76, 1237.2, 1248.7, 1269.28, 1276.4, 1280.47, 1283.08, 1290.1, 1295.54, 1302.79, 1303.24, 1335.71, 1339.4, 1348.7, 1356.25, 1402.07, 1428.18, 1430.12, 1439.24, 1439.74, 1441.44, 1443.49, 1446.61, 1459.04, 1459.6, 1468.57, 1483.33, 1532.95, 1563.57, 1578.37, 1582.09, 1597.06, 1601.67, 2939.67, 2953.9, 2957.2, 2979.38, 2981.45, 2994.08, 2997.66, 3015.38, 3043.46, 3045.23, 3053.2, 3095.43, 3098.41, 3098.73, 3103.22, 3105.69, 3106.31, 3114.21, 3115.95, 3117.98, 3120.95, 3121.66, 3125.67, 3130.95, 3131.08, 3132.45.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.451108
Thermal correction to Energy= 0.474770
Thermal correction to Enthalpy= 0.475714
Thermal correction to Gibbs Free Energy= 0.394561

Sum of electronic and zero-point Energies= -1136.243913
Sum of electronic and thermal Energies= -1136.220252
Sum of electronic and thermal Enthalpies= -1136.219308
Sum of electronic and thermal Free Energies= -1136.300460

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 2.07612300 | -1.98758000 | -1.93635900 |
| C | 0.84073500 | -1.95995600 | -1.00440300 |
| H | 1.81605200 | -2.31557100 | -2.94585500 |
| H | 2.46981400 | -0.96861800 | -1.99987100 |
| C | -0.20559500 | -3.05448300 | -1.31006200 |
| H | -0.34117100 | -3.12718500 | -2.39461800 |
| H | 0.09961900 | -4.03265400 | -0.93281700 |
| C | -1.47903300 | -2.52354900 | -0.64392000 |
| H | -2.39287300 | -2.97645600 | -1.03568000 |
| H | -1.44981200 | -2.70544700 | 0.43383500 |
| C | -1.42979600 | -0.99847300 | -0.92833500 |

| | | | |
|---|---|---|---|
| H | -1.96764400 | -0.80202800 | -1.86152300 |
| O | 0.57975100 | 0.36208400 | -0.50785000 |
| N | 0.03152900 | -0.74139500 | -1.23949200 |
| C | 0.64648800 | 1.50973300 | -1.37489600 |
| H | 1.21213700 | 1.23538300 | -2.27401900 |
| H | -0.36187600 | 1.80907800 | -1.68343700 |
| C | -3.30019900 | 0.39804700 | 0.18694400 |
| C | -3.69771500 | 1.18857600 | 1.30632000 |
| C | -4.26721000 | 0.20396500 | -0.84228700 |
| C | -4.96385500 | 1.74473700 | 1.38645200 |
| H | -2.98037200 | 1.35416200 | 2.10490800 |
| C | -5.53248800 | 0.76675100 | -0.75103300 |
| H | -4.01520400 | -0.39123400 | -1.71354900 |
| C | -5.89561600 | 1.54023900 | 0.35897300 |
| H | -5.23391300 | 2.34318900 | 2.25108500 |
| H | -6.24866700 | 0.60246400 | -1.55039500 |
| H | -6.88696700 | 1.97628500 | 0.42216400 |
| C | -1.99174800 | -0.14723300 | 0.15796300 |
| H | -1.34512000 | 0.06965600 | 1.00170900 |
| C | 3.10882200 | -2.88877000 | -1.23364800 |
| H | 4.14214300 | -2.61639000 | -1.46713100 |
| H | 2.97856400 | -3.93959400 | -1.52388900 |
| C | 2.76542600 | -2.70380600 | 0.22750200 |
| C | 1.48335600 | -2.15588300 | 0.37362900 |
| C | 3.53683200 | -3.01917300 | 1.34553300 |
| C | 0.97107400 | -1.91314300 | 1.64859900 |
| C | 3.02149000 | -2.77390500 | 2.62056700 |
| H | 4.53072500 | -3.44260000 | 1.22908900 |
| C | 1.74652200 | -2.22195500 | 2.76943800 |
| H | -0.01012200 | -1.47326100 | 1.78331900 |
| H | 3.61619400 | -3.00424100 | 3.49916600 |
| H | 1.35792100 | -2.02288400 | 3.76337100 |
| C | 1.31625100 | 2.62950100 | -0.61971000 |
| C | 2.52098100 | 2.41391800 | 0.06273100 |
| C | 0.75071700 | 3.90874100 | -0.60921900 |
| C | 3.14869200 | 3.46178000 | 0.73430300 |
| H | 2.95718600 | 1.42062500 | 0.07592000 |
| C | 1.38408100 | 4.96166300 | 0.05383500 |
| H | -0.19084300 | 4.08129300 | -1.12314700 |
| C | 2.58440200 | 4.73968200 | 0.72839300 |
| H | 4.07898500 | 3.28178500 | 1.26407500 |
| H | 0.93468600 | 5.94977600 | 0.05123700 |
| H | 3.07555900 | 5.55491700 | 1.25023000 |

**Vibrational frequencies**

12.88, 20.89, 31.01, 38.3, 41.66, 66.91, 68.59, 86.14, 96.46, 122.04, 134.94, 169.36, 185.88, 188.23, 227.6, 235.89, 244.35, 263.31, 291.53, 316.99, 355, 369.75, 391.18, 410.2, 415.95, 440.36, 445.02, 472.63, 478.28, 499.3, 513.23, 535.16, 548.69, 581.07, 593.39, 599.32, 616.72, 623.75, 644.88, 659.22, 675.35, 689.69, 704.94, 710.77, 737.42, 753.14, 765.48, 767.92, 785.68, 822.83, 834.34, 837.72, 846.55, 854.76, 863.62, 874.08, 879.91, 896.85, 911.34, 926.64, 951.51, 954.34, 976.04, 980.7, 988.15, 988.65, 989.95, 992.09, 994.47, 1004, 1007.18, 1012.45, 1019.81, 1030.56, 1036.21, 1038.29, 1046.09, 1047.55, 1068.92, 1089.46, 1090.19, 1100.43, 1106.5, 1127.36, 1151.35, 1154.56, 1170.95, 1175.77, 1178.39, 1185.27, 1189.37, 1197.67, 1201.74, 1212.85, 1225.29, 1225.96, 1226.43, 1239.28, 1276.1, 1289.14, 1311.37, 1314.81, 1319.08, 1325.33, 1329.69, 1334.53, 1339.9, 1343.32, 1355.77, 1356.07, 1362.85, 1392.57, 1438.2, 1478.97, 1481.26, 1481.55, 1484.15, 1486.39, 1498.67, 1500.11, 1503.55, 1505.49, 1515.47, 1526.89, 1575.8, 1598.08, 1619.46,

1623.93, 1638.78, 1644.09, 3007.05, 3010.01, 3026.61, 3036.53, 3045.95, 3046.8, 3051.22, 3072.23, 3097.1, 3097.91, 3107.47, 3154.71, 3156.66, 3157.69, 3162.78, 3164.71, 3164.74, 3174.16, 3174.29, 3180, 3181.09, 3182.35, 3184.11, 3191.38, 3191.72, 3191.99.

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## 6c *trans*

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.471306 (Hartr
Thermal correction to Energy= 0.494097
Thermal correction to Enthalpy= 0.495041
Thermal correction to Gibbs Free Energy= 0.417810

Sum of electronic and zero-point Energies= -1136.323541
Sum of electronic and thermal Energies= -1136.300750
Sum of electronic and thermal Enthalpies= -1136.299806
Sum of electronic and thermal Free Energies= -1136.377037

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.32539700 | -1.22242300 | 2.22596100 |
| C | 0.17313300 | -1.57093700 | 0.81141800 |
| H | -0.13678200 | -2.08368200 | 2.87410500 |
| H | 0.21706900 | -0.36664300 | 2.63154200 |
| C | 1.46536400 | -2.38545800 | 0.75449900 |
| H | 2.12586200 | -2.04480900 | 1.55585900 |
| H | 1.26982600 | -3.44830900 | 0.90187000 |
| C | 2.09110100 | -2.06034900 | -0.61887500 |
| H | 3.16404600 | -1.89150900 | -0.52344400 |
| H | 1.95046200 | -2.87351400 | -1.33229700 |
| C | 1.35990600 | -0.79526100 | -1.10436800 |
| O | -0.51852000 | 0.38583700 | -0.36356700 |
| N | 0.60575100 | -0.35060300 | 0.07935100 |
| C | -0.56045600 | 1.66357400 | 0.24490400 |
| H | -0.41992000 | 1.55902100 | 1.32828100 |
| H | 0.24714400 | 2.29934600 | -0.13753200 |
| C | -1.84567600 | -1.01199000 | 2.10033000 |
| H | -2.09144000 | 0.03186500 | 1.87479200 |
| H | -2.38949700 | -1.28760000 | 3.00601500 |
| C | -2.19961400 | -1.88731100 | 0.92176100 |
| C | -1.05616700 | -2.22734900 | 0.19481500 |
| C | -3.45109600 | -2.33990500 | 0.52265800 |
| C | -1.15512800 | -3.03522300 | -0.93232700 |
| C | -3.55098900 | -3.14455900 | -0.61143700 |
| H | -4.33888300 | -2.07635000 | 1.08870800 |
| C | -2.41056700 | -3.49261200 | -1.33222400 |
| H | -0.27355500 | -3.31919800 | -1.49741700 |
| H | -4.52069900 | -3.50890000 | -0.93143300 |
| H | -2.49864500 | -4.12718700 | -2.20670300 |
| C | -1.89682700 | 2.29800000 | -0.04769900 |
| C | -2.03859800 | 3.67929600 | 0.09043900 |
| C | -3.00181200 | 1.53279200 | -0.41995200 |
| C | -3.26803700 | 4.28929100 | -0.12879100 |
| H | -1.17813100 | 4.28109000 | 0.36771200 |
| C | -4.23199400 | 2.14637200 | -0.64478000 |
| H | -2.89077400 | 0.46134300 | -0.54369100 |
| C | -4.37046300 | 3.52213400 | -0.49731300 |
| H | -3.36470300 | 5.36356600 | -0.01929600 |
| H | -5.08418700 | 1.54369600 | -0.93857800 |

| | | | |
|---|---|---|---|
| H | -5.32885800 | 3.99681100 | -0.67357400 |
| C | 2.25276000 | 0.33026400 | -1.64803400 |
| H | 2.61377300 | 0.02873600 | -2.63549900 |
| C | 3.43697900 | 0.68013700 | -0.77875400 |
| C | 3.28263700 | 1.36243700 | 0.43177500 |
| C | 4.72713200 | 0.30855700 | -1.16542600 |
| C | 4.38400000 | 1.66485300 | 1.22659200 |
| H | 2.29035600 | 1.65228600 | 0.75409500 |
| C | 5.83207300 | 0.60826600 | -0.37348500 |
| H | 4.86746300 | -0.21928500 | -2.10383400 |
| C | 5.66327100 | 1.28801100 | 0.82793600 |
| H | 4.24210100 | 2.19750000 | 2.16034700 |
| H | 6.82354400 | 0.31184400 | -0.69672800 |
| H | 6.52110200 | 1.52678400 | 1.44615200 |
| H | 0.63848500 | -1.05284500 | -1.89080500 |
| H | 1.61952300 | 1.20983700 | -1.80331200 |

**Vibrational frequencies**

21.71, 31.24, 37.1, 43.6, 54.73, 63.04, 87.23, 103.47, 116.87, 122.79, 140.93, 173.27, 206.36, 225.84, 233.07, 236.69, 268.23, 274.97, 303.64, 332.73, 364.55, 408.41, 414.19, 420.56, 434.52, 441.39, 465.61, 470.37, 486.88, 496.72, 524.65, 554.78, 566.91, 601.51, 618.69, 630.23, 630.99, 643.18, 666.55, 677.52, 714.24, 725.6, 735.57, 753.83, 756.32, 766.8, 782.29, 789.5, 811.52, 831.14, 846.43, 866.23, 882.39, 882.51, 893.38, 912.42, 923.83, 940.37, 951.6, 960.44, 983.72, 988.44, 1003.92, 1012.68, 1013.39, 1017.36, 1019.61, 1021.46, 1023.78, 1027.81, 1030.49, 1038.89, 1054.51, 1060.35, 1062.54, 1063.9, 1076.59, 1089.47, 1098.54, 1110.37, 1111.3, 1120.77, 1147.76, 1157.66, 1170.29, 1171.11, 1174.12, 1175.68, 1182.48, 1196.48, 1200.81, 1202.87, 1208.66, 1229.38, 1233.84, 1235.73, 1242.13, 1253.43, 1256.73, 1293.45, 1304.3, 1316.12, 1318.37, 1325.99, 1333.6, 1337.88, 1344.02, 1349.18, 1353.6, 1359.12, 1363.18, 1372.98, 1405.79, 1417.58, 1471.87, 1479.35, 1481.18, 1493.15, 1494.01, 1495.15, 1499.91, 1505.88, 1510.01, 1524.85, 1539.14, 1540.87, 1658.35, 1659.68, 1660.73, 1678.84, 1683.19, 1683.43, 3031.19, 3032.48, 3052.46, 3057.53, 3068.05, 3069.32, 3070.56, 3085.52, 3098.01, 3111.12, 3120.12, 3123.1, 3136.44, 3174.94, 3180.57, 3181.26, 3187.82, 3191.99, 3194, 3196.91, 3197.07, 3203.58, 3204.86, 3210.28, 3213.03, 3216.55, 3224.63.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.466192
Thermal correction to Energy= 0.489565
Thermal correction to Enthalpy= 0.490509
Thermal correction to Gibbs Free Energy= 0.410798

Sum of electronic and zero-point Energies= -1136.800789
Sum of electronic and thermal Energies= -1136.777416
Sum of electronic and thermal Enthalpies= -1136.776472
Sum of electronic and thermal Free Energies= -1136.856183

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.57601800 | 1.22304400 | 2.61939500 |
| C | 0.09057200 | 0.59619000 | 1.28619600 |
| H | 0.03215900 | 0.74358900 | 3.43910300 |
| H | 1.63898500 | 1.03386200 | 2.77672900 |
| C | -0.34034300 | -0.87560500 | 1.40912600 |
| H | 0.33100700 | -1.37920200 | 2.10965100 |
| H | -1.35512000 | -0.96149000 | 1.80062400 |
| C | -0.17776100 | -1.47528900 | -0.00463100 |
| H | 0.23066300 | -2.48520400 | 0.04370100 |
| H | -1.13512200 | -1.54003400 | -0.52520500 |
| C | 0.76852900 | -0.50549900 | -0.74928300 |
| O | 1.52976800 | 1.69426600 | -0.33105000 |
| N | 1.21024700 | 0.44235100 | 0.30109700 |
| C | 2.87379500 | 2.10195200 | -0.01627700 |
| H | 2.96847500 | 2.28981100 | 1.05791500 |

| | | | |
|---|---|---|---|
| H | 3.57025500 | 1.30139600 | -0.28400100 |
| C | 0.20231000 | 2.71975500 | 2.57633500 |
| H | 1.03320900 | 3.33518000 | 2.21438600 |
| H | -0.07760400 | 3.10976500 | 3.55887800 |
| C | -0.94216400 | 2.75668300 | 1.59095500 |
| C | -1.01500200 | 1.56672300 | 0.85774100 |
| C | -1.85763800 | 3.78381700 | 1.37484100 |
| C | -2.01457300 | 1.40431200 | -0.10240100 |
| C | -2.85498200 | 3.61832500 | 0.41311000 |
| H | -1.80074600 | 4.70298300 | 1.94967600 |
| C | -2.93302900 | 2.43320100 | -0.32005600 |
| H | -2.10004100 | 0.48896500 | -0.67597600 |
| H | -3.57596100 | 4.40982700 | 0.23883800 |
| H | -3.71472200 | 2.30830800 | -1.06162700 |
| C | 3.17857900 | 3.35311600 | -0.80054400 |
| C | 3.16227400 | 4.60765200 | -0.18523500 |
| C | 3.48133200 | 3.27694000 | -2.16507000 |
| C | 3.44527100 | 5.76317000 | -0.91308400 |
| H | 2.92927200 | 4.68162500 | 0.87201100 |
| C | 3.76078700 | 4.42824300 | -2.89668100 |
| H | 3.50080600 | 2.30954500 | -2.65600000 |
| C | 3.74433400 | 5.67541800 | -2.27108000 |
| H | 3.43176900 | 6.72914400 | -0.42022400 |
| H | 3.99628700 | 4.35348900 | -3.95276200 |
| H | 3.96541100 | 6.57224900 | -2.83939700 |
| C | 1.95666900 | -1.16097200 | -1.49021800 |
| H | 2.63049000 | -0.35967900 | -1.80886900 |
| C | 2.73002000 | -2.22701900 | -0.74125700 |
| C | 2.63783900 | -3.56853600 | -1.13481500 |
| C | 3.55268400 | -1.91963700 | 0.35187900 |
| C | 3.33665900 | -4.57160200 | -0.46326200 |
| H | 2.01190900 | -3.83078400 | -1.98237200 |
| C | 4.25241100 | -2.91876600 | 1.02674200 |
| H | 3.63684300 | -0.89180100 | 0.68165700 |
| C | 4.14682600 | -4.24968300 | 0.62362400 |
| H | 3.24817300 | -5.60209100 | -0.79053900 |
| H | 4.88308600 | -2.65627300 | 1.86967600 |
| H | 4.69289800 | -5.02587800 | 1.14849700 |
| H | 0.20670400 | 0.06052600 | -1.50313400 |
| H | 1.56004500 | -1.60321800 | -2.40970800 |

**Vibrational frequencies**

24.31, 25.9, 29.38, 35.43, 42.18, 47.82, 70.68, 80.55, 91.18, 97.48, 141.81, 170.78, 184.95, 213.48, 223.97, 247.19, 256.55, 272.7, 296.22, 330.18, 353.29, 398.28, 403.15, 417.07, 417.35, 435.82, 460.6, 469.8, 484.54, 498.35, 525.4, 547.35, 560.12, 595.93, 617.1, 629.78, 636.21, 637.3, 658.46, 674.64, 709.89, 713.71, 727.89, 738.92, 748.93, 764.21, 769.29, 773.68, 806.03, 820.74, 843.5, 856.02, 859.04, 860.08, 872.66, 890.42, 903.77, 930.31, 932.81, 937.47, 955.97, 970.19, 988.54, 989.04, 990.35, 990.94, 997.01, 999.97, 1004.61, 1006.18, 1010.26, 1016.38, 1018.23, 1038, 1050.19, 1050.33, 1051.85, 1053.8, 1071.91, 1082.91, 1098.15, 1108.82, 1110.34, 1126.68, 1156.13, 1166.4, 1177.07, 1180.43, 1180.97, 1191.19, 1198.14, 1199.62, 1202.46, 1218.55, 1222.75, 1226.34, 1227.63, 1232.68, 1248.13, 1279.36, 1291.56, 1311.66, 1317.73, 1325.11, 1338.51, 1340.89, 1341.72, 1345.47, 1353.98, 1355.92, 1358.67, 1367.84, 1389.56, 1409.31, 1473.76, 1475.5, 1482.81, 1483.97, 1485.37, 1489.05, 1489.68, 1504.61, 1513.55, 1515.79, 1525.35, 1528.14, 1619.41, 1621.72, 1625.99, 1641.38, 1641.7, 1646.06, 2996.51, 3024.75, 3027.84, 3036.33, 3038.32, 3049.22, 3062.86, 3063.8, 3065.98, 3068.89, 3093.59, 3099.39, 3107.69, 3154.96, 3156.3, 3160.58, 3162.87, 3164.51, 3166.29, 3172.89, 3173.34, 3178.9, 3181.06, 3184.93, 3189.53, 3190.66, 3199.59.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.454235
Thermal correction to Energy= 0.478205
Thermal correction to Enthalpy= 0.479150
Thermal correction to Gibbs Free Energy= 0.399473
Sum of electronic and zero-point Energies= -1136.640760
Sum of electronic and thermal Energies= -1136.616789
Sum of electronic and thermal Enthalpies= -1136.615845
Sum of electronic and thermal Free Energies= -1136.695521

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -1.28524200 | -1.41511200 | 2.10397300 |
| C | -0.75147900 | -1.69906000 | 0.67600500 |
| H | -1.46521400 | -2.38200700 | 2.59917100 |
| H | -0.54359700 | -0.86936100 | 2.70214900 |
| C | 0.13976200 | -2.95081600 | 0.55795500 |
| H | 0.73266900 | -3.05160600 | 1.47844100 |
| H | -0.46874900 | -3.85828500 | 0.45272300 |
| C | 1.07319000 | -2.69348300 | -0.65319300 |
| H | 2.11254600 | -2.94237700 | -0.40343700 |
| H | 0.79429200 | -3.30018400 | -1.52548700 |
| C | 0.91833600 | -1.18962000 | -0.97405700 |
| O | -0.42207700 | 0.57780900 | -0.14845900 |
| N | 0.24491300 | -0.65334100 | 0.23757000 |
| C | -0.01248300 | 1.64748500 | 0.71498000 |
| H | -0.33578100 | 1.44271100 | 1.75267400 |
| H | 1.08751000 | 1.72812600 | 0.72607600 |
| C | -2.63246300 | -0.67771900 | 1.93527600 |
| H | -2.50265400 | 0.41704800 | 1.94682900 |
| H | -3.35199500 | -0.92196000 | 2.73054800 |
| C | -3.09754200 | -1.13255200 | 0.56945100 |
| C | -2.04213900 | -1.72722000 | -0.14719300 |
| C | -4.37318000 | -1.03207100 | 0.00563100 |
| C | -2.26845800 | -2.23664600 | -1.43227300 |
| C | -4.59342700 | -1.53386300 | -1.28433000 |
| H | -5.19286800 | -0.57465800 | 0.56444300 |
| C | -3.54805900 | -2.13655600 | -1.99700800 |
| H | -1.47038300 | -2.72423600 | -1.99425100 |
| H | -5.58655400 | -1.46626000 | -1.73226600 |
| H | -3.73215800 | -2.53655300 | -2.99577300 |
| C | -0.61930700 | 2.94683200 | 0.23322000 |
| C | -0.10743900 | 4.15795800 | 0.73150900 |
| C | -1.69218900 | 2.98403500 | -0.67066400 |
| C | -0.65869700 | 5.38113300 | 0.33963700 |
| H | 0.73247800 | 4.14313500 | 1.43066200 |
| C | -2.23883200 | 4.21137800 | -1.06831100 |
| H | -2.09230600 | 2.05203700 | -1.06835300 |
| C | -1.72865100 | 5.41203700 | -0.56408400 |
| H | -0.24833500 | 6.31177500 | 0.73557900 |
| H | -3.06927800 | 4.22559500 | -1.77668000 |
| H | -2.15659800 | 6.36626300 | -0.87567500 |
| C | 2.21438700 | -0.42265800 | -1.32343000 |
| H | 1.97376700 | 0.65252300 | -1.30561300 |
| C | 3.43695000 | -0.70799300 | -0.47421600 |
| C | 3.48477600 | -0.40196700 | 0.89964300 |
| C | 4.57408300 | -1.29706000 | -1.05689800 |

| | | | |
|---|---|---|---|
| C | 4.62870500 | -0.67499200 | 1.65832400 |
| H | 2.61123500 | 0.04289500 | 1.37664700 |
| C | 5.72151100 | -1.56883600 | -0.30241700 |
| H | 4.55970500 | -1.54301100 | -2.12168100 |
| C | 5.75309100 | -1.25806500 | 1.06131800 |
| H | 4.64291400 | -0.42796800 | 2.72179600 |
| H | 6.59094100 | -2.02291300 | -0.78164000 |
| H | 6.64600100 | -1.46650200 | 1.65312200 |
| H | 0.23444200 | -1.05620400 | -1.83287200 |
| H | 2.45921200 | -0.65401600 | -2.37176000 |

**Vibrational frequencies**

24.67, 32.01, 37.00, 41.73, 48.42, 67.53, 75.11, 93.62, 100.5, 108.32, 117.6, 168.61, 185.15, 197.5, 215.53, 217.9, 234.37, 256.12, 282.33, 308.4, 341.19, 392.4, 397.21, 401.84, 413.05, 425.73, 447.52, 456.44, 467.59, 471.83, 504.05, 533.28, 544.05, 580.48, 596.78, 609.81, 613.74, 620.04, 637.63, 654.14, 690.15, 692.8, 708.16, 716.63, 720.97, 727.08, 739.47, 749.08, 782.67, 794.27, 816.7, 826.39, 831.4, 834.69, 842.6, 863.2, 872.08, 886.04, 897.16, 902.87, 917.32, 935.42, 952.2, 955.39, 955.54, 960.16, 964.78, 967.33, 968.62, 983.98, 988.45, 989.27, 1000.95, 1016.74, 1021.89, 1024.16, 1026.8, 1029.45, 1037.72, 1050.57, 1065.49, 1078.95, 1080.31, 1091.56, 1127.61, 1134.91, 1146.07, 1146.72, 1147.47, 1151.79, 1159.38, 1163.7, 1169.57, 1187.44, 1189.8, 1190.12, 1191.91, 1206.2, 1213.68, 1239.98, 1249.64, 1268.65, 1276.29, 1281.41, 1289.76, 1294.98, 1298.05, 1311.29, 1321.39, 1332.25, 1343.04, 1348.95, 1354.44, 1361.58, 1425.86, 1428.33, 1432.82, 1435.62, 1439.21, 1441.95, 1443.15, 1455.39, 1455.87, 1460.3, 1480.21, 1481.88, 1577.31, 1578.51, 1580.9, 1596.11, 1598.37, 1601.77, 2918.67, 2925.3, 2968.93, 2970.1, 2977.35, 2982.5, 2996.11, 3002.26, 3012.97, 3013.31, 3037.34, 3044.05, 3053.47, 3092.39, 3094.05, 3095.39, 3103.44, 3103.55, 3104.6, 3113.26, 3115.45, 3115.76, 3124.94, 3125.97, 3127.79, 3132.37, 3144.34.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.464748 (Hartr
Thermal correction to Energy= 0.488433
Thermal correction to Enthalpy= 0.489377
Thermal correction to Gibbs Free Energy= 0.409146

Sum of electronic and zero-point Energies= -1136.879211
Sum of electronic and thermal Energies= -1136.855527
Sum of electronic and thermal Enthalpies= -1136.854582
Sum of electronic and thermal Free Energies= -1136.934813

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.20039100 | -1.60567700 | 2.32276400 |
| C | 0.22716200 | -1.73490600 | 0.83997700 |
| H | 0.20627700 | -2.46238500 | 2.87086300 |
| H | 0.21209100 | -0.69801500 | 2.76918600 |
| C | 1.59577600 | -2.40564600 | 0.63209600 |
| H | 2.26122000 | -2.10308800 | 1.44571900 |
| H | 1.50800100 | -3.49386600 | 0.65609100 |
| C | 2.12698600 | -1.86478800 | -0.71717200 |
| H | 3.17775600 | -1.58002400 | -0.63361000 |
| H | 2.05215500 | -2.61000900 | -1.51317900 |
| C | 1.23789800 | -0.64600400 | -1.04080100 |
| O | -0.69377200 | 0.31440400 | -0.09934600 |
| N | 0.52293500 | -0.39429600 | 0.23260000 |
| C | -0.78559200 | 1.52242900 | 0.68404200 |
| H | -0.92467100 | 1.26372300 | 1.74112800 |
| H | 0.14197900 | 2.09432000 | 0.58777000 |
| C | -1.74061100 | -1.67692400 | 2.35138400 |
| H | -2.18986400 | -0.67698900 | 2.32886600 |
| H | -2.12051200 | -2.17843400 | 3.24665500 |
| C | -2.06752600 | -2.42809900 | 1.08165500 |
| C | -0.96158100 | -2.46838800 | 0.22254000 |

| | | | |
|---|---|---|---|
| C | -3.26868700 | -3.03957300 | 0.72443600 |
| C | -1.05485900 | -3.13067600 | -1.00379400 |
| C | -3.36051700 | -3.69635400 | -0.50504700 |
| H | -4.12284500 | -3.01490500 | 1.39551200 |
| C | -2.25884700 | -3.74243400 | -1.36307700 |
| H | -0.20501700 | -3.19170900 | -1.67602900 |
| H | -4.28849600 | -4.18133800 | -0.79177100 |
| H | -2.33586100 | -4.26340900 | -2.31236100 |
| C | -1.95300100 | 2.32302400 | 0.16578600 |
| C | -1.73507500 | 3.50091400 | -0.55733300 |
| C | -3.27036300 | 1.90405400 | 0.39325700 |
| C | -2.80895100 | 4.25387800 | -1.03490300 |
| H | -0.71758500 | 3.83361200 | -0.74232700 |
| C | -4.34512200 | 2.65033600 | -0.08736300 |
| H | -3.45466100 | 0.98836500 | 0.94609000 |
| C | -4.11657100 | 3.82900300 | -0.80089700 |
| H | -2.62411700 | 5.16829200 | -1.58975300 |
| H | -5.36105700 | 2.31486100 | 0.09594200 |
| H | -4.95360000 | 4.41218400 | -1.17159000 |
| C | 1.96978800 | 0.61196400 | -1.55450300 |
| H | 1.24975900 | 1.43791700 | -1.53518600 |
| C | 3.24262700 | 0.99962700 | -0.82988800 |
| C | 4.46632500 | 0.99420900 | -1.51464400 |
| C | 3.24739800 | 1.37171100 | 0.52367000 |
| C | 5.65653100 | 1.34665000 | -0.87557800 |
| H | 4.48559800 | 0.71079800 | -2.56389100 |
| C | 4.43523900 | 1.72159500 | 1.16663100 |
| H | 2.31487300 | 1.36935600 | 1.07619500 |
| C | 5.64523700 | 1.71165400 | 0.47049100 |
| H | 6.59023600 | 1.33604000 | -1.42963500 |
| H | 4.41504400 | 2.00548800 | 2.21463000 |
| H | 6.56800200 | 1.98644100 | 0.97164000 |
| H | 0.49201700 | -0.91202400 | -1.80243500 |
| H | 2.21099000 | 0.44425600 | -2.60969300 |

**Vibrational frequencies**

18.56, 25.42, 35.75, 37.35, 49.27, 52.93, 73.71, 76.9, 84.84, 100.41, 132.83, 163.12, 177.5, 205.05, 216.29, 228.51, 248.49, 263.56, 278.35, 322.2, 332.72, 393.29, 394.67, 406.69, 412.09, 424.33, 452.7, 462.61, 477.89, 487.54, 515, 537.86, 551.26, 589.89, 606.75, 619.14, 624.37, 629.58, 644.77, 664.71, 704.36, 712.29, 721.09, 732.35, 744.82, 757.37, 761.66, 772.73, 798.32, 811.6, 839.17, 849.6, 862.5, 865.73, 871.25, 887.24, 894.1, 924.34, 930.98, 931.38, 952.72, 962.09, 983.12, 984.29, 988.4, 989.62, 992.79, 993.16, 999.81, 1003.1, 1003.27, 1011.62, 1012.79, 1027.14, 1044.1, 1047.4, 1048.25, 1051.4, 1060.91, 1078.5, 1092.34, 1104.84, 1107.18, 1122.8, 1152.75, 1164.89, 1174.51, 1177.81, 1177.96, 1185.74, 1194.88, 1197.97, 1198.47, 1216.2, 1221, 1222.23, 1225.76, 1230.83, 1249.17, 1278.45, 1290.38, 1307.57, 1311.18, 1323.53, 1330.65, 1339.63, 1346.91, 1351.67, 1354.57, 1356.02, 1362.82, 1363.7, 1384.13, 1399.51, 1473.7, 1475.37, 1481.35, 1482.79, 1489.96, 1491.27, 1492.77, 1503.87, 1516.17, 1518.17, 1523.08, 1527.15, 1617.92, 1620.75, 1624.85, 1637.23, 1639.62, 1644.01, 2986.14, 3009.41, 3021.52, 3034.48, 3036.19, 3049.64, 3058.04, 3066.34, 3066.84, 3069.41, 3091, 3096.47, 3107.26, 3151.19, 3153.77, 3157.64, 3160.81, 3162.6, 3162.99, 3171.86, 3172.57, 3173.2, 3181.2, 3184.39, 3184.88, 3190.09, 3196.48.

**6c** ***cis***

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.471306 (Hartr
Thermal correction to Energy= 0.494097
Thermal correction to Enthalpy= 0.495041
Thermal correction to Gibbs Free Energy= 0.417810
Sum of electronic and zero-point Energies= -1136.323541
Sum of electronic and thermal Energies= -1136.300750
Sum of electronic and thermal Enthalpies= -1136.299806
Sum of electronic and thermal Free Energies= -1136.377037

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.32539700 | -1.22242300 | 2.22596100 |
| C | 0.17313300 | -1.57093700 | 0.81141800 |
| H | -0.13678200 | -2.08368200 | 2.87410500 |
| H | 0.21706900 | -0.36664300 | 2.63154200 |
| C | 1.46536400 | -2.38545800 | 0.75449900 |
| H | 2.12586200 | -2.04480900 | 1.55585900 |
| H | 1.26982600 | -3.44830900 | 0.90187000 |
| C | 2.09110100 | -2.06034900 | -0.61887500 |
| H | 3.16404600 | -1.89150900 | -0.52344400 |
| H | 1.95046200 | -2.87351400 | -1.33229700 |
| C | 1.35990600 | -0.79526100 | -1.10436800 |
| O | -0.51852000 | 0.38583700 | -0.36356700 |
| N | 0.60575100 | -0.35060300 | 0.07935100 |
| C | -0.56045600 | 1.66357400 | 0.24490400 |
| H | -0.41992000 | 1.55902100 | 1.32828100 |
| H | 0.24714400 | 2.29934600 | -0.13753200 |
| C | -1.84567600 | -1.01199000 | 2.10033000 |
| H | -2.09144000 | 0.03186500 | 1.87479200 |
| H | -2.38949700 | -1.28760000 | 3.00601500 |
| C | -2.19961400 | -1.88731100 | 0.92176100 |
| C | -1.05616700 | -2.22734900 | 0.19481500 |
| C | -3.45109600 | -2.33990500 | 0.52265800 |
| C | -1.15512800 | -3.03522300 | -0.93232700 |
| C | -3.55098900 | -3.14455900 | -0.61143700 |
| H | -4.33888300 | -2.07635000 | 1.08870800 |
| C | -2.41056700 | -3.49261200 | -1.33222400 |
| H | -0.27355500 | -3.31919800 | -1.49741700 |
| H | -4.52069900 | -3.50890000 | -0.93143300 |
| H | -2.49864500 | -4.12718700 | -2.20670300 |
| C | -1.89682700 | 2.29800000 | -0.04769900 |
| C | -2.03859800 | 3.67929600 | 0.09043900 |
| C | -3.00181200 | 1.53279200 | -0.41995200 |
| C | -3.26803700 | 4.28929100 | -0.12879100 |
| H | -1.17813100 | 4.28109000 | 0.36771200 |
| C | -4.23199400 | 2.14637200 | -0.64478000 |
| H | -2.89077400 | 0.46134300 | -0.54369100 |
| C | -4.37046300 | 3.52213400 | -0.49731300 |
| H | -3.36470300 | 5.36356600 | -0.01929600 |
| H | -5.08418700 | 1.54369600 | -0.93857800 |
| H | -5.32885800 | 3.99681100 | -0.67357400 |
| C | 2.25276000 | 0.33026400 | -1.64803400 |
| H | 2.61377300 | 0.02873600 | -2.63549900 |
| C | 3.43697900 | 0.68013700 | -0.77875400 |

| | | | |
|---|---|---|---|
| C | 3.28263700 | 1.36243700 | 0.43177500 |
| C | 4.72713200 | 0.30855700 | -1.16542600 |
| C | 4.38400000 | 1.66485300 | 1.22659200 |
| H | 2.29035600 | 1.65228600 | 0.75409500 |
| C | 5.83207300 | 0.60826600 | -0.37348500 |
| H | 4.86746300 | -0.21928500 | -2.10383400 |
| C | 5.66327100 | 1.28801100 | 0.82793600 |
| H | 4.24210100 | 2.19750000 | 2.16034700 |
| H | 6.82354400 | 0.31184400 | -0.69672800 |
| H | 6.52110200 | 1.52678400 | 1.44615200 |
| H | 0.63848500 | -1.05284500 | -1.89080500 |
| H | 1.61952300 | 1.20983700 | -1.80331200 |

**Vibrational frequencies**

21.71, 31.24, 37.1, 43.6, 54.73, 63.04, 87.23, 103.47, 116.87, 122.79, 140.93, 173.27, 206.36, 225.84, 233.07, 236.69, 268.23, 274.97, 303.64, 332.73, 364.55, 408.41, 414.19, 420.56, 434.52, 441.39, 465.61, 470.37, 486.88, 496.72, 524.65, 554.78, 566.91, 601.51, 618.69, 630.23, 630.99, 643.18, 666.55, 677.52, 714.24, 725.6, 735.57, 753.83, 756.32, 766.8, 782.29, 789.5, 811.52, 831.14, 846.43, 866.23, 882.39, 882.51, 893.38, 912.42, 923.83, 940.37, 951.6, 960.44, 983.72, 988.44, 1003.92, 1012.68, 1013.39, 1017.36, 1019.61, 1021.46, 1023.78, 1027.81, 1030.49, 1038.89, 1054.51, 1060.35, 1062.54, 1063.9, 1076.59, 1089.47, 1098.54, 1110.37, 1111.3, 1120.77, 1147.76, 1157.66, 1170.29, 1171.11, 1174.12, 1175.68, 1182.48, 1196.48, 1200.81, 1202.87, 1208.66, 1229.38, 1233.84, 1235.73, 1242.13, 1253.43, 1256.73, 1293.45, 1304.3, 1316.12, 1318.37, 1325.99, 1333.6, 1337.88, 1344.02, 1349.18, 1353.6, 1359.12, 1363.18, 1372.98, 1405.79, 1417.58, 1471.87, 1479.35, 1481.18, 1493.15, 1494.01, 1495.15, 1499.91, 1505.88, 1510.01, 1524.85, 1539.14, 1540.87, 1658.35, 1659.68, 1660.73, 1678.84, 1683.19, 1683.43, 3031.19, 3032.48, 3052.46, 3057.53, 3068.05, 3069.32, 3070.56, 3085.52, 3098.01, 3111.12, 3120.12, 3123.1, 3136.44, 3174.94, 3180.57, 3181.26, 3187.82, 3191.99, 3194, 3196.91, 3197.07, 3203.58, 3204.86, 3210.28, 3213.03, 3216.55, 3224.63.

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.465268 (Hartr
Thermal correction to Energy= 0.488911
Thermal correction to Enthalpy= 0.489855
Thermal correction to Gibbs Free Energy= 0.407541

Sum of electronic and zero-point Energies= -1136.798857
Sum of electronic and thermal Energies= -1136.775214
Sum of electronic and thermal Enthalpies= -1136.774270
Sum of electronic and thermal Free Energies= -1136.856584

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.91457600 | -1.72988100 | -2.10436800 |
| C | 0.70035300 | -1.63710200 | -1.14430800 |
| H | 1.60553600 | -1.91204800 | -3.13565500 |
| H | 2.44367800 | -0.77372400 | -2.07650300 |
| C | -0.46837600 | -2.57470800 | -1.53284500 |
| H | -0.59305100 | -2.56134600 | -2.62024700 |
| H | -0.28869900 | -3.60574600 | -1.22500000 |
| C | -1.68690800 | -1.94506700 | -0.85017600 |
| H | -2.63188900 | -2.26183400 | -1.29491400 |
| H | -1.71150100 | -2.22340600 | 0.20749800 |
| C | -1.44705900 | -0.43215100 | -0.99716900 |
| H | -1.93058100 | -0.08376500 | -1.91695100 |
| O | 0.67734000 | 0.64564400 | -0.40052400 |
| N | 0.03642300 | -0.31488200 | -1.23543400 |
| C | 1.05621300 | 1.79817100 | -1.17097300 |
| H | 1.67981100 | 1.47593800 | -2.01282700 |
| H | 0.16731600 | 2.28687900 | -1.58510800 |
| C | -3.50595500 | 0.38805200 | 0.23252500 |
| C | -4.28856200 | 1.08887900 | -0.69546500 |

| | | | |
|---|---|---|---|
| C | -4.16259500 | -0.35309600 | 1.22154700 |
| C | -5.68009900 | 1.04494500 | -0.64084400 |
| H | -3.80328800 | 1.68238400 | -1.46451800 |
| C | -5.55549800 | -0.39944700 | 1.28150700 |
| H | -3.57786600 | -0.89491900 | 1.95803900 |
| C | -6.32006400 | 0.29789000 | 0.34838500 |
| H | -6.26554500 | 1.59862800 | -1.36720000 |
| H | -6.04182800 | -0.97793300 | 2.05971200 |
| H | -7.40304300 | 0.26548900 | 0.39411400 |
| C | -1.99370600 | 0.42791700 | 0.15735400 |
| H | -1.66463900 | 1.46032700 | 0.01823500 |
| C | 2.82494400 | -2.82769000 | -1.52118300 |
| H | 3.88250600 | -2.67193000 | -1.75015500 |
| H | 2.55593400 | -3.81574900 | -1.91468500 |
| C | 2.52661600 | -2.74926900 | -0.04045400 |
| C | 1.33666700 | -2.04761000 | 0.19307000 |
| C | 3.26598300 | -3.27019700 | 1.01830200 |
| C | 0.89163100 | -1.85466400 | 1.49920800 |
| C | 2.81504100 | -3.07791400 | 2.32533300 |
| H | 4.18833100 | -3.81207700 | 0.83225400 |
| C | 1.63557500 | -2.37044100 | 2.56285100 |
| H | -0.00922000 | -1.29100600 | 1.70338600 |
| H | 3.38777300 | -3.46994000 | 3.15902600 |
| H | 1.29888400 | -2.21045700 | 3.58158100 |
| C | 1.80502200 | 2.74890800 | -0.27142500 |
| C | 2.90109100 | 2.30775300 | 0.48050900 |
| C | 1.43031500 | 4.09277700 | -0.19215200 |
| C | 3.60521200 | 3.19467800 | 1.29056400 |
| H | 3.19333300 | 1.26482800 | 0.43833600 |
| C | 2.14143600 | 4.98551200 | 0.61041300 |
| H | 0.57638500 | 4.44470200 | -0.76235300 |
| C | 3.22972400 | 4.53757000 | 1.35546900 |
| H | 4.44877500 | 2.83887300 | 1.87214900 |
| H | 1.83946900 | 6.02608700 | 0.65857200 |
| H | 3.78042900 | 5.22762400 | 1.98535800 |
| H | -1.56921400 | 0.09421900 | 1.10632000 |

**Vibrational frequencies**

10.95, 15.35, 20.15, 22.99, 40.42, 45.4, 67.36, 81.21, 89.46, 90.25, 127.67, 175.74, 187.09, 199.44, 228, 245.31, 248.07, 270.19, 298.59, 329.41, 352.99, 367.92, 396.54, 411.47, 414.75, 426.38, 437.91, 477.66, 499.08, 509.02, 533.61, 543.65, 555.11, 585.34, 599.76, 603.64, 633.76, 635.46, 655.96, 667.43, 706.02, 712.13, 716.27, 737.34, 754.59, 758.67, 772.04, 790.77, 814.25, 833.73, 843.67, 851.11, 858.16, 859.66, 875.35, 884.71, 888.93, 923.86, 929.46, 949.37, 953.79, 961.02, 977.1, 988.66, 988.74, 994.35, 996.22, 1004.67, 1005.36, 1006.49, 1016.04, 1016.57, 1020.9, 1040.45, 1047.27, 1047.66, 1049.27, 1058.29, 1074.83, 1088.14, 1092.96, 1106.06, 1110.72, 1120.75, 1138.2, 1156.22, 1176.34, 1176.89, 1177.43, 1182.19, 1196.5, 1198.49, 1204.01, 1213.79, 1221.9, 1226.43, 1230.84, 1231.66, 1237.62, 1278.26, 1291.18, 1309.44, 1320.9, 1324.88, 1329.06, 1331.38, 1336.19, 1342.94, 1350.99, 1352.74, 1355.24, 1361.31, 1391.03, 1395.49, 1475.87, 1477.89, 1479.94, 1481.69, 1483.83, 1487.06, 1490.41, 1497.87, 1502.23, 1504.5, 1524.2, 1525.87, 1620.44, 1621.1, 1623.82, 1641.38, 1641.85, 1644.85, 3002.61, 3009.26, 3012.04, 3036.16, 3042.33, 3043.63, 3048.49, 3056.65, 3066.95, 3093.69, 3096.12, 3097.57, 3103.36, 3153.63, 3156.7, 3157.86, 3159.46, 3164.73, 3166.51, 3169.46, 3174.68, 3176.74, 3181.47, 3184.82, 3188.9, 3191.31, 3202.95.

**mPWPW91/6-311+G(*d*,*p*)**

Zero-point correction= 0.453890
Thermal correction to Energy= 0.477852
Thermal correction to Enthalpy= 0.478796
Thermal correction to Gibbs Free Energy= 0.398792

Sum of electronic and zero-point Energies= -1136.635355
Sum of electronic and thermal Energies= -1136.611393
Sum of electronic and thermal Enthalpies= -1136.610449
Sum of electronic and thermal Free Energies= -1136.690454

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.88653200 | -1.74008100 | -1.97917200 |
| C | 0.75077900 | -2.05602500 | -0.96707200 |
| H | 1.62627700 | -2.06051700 | -2.99705000 |
| H | 2.03316200 | -0.65014200 | -1.99553600 |
| C | -0.03570700 | -3.35109500 | -1.29089900 |
| H | -0.21173800 | -3.40392400 | -2.37682600 |
| H | 0.51178200 | -4.25310100 | -0.98866300 |
| C | -1.35750700 | -3.16187600 | -0.53869100 |
| H | -2.16559900 | -3.80011600 | -0.92302700 |
| H | -1.22369300 | -3.40293100 | 0.52758300 |
| C | -1.67382800 | -1.66174900 | -0.70393700 |
| H | -2.31084800 | -1.52348900 | -1.59397000 |
| O | -0.01299700 | 0.11919900 | -0.27620300 |
| N | -0.33818700 | -1.04470600 | -1.05177400 |
| C | -0.05975200 | 1.29124700 | -1.11810800 |
| H | 0.44121400 | 1.05776900 | -2.07302200 |
| H | -1.10539500 | 1.55727400 | -1.34767000 |
| C | -3.14176900 | 0.24993200 | 0.28562100 |
| C | -2.88725500 | 1.35695600 | 1.11259100 |
| C | -4.11341600 | 0.38766100 | -0.72345400 |
| C | -3.57377400 | 2.56420800 | 0.93678200 |
| H | -2.13331500 | 1.27467100 | 1.89803100 |
| C | -4.79931600 | 1.59348000 | -0.90616900 |
| H | -4.34411200 | -0.46040600 | -1.37267300 |
| C | -4.53064000 | 2.68940300 | -0.07661800 |
| H | -3.35352000 | 3.41038000 | 1.59016700 |
| H | -5.54951900 | 1.67558200 | -1.69508000 |
| H | -5.06558300 | 3.63023500 | -0.21683900 |
| C | -2.42396700 | -1.06796700 | 0.50587500 |
| H | -1.73998200 | -0.97337200 | 1.35982200 |
| C | 3.15606400 | -2.41035200 | -1.41518500 |
| H | 4.08069000 | -1.88266100 | -1.69125100 |
| H | 3.25843400 | -3.44611600 | -1.78288700 |
| C | 2.89933700 | -2.40628300 | 0.07605300 |
| C | 1.53625900 | -2.18547400 | 0.35011900 |
| C | 3.81725100 | -2.59244600 | 1.11429000 |
| C | 1.09247900 | -2.14645200 | 1.67679100 |
| C | 3.36790300 | -2.55280200 | 2.44114200 |
| H | 4.87457900 | -2.75941800 | 0.89584000 |
| C | 2.01290200 | -2.32903100 | 2.71889700 |
| H | 0.04639000 | -1.95409200 | 1.91368500 |
| H | 4.07653900 | -2.68622400 | 3.26061100 |
| H | 1.67142800 | -2.28597000 | 3.75483500 |
| C | 0.62977000 | 2.44008500 | -0.41854600 |
| C | 1.72468700 | 2.23394000 | 0.43755200 |

| | | | |
|---|---|---|---|
| C | 0.19469100 | 3.75467900 | -0.65654700 |
| C | 2.37006500 | 3.32148800 | 1.03745600 |
| H | 2.06034000 | 1.21773300 | 0.64274100 |
| C | 0.84851600 | 4.84236600 | -0.06782200 |
| H | -0.66817900 | 3.92635600 | -1.30416000 |
| C | 1.93868800 | 4.62894200 | 0.78431400 |
| H | 3.21493800 | 3.14474200 | 1.70580300 |
| H | 0.49887800 | 5.85732000 | -0.26572600 |
| H | 2.44401500 | 5.47543000 | 1.25241600 |
| H | -3.17598700 | -1.82507300 | 0.78941700 |

**Vibrational frequencies**

16.22, 26.24, 34.53, 36.28, 52.22, 57.67, 78.69, 92.85, 106.16, 120.09, 136.02, 178.82, 185.35, 190.79, 218.45, 236.77, 256.86, 277.44, 287.77, 315.15, 332.09, 360.64, 370.12, 401.53, 402.29, 429.05, 433.09, 462.15, 470.87, 486.01, 520.57, 532.76, 547.25, 571.94, 579.32, 585.17, 600.1, 613.5, 614.94, 646.64, 685.32, 689.38, 692.71, 718.5, 721.88, 726.43, 742.62, 769.03, 792.84, 805.03, 819.93, 828, 829.46, 830.57, 843.05, 850.29, 867.99, 888.92, 892.3, 917.54, 921.52, 931.95, 951.46, 951.93, 957.12, 960.61, 965.99, 966.51, 974.1, 982.3, 987.96, 988.39, 994.74, 1004.85, 1015.44, 1023.43, 1025.77, 1026.84, 1045.75, 1059.65, 1063.94, 1072.51, 1076.72, 1088.27, 1109.41, 1129.7, 1144.88, 1146.54, 1147.39, 1156.51, 1160.92, 1168.35, 1169.74, 1180.96, 1188.26, 1193.83, 1195.14, 1203.06, 1205.13, 1236.14, 1251.38, 1264.35, 1279.15, 1282, 1290.4, 1294.48, 1299.29, 1301.42, 1314.81, 1332.8, 1340.28, 1347.05, 1349, 1356.92, 1411.62, 1427.41, 1432.53, 1436.22, 1438.53, 1441.23, 1442.97, 1447.8, 1451.88, 1458.8, 1479.96, 1481.08, 1577.78, 1578.64, 1580.11, 1597.1, 1598.09, 1600.29, 2943.84, 2946.08, 2954.98, 2955.93, 2977.12, 2979.72, 2981.56, 2995.13, 3012.29, 3029.42, 3035.79, 3046.02, 3048.49, 3094.69, 3095.69, 3095.98, 3102.63, 3104.3, 3106.33, 3110.74, 3113.73, 3118.48, 3120.63, 3126.62, 3129.19, 3135.67, 3138.41.

**TPSSh/6-311+G(*d*,*p*)**

Zero-point correction= 0.464760 (Hartr
Thermal correction to Energy= 0.488258
Thermal correction to Enthalpy= 0.489203
Thermal correction to Gibbs Free Energy= 0.409920

Sum of electronic and zero-point Energies= -1136.874163
Sum of electronic and thermal Energies= -1136.850664
Sum of electronic and thermal Enthalpies= -1136.849720
Sum of electronic and thermal Free Energies= -1136.929003

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.87584100 | -1.73390100 | -1.97640500 |
| C | 0.74663100 | -2.05075400 | -0.96578200 |
| H | 1.61208900 | -2.04316400 | -2.99085800 |
| H | 2.03229600 | -0.65094400 | -1.97935300 |
| C | -0.03331700 | -3.34679600 | -1.28159200 |
| H | -0.22423100 | -3.39682900 | -2.35925400 |
| H | 0.51870700 | -4.24149500 | -0.98667000 |
| C | -1.34312000 | -3.16005800 | -0.51261800 |
| H | -2.14806900 | -3.80540300 | -0.87436800 |
| H | -1.18910000 | -3.38079000 | 0.54933100 |
| C | -1.67084600 | -1.66817100 | -0.69763000 |
| H | -2.30663500 | -1.54657100 | -1.58224100 |
| O | -0.02504500 | 0.11120500 | -0.27691000 |
| N | -0.34436100 | -1.04741000 | -1.05399800 |
| C | -0.05171700 | 1.27489900 | -1.12235300 |
| H | 0.46780300 | 1.03543900 | -2.05749900 |
| H | -1.08627800 | 1.53929900 | -1.36975900 |
| C | -3.12702200 | 0.25202000 | 0.26731800 |
| C | -2.86845500 | 1.36452100 | 1.07716900 |
| C | -4.09248000 | 0.37911800 | -0.74236100 |
| C | -3.54683300 | 2.56907300 | 0.88432900 |

| | | | |
|---|---|---|---|
| H | -2.12035800 | 1.28903000 | 1.86066700 |
| C | -4.77057800 | 1.58188000 | -0.94171500 |
| H | -4.32342000 | -0.47191200 | -1.37762100 |
| C | -4.49854300 | 2.68437900 | -0.12912000 |
| H | -3.32467400 | 3.41864500 | 1.52264700 |
| H | -5.51472200 | 1.65664900 | -1.72893500 |
| H | -5.02600600 | 3.62059200 | -0.28230700 |
| C | -2.41396200 | -1.06377700 | 0.50711400 |
| H | -1.72910900 | -0.95554700 | 1.35080500 |
| C | 3.13710100 | -2.42041400 | -1.42036000 |
| H | 4.06187200 | -1.90978900 | -1.70428100 |
| H | 3.21577900 | -3.45493900 | -1.77911200 |
| C | 2.88713700 | -2.39964000 | 0.07072200 |
| C | 1.53200200 | -2.16762900 | 0.34673900 |
| C | 3.80546500 | -2.58054500 | 1.10409300 |
| C | 1.09372900 | -2.10982700 | 1.67019200 |
| C | 3.36253600 | -2.52242200 | 2.42777100 |
| H | 4.85507800 | -2.75658800 | 0.88539300 |
| C | 2.01424100 | -2.28616900 | 2.70730100 |
| H | 0.05549600 | -1.90873500 | 1.90684300 |
| H | 4.06908200 | -2.65110400 | 3.24197300 |
| H | 1.67922200 | -2.22909600 | 3.73845000 |
| C | 0.62671300 | 2.42010400 | -0.40927300 |
| C | 1.68973200 | 2.20795500 | 0.47709300 |
| C | 0.21086700 | 3.73240300 | -0.66526200 |
| C | 2.32448300 | 3.28960600 | 1.08957100 |
| H | 2.00847000 | 1.19504500 | 0.69459600 |
| C | 0.85358200 | 4.81399100 | -0.06298000 |
| H | -0.62534600 | 3.90731700 | -1.33664900 |
| C | 1.91256700 | 4.59549100 | 0.81966600 |
| H | 3.14315100 | 3.10997000 | 1.77973900 |
| H | 0.52051000 | 5.82546700 | -0.27426800 |
| H | 2.40833700 | 5.43511000 | 1.29659300 |
| H | -3.16321000 | -1.81170000 | 0.79910500 |

**Vibrational frequencies**

15.32, 24.82, 34.12, 38.99, 54.33, 59.73, 78.6, 93.1, 106.68, 120.6, 138.55, 180.01, 188.89, 193.22, 221.14, 239.86, 260.2, 280.51, 290.46, 318.29, 332.95, 364.7, 374.3, 412.39, 413.65, 435.38, 441.67, 470.46, 479.97, 495.13, 528.91, 541.36, 555.61, 583.13, 587.63, 596.7, 609.2, 622.38, 623.78, 656.62, 699.62, 707.56, 711.27, 736.93, 744.63, 748.18, 766.35, 785.06, 810.35, 819.78, 836.52, 848.23, 860.84, 863.06, 869.39, 879.4, 892.36, 921, 921.71, 946.59, 952.05, 955.97, 979.44, 988.95, 989.42, 993.09, 997.08, 1001.67, 1002.06, 1007.16, 1010.14, 1010.52, 1024.7, 1039.11, 1045.6, 1046.64, 1047.65, 1053.46, 1072.42, 1087.63, 1092.98, 1101, 1104.68, 1115.34, 1144.12, 1159.42, 1174.75, 1175.6, 1177.07, 1188.71, 1193.85, 1199.8, 1204.74, 1212.67, 1218.55, 1221.38, 1225.93, 1238.38, 1239.1, 1275.08, 1290.63, 1303.17, 1319.98, 1325.19, 1329.33, 1332.18, 1340.96, 1343.01, 1354.06, 1354.94, 1359.95, 1362.4, 1391.33, 1395.61, 1466.21, 1478.5, 1479.98, 1481.46, 1482.91, 1488.62, 1497.26, 1501.64, 1504.36, 1509.32, 1524.09, 1525.1, 1618.8, 1620.57, 1621.72, 1638.4, 1640.19, 1642.63, 3010.23, 3011.59, 3012.08, 3013.72, 3032.59, 3037.51, 3047.24, 3049.69, 3067.81, 3085.91, 3094.91, 3098.56, 3103.26, 3152.91, 3153.51, 3154.45, 3160.95, 3162.13, 3165.21, 3169.41, 3172.57, 3178.02, 3180.09, 3186.13, 3188.9, 3194.81, 3197.34.

## 19c

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.325560
Thermal correction to Energy= 0.344276
Thermal correction to Enthalpy= 0.345220
Thermal correction to Gibbs Free Energy= 0.276319
Sum of electronic and zero-point Energies= -843.367984
Sum of electronic and thermal Energies= -843.349268
Sum of electronic and thermal Enthalpies= -843.348324
Sum of electronic and thermal Free Energies= -843.417225

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.67411900 | -2.24991500 | -0.78424800 |
| C | 5.04408600 | -1.58257300 | -1.00849500 |
| C | 5.06746100 | -0.51294200 | 0.05558800 |
| C | 3.86690500 | -0.30353900 | 0.58601200 |
| C | 2.81532400 | -1.20064200 | -0.04626900 |
| H | 3.79489700 | -3.12179900 | -0.13644200 |
| H | 5.11780700 | -1.12761700 | -2.00190700 |
| H | 5.87215800 | -2.28888600 | -0.91708700 |
| H | 5.96322800 | 0.03712500 | 0.32018900 |
| H | 3.62815400 | 0.44430500 | 1.33188500 |
| H | 3.18531500 | -2.57152600 | -1.70479500 |
| C | 1.86919300 | -1.87079800 | 0.97317600 |
| H | 1.33464900 | -2.68291800 | 0.46866800 |
| H | 2.51336900 | -2.33561100 | 1.72503800 |
| C | 0.85934200 | -0.94753500 | 1.67821500 |
| H | 0.63837600 | -1.33311900 | 2.67676200 |
| H | 1.29681300 | 0.04779300 | 1.80949900 |
| C | -0.42457700 | -0.79998300 | 0.92153600 |
| H | -0.35522400 | -0.66682900 | -0.15424400 |
| C | -1.63381200 | -0.83290000 | 1.48623800 |
| H | -1.76770900 | -0.97294400 | 2.55328000 |
| O | 1.70469000 | 0.71326200 | -0.56950000 |
| N | 2.04900900 | -0.48611300 | -1.08093100 |
| C | 0.93880100 | 1.49573300 | -1.50411900 |
| H | 1.63658200 | 2.15451900 | -2.02846400 |
| H | 0.48017000 | 0.81339000 | -2.22168800 |
| C | -0.08977600 | 2.26981500 | -0.72899500 |
| C | -1.44419700 | 1.96981700 | -0.84782600 |
| C | 0.31421100 | 3.26748400 | 0.15991300 |
| C | -2.38901900 | 2.65369000 | -0.08785500 |
| H | -1.77018800 | 1.18829700 | -1.52714100 |
| C | -0.62526100 | 3.94870400 | 0.92287300 |
| H | 1.36950700 | 3.50222400 | 0.25495900 |
| C | -1.97903900 | 3.64225800 | 0.79866100 |
| H | -3.43696500 | 2.39508400 | -0.18074300 |
| H | -0.30413400 | 4.72129600 | 1.61164500 |
| H | -2.71179900 | 4.17462500 | 1.39351300 |
| C | -2.82355600 | -0.65910300 | 0.70926200 |
| N | -3.77962600 | -0.50909700 | 0.08518700 |

**Vibrational frequencies**

19.2, 39.2, 45.03, 59.61, 73.43, 94.1, 109.18, 119, 136.6, 146.83, 171.19, 198.02, 235.82, 249.01, 277.79, 291.04, 329.59, 341.25, 366.11, 397.3, 416.98, 443.52, 479.7, 502.01, 534.56, 548.92, 584.95, 610.93, 631.61, 651.04, 718.56, 728.95, 764.68, 778.62, 813.12, 827.25,

847.76, 851.32, 880.58, 893.82, 915.76, 945.26, 947.94, 971.05, 987.87, 990.75, 1004.46, 1008.38, 1010.54, 1021.63, 1027.9, 1031.75, 1046.71, 1064.77, 1066.41, 1077.45, 1114.54, 1120.25, 1130.24, 1148.16, 1174.98, 1179.47, 1185.26, 1206.3, 1208.39, 1235.52, 1246.39, 1250.45, 1275.7, 1278.16, 1315.9, 1328.7, 1331.85, 1336.75, 1344.9, 1355.87, 1370.4, 1381.79, 1388.73, 1401.72, 1475.83, 1479.67, 1486.19, 1497.48, 1498.25, 1509.8, 1547.15, 1667.08, 1689.15, 1704.54, 1719.35, 2382.86, 3055.56, 3055.79, 3062.62, 3064.54, 3072.27, 3099.13, 3103.62, 3106.57, 3127.53, 3143.29, 3172.78, 3173.96, 3183.16, 3186.12, 3188.81, 3191.24, 3197.54, 3207.51, 3217.52.

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## 19d

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.399312
Thermal correction to Energy= 0.422018
Thermal correction to Enthalpy= 0.422962
Thermal correction to Gibbs Free Energy= 0.343895

Sum of electronic and zero-point Energies= -1018.225238
Sum of electronic and thermal Energies= -1018.202532
Sum of electronic and thermal Enthalpies= -1018.201588
Sum of electronic and thermal Free Energies= -1018.280655

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 4.06706900 | -1.94253200 | -0.72889600 |
| C | 5.28141500 | -0.99464100 | -0.75428700 |
| C | 4.95814900 | -0.01437900 | 0.34627400 |
| C | 3.68955700 | -0.09224500 | 0.73494100 |
| C | 2.92951100 | -1.14792400 | -0.05171500 |
| H | 4.30026700 | -2.81678100 | -0.11571200 |
| H | 5.36918400 | -0.47099400 | -1.71214200 |
| H | 6.22477200 | -1.51994600 | -0.58898500 |
| H | 5.68082600 | 0.69230200 | 0.73833400 |
| H | 3.21593800 | 0.54280000 | 1.47297400 |
| H | 3.75954300 | -2.28899900 | -1.71629100 |
| C | 2.05033300 | -2.06671600 | 0.82293000 |
| H | 1.73343800 | -2.92189200 | 0.21637900 |
| H | 2.70746500 | -2.45834700 | 1.60477300 |
| C | 0.81911400 | -1.41706300 | 1.48390200 |
| H | 0.60941200 | -1.91368300 | 2.43449400 |
| H | 1.03277500 | -0.36666600 | 1.70898500 |
| C | -0.40700300 | -1.47156500 | 0.62792900 |
| H | -0.31865300 | -1.13785600 | -0.40245000 |
| C | -1.59791400 | -1.91147500 | 1.03178200 |
| H | -1.77733800 | -2.28380000 | 2.03396600 |
| O | 1.48431700 | 0.51235200 | -0.61386100 |
| N | 2.13755800 | -0.54518700 | -1.13524100 |
| C | 0.65652500 | 1.14602200 | -1.60475500 |
| H | 1.31316200 | 1.65381900 | -2.31631500 |
| H | 0.09126000 | 0.37127800 | -2.12828600 |
| C | -0.24890700 | 2.10306700 | -0.88586200 |
| C | -1.56284600 | 1.74099300 | -0.59409600 |
| C | 0.23320400 | 3.34257500 | -0.46589900 |
| C | -2.38565300 | 2.61291300 | 0.11294400 |
| H | -1.94232700 | 0.77838300 | -0.92441800 |
| C | -0.58768600 | 4.21243100 | 0.24137500 |
| H | 1.25678700 | 3.62165200 | -0.69478400 |
| C | -1.89958700 | 3.84662100 | 0.53191900 |
| H | -3.40767800 | 2.32809600 | 0.33444200 |

| | | | |
|---|---|---|---|
| H | -0.20804300 | 5.17470400 | 0.56417600 |
| H | -2.54160200 | 4.52491000 | 1.08176200 |
| O | -2.73986600 | -1.45170200 | -1.02194400 |
| C | -2.74566000 | -1.90078700 | 0.09916800 |
| O | -3.83269900 | -2.45852300 | 0.65503600 |
| C | -5.00571400 | -2.50388700 | -0.17100400 |
| H | -5.27150200 | -1.48400500 | -0.45828000 |
| H | -4.76965600 | -3.05521800 | -1.08370700 |
| C | -6.09836400 | -3.17146700 | 0.63229200 |
| H | -6.30556900 | -2.60827100 | 1.54336000 |
| H | -7.01405400 | -3.22209200 | 0.04037500 |
| H | -5.80761900 | -4.18566800 | 0.90944300 |

**Vibrational frequencies**

21.72, 32.31, 35.47, 38.41, 51.44, 63.21, 71.43, 76.56, 88.82, 104.17, 125.43, 139.43, 166.25, 180.19, 183.82, 229.33, 243.29, 251.15, 264.76, 282.36, 290.77, 341.98, 348.25, 378.55, 381.2, 394.9, 415.82, 439.29, 462.35, 505.11, 514.25, 553.05, 617.27, 632.87, 654.31, 716.98, 728.51, 734.96, 757.57, 771.91, 779.45, 819.23, 826.41, 850.95, 854.34, 872.77, 880.08, 891.21, 911.3, 932.63, 948.2, 956.18, 978.42, 989.39, 993.03, 1003.41, 1011.81, 1013.85, 1020.56, 1021.74, 1026.02, 1051.1, 1063.98, 1073.21, 1082.28, 1095.94, 1119.5, 1124.75, 1132.1, 1147.46, 1152.19, 1178.76, 1182.39, 1186.22, 1190.7, 1203.17, 1213.22, 1226.73, 1238.28, 1256.04, 1256.48, 1271.25, 1295.95, 1313.99, 1320.04, 1331.66, 1336.24, 1342.73, 1357, 1366.34, 1375.41, 1385.97, 1391.02, 1407.8, 1410.35, 1444.49, 1477.96, 1482.3, 1487.55, 1493.44, 1498.75, 1501.5, 1505.36, 1519.14, 1528.84, 1548.11, 1666.52, 1687.96, 1700.49, 1736.22, 1813.98, 3051.42, 3051.67, 3062.87, 3065.17, 3071.31, 3078.19, 3087.01, 3096.42, 3099.94, 3107.38, 3126.3, 3130.31, 3135.7, 3145.27, 3152.58, 3179.54, 3184.8, 3185.99, 3189.94, 3196.1, 3199.77, 3202.06, 3210.16, 3224.7.

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## 19e

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.360420
Thermal correction to Energy= 0.379632
Thermal correction to Enthalpy= 0.380576
Thermal correction to Gibbs Free Energy= 0.311584

Sum of electronic and zero-point Energies= -865.604793
Sum of electronic and thermal Energies= -865.585581
Sum of electronic and thermal Enthalpies= -865.584636
Sum of electronic and thermal Free Energies= -865.653628

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 4.18680200 | -1.85411900 | -0.77542500 |
| C | 5.26067900 | -0.83639100 | -0.34875900 |
| C | 4.72705700 | -0.32929300 | 0.96954000 |
| C | 3.45339500 | -0.66003300 | 1.15729700 |
| C | 2.90303900 | -1.44943300 | -0.01877700 |
| H | 4.48352600 | -2.85463200 | -0.45064700 |
| H | 5.34699000 | -0.01091500 | -1.06346600 |
| H | 6.25158500 | -1.28733800 | -0.25827700 |
| H | 5.31893900 | 0.26587700 | 1.65560400 |
| H | 2.84563900 | -0.37353600 | 2.00631800 |
| H | 4.00904300 | -1.88117100 | -1.85127800 |
| C | 2.07509900 | -2.68777000 | 0.38248500 |
| H | 1.92560900 | -3.30071100 | -0.51422000 |
| H | 2.70655300 | -3.26860000 | 1.06202800 |
| C | 0.72187500 | -2.41780400 | 1.05010400 |
| H | 0.44691800 | -3.31107000 | 1.62356000 |
| H | 0.80270800 | -1.60635700 | 1.77893500 |
| C | -0.39192800 | -2.10651700 | 0.08893900 |

| | | | |
|---|---|---|---|
| H | -0.36076600 | -2.53893600 | -0.90564400 |
| C | -1.43429200 | -1.33967800 | 0.39535600 |
| O | 1.39096400 | 0.24599200 | -0.19010800 |
| N | 2.12332400 | -0.60571300 | -0.93609200 |
| C | 0.53169600 | 1.00910500 | -1.02604300 |
| H | 1.15135400 | 1.60800100 | -1.70218600 |
| H | -0.07250400 | 0.32137000 | -1.62391600 |
| C | -0.34243200 | 1.89431800 | -0.18001400 |
| C | -0.09321600 | 2.10629900 | 1.17385000 |
| C | -1.41581800 | 2.54903400 | -0.78651100 |
| C | -0.90106000 | 2.97349600 | 1.90463400 |
| H | 0.72684800 | 1.58539200 | 1.65154600 |
| C | -2.21977600 | 3.41739600 | -0.05722700 |
| H | -1.61915700 | 2.38036400 | -1.83986200 |
| C | -1.96232700 | 3.63310800 | 1.29418700 |
| H | -0.69915500 | 3.13219700 | 2.95777300 |
| H | -3.04708900 | 3.92229900 | -0.54225400 |
| H | -2.58638100 | 4.30894400 | 1.86686600 |
| O | -1.55838900 | -0.76006600 | 1.61878800 |
| C | -2.71000500 | 0.04750400 | 1.77871900 |
| H | -2.63355500 | 0.51414000 | 2.75892700 |
| H | -2.75115400 | 0.82992800 | 1.01395600 |
| H | -3.61861900 | -0.56275000 | 1.73547800 |
| H | -2.23859200 | -1.13543700 | -0.30854800 |

**Vibrational frequencies**

19.20, 39.49, 65.97, 75.4, 81.59, 92.86, 118.72, 137.62, 155.01, 179.94, 182.89, 195.18, 204.12, 223.72, 243.57, 253.13, 291.15, 296.63, 352.88, 375.9, 406.71, 408.38, 433.11, 465.98, 477.85, 494.96, 554.65, 615.19, 631.28, 647.81, 707.32, 709.91, 726.85, 735.11, 748.77, 770.45, 820.64, 845.09, 855.55, 870.84, 875.61, 926.83, 929.6, 947.32, 957.9, 975.03, 986.46, 993, 1006.18, 1010.31, 1019.17, 1019.79, 1032.82, 1059.39, 1065.34, 1071.04, 1094.41, 1106.74, 1118.37, 1131.99, 1156.06, 1180.27, 1183.28, 1183.95, 1189.64, 1196.68, 1208.26, 1212.1, 1221.77, 1242.87, 1248.15, 1265.43, 1271.51, 1291.1, 1306.03, 1328.12, 1331.06, 1335.83, 1358.83, 1359.83, 1376.92, 1387.84, 1413.81, 1430.64, 1472.44, 1476.49, 1480.39, 1492.47, 1496.32, 1499.97, 1501.53, 1507.55, 1520.18, 1549.19, 1662.39, 1687.71, 1697.96, 1756.8, 3032.09, 3039.34, 3046.45, 3051.81, 3063.31, 3068.67, 3087.09, 3097.71, 3102.5, 3106.58, 3110.71, 3129.27, 3146.58, 3168.78, 3177.74, 3180.87, 3190.34, 3197.03, 3204.31, 3217.85, 3233.21, 3233.68.

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## 19f

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.354164
Thermal correction to Energy= 0.372959
Thermal correction to Enthalpy= 0.373903
Thermal correction to Gibbs Free Energy= 0.304273

Sum of electronic and zero-point Energies= -790.401755
Sum of electronic and thermal Energies= -790.382960
Sum of electronic and thermal Enthalpies= -790.382015
Sum of electronic and thermal Free Energies= -790.451645

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.77494500 | -2.05360200 | -0.71782400 |
| C | 5.04475600 | -1.18160400 | -0.71301300 |
| C | 4.81147300 | -0.26856400 | 0.46609900 |
| C | 3.54913100 | -0.29433900 | 0.88077500 |
| C | 2.70502100 | -1.23819900 | 0.03985800 |
| H | 3.96570700 | -2.97744400 | -0.16574000 |
| H | 5.13777200 | -0.59379200 | -1.63261200 |

| | | | |
|---|---|---|---|
| H | 5.95800100 | -1.77344100 | -0.61759800 |
| H | 5.58733000 | 0.35863300 | 0.88989200 |
| H | 3.13175100 | 0.31113900 | 1.67526600 |
| H | 3.42525100 | -2.31736100 | -1.71684800 |
| C | 1.78266300 | -2.15770500 | 0.86972600 |
| H | 1.43447800 | -2.97154200 | 0.22439000 |
| H | 2.42022200 | -2.60852200 | 1.63631900 |
| C | 0.57161900 | -1.48123500 | 1.53428900 |
| H | 0.31512500 | -2.01604400 | 2.45277300 |
| H | 0.84023000 | -0.45963600 | 1.82656300 |
| C | -0.64182900 | -1.44601700 | 0.64604000 |
| H | -0.48032000 | -1.13114200 | -0.38425600 |
| C | -1.87190600 | -1.78364800 | 1.02408100 |
| H | -2.03309100 | -2.11601400 | 2.04908500 |
| O | 1.42748600 | 0.59705100 | -0.39244600 |
| N | 1.93178400 | -0.50929700 | -0.97883500 |
| C | 0.65867600 | 1.35958700 | -1.32919800 |
| H | 1.32445100 | 1.72399000 | -2.11526300 |
| H | -0.08400400 | 0.69326600 | -1.77899100 |
| C | -3.07955100 | -1.73180000 | 0.13598700 |
| C | 0.00704200 | 2.49059900 | -0.58563500 |
| C | -0.85726900 | 2.21504400 | 0.47569400 |
| C | 0.24864100 | 3.81316300 | -0.94410800 |
| C | -1.46860700 | 3.25296200 | 1.16671000 |
| H | -1.04369500 | 1.18284800 | 0.75714700 |
| C | -0.37145800 | 4.85451500 | -0.25816800 |
| H | 0.92654300 | 4.03150000 | -1.76252800 |
| C | -1.22910200 | 4.57530600 | 0.79868700 |
| H | -2.13618100 | 3.03189600 | 1.99126200 |
| H | -0.17856200 | 5.88122900 | -0.54601500 |
| H | -1.71015500 | 5.38423500 | 1.33600100 |
| H | -2.81290600 | -1.39388800 | -0.86719700 |
| H | -3.55135000 | -2.71486900 | 0.05290500 |
| H | -3.83318500 | -1.04816800 | 0.53775900 |

**Vibrational frequencies**

23.47, 31.16, 38.83, 48, 53.31, 69.26, 108.72, 127.31, 148.48, 168.28, 184.48, 211.05, 225.65, 242.75, 251.31, 291.07, 311.99, 320.63, 354.66, 393.32, 412.44, 449.43, 474.84, 497.71, 513, 555.32, 617.92, 632.09, 649.66, 713.81, 725.69, 763.3, 769.93, 782.62, 825.43, 845.04, 852.76, 874.73, 885.03, 920.51, 944.62, 947.62, 952.98, 980.16, 991.23, 996.56, 1004.76, 1006.17, 1008.02, 1021.24, 1024.93, 1043.27, 1063.77, 1072.99, 1074.73, 1089.49, 1104.78, 1119.38, 1120.49, 1143.51, 1149.52, 1179.56, 1181.88, 1189.76, 1207.33, 1208.24, 1236.36, 1250.58, 1258.04, 1260.4, 1285.31, 1320.1, 1323.63, 1338.04, 1338.87, 1342.59, 1357.62, 1371.08, 1385.37, 1390.86, 1415.05, 1418.95, 1474.63, 1478.99, 1482.55, 1485.43, 1495.44, 1497.58, 1499.77, 1513.24, 1546.41, 1667.66, 1686.05, 1701.73, 1758.86, 3039.94, 3044.85, 3046.52, 3048.71, 3067.07, 3067.43, 3089.36, 3090.9, 3093.79, 3104.47, 3118.72, 3119.08, 3127.44, 3132.25, 3138.28, 3175.48, 3177.67, 3185.32, 3192.28, 3196.9, 3214.55, 3215.71.

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## 19g

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.382530 (Hartr
Thermal correction to Energy= 0.402357
Thermal correction to Enthalpy= 0.403301
Thermal correction to Gibbs Free Energy= 0.333033
Sum of electronic and zero-point Energies= -829.684439
Sum of electronic and thermal Energies= -829.664613
Sum of electronic and thermal Enthalpies= -829.663668
Sum of electronic and thermal Free Energies= -829.733936

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 4.00836100 | -2.09612500 | -0.73969700 |
| C | 5.23152500 | -1.18396600 | -0.53193900 |
| C | 4.86616600 | -0.42343000 | 0.71984500 |
| C | 3.57870800 | -0.54675300 | 1.02628800 |
| C | 2.84719100 | -1.42071800 | 0.02167100 |
| H | 4.20050200 | -3.07306800 | -0.28904100 |
| H | 5.36810700 | -0.48849600 | -1.36695600 |
| H | 6.16149700 | -1.74779200 | -0.42949900 |
| H | 5.57636300 | 0.18234900 | 1.27086300 |
| H | 3.07752700 | -0.05141100 | 1.84819600 |
| H | 3.74664700 | -2.24835200 | -1.78768500 |
| C | 1.91217200 | -2.47374200 | 0.65929200 |
| H | 1.61994100 | -3.18462800 | -0.12225000 |
| H | 2.52497000 | -3.02588300 | 1.37838500 |
| C | 0.65440500 | -1.94942100 | 1.36142700 |
| H | 0.30004200 | -2.73102000 | 2.04297000 |
| H | 0.91717300 | -1.09548400 | 1.99694700 |
| C | -0.46029500 | -1.56841000 | 0.41465000 |
| H | -0.28002800 | -1.78262700 | -0.63788000 |
| C | -1.61417800 | -0.99001400 | 0.75009900 |
| O | 1.50273900 | 0.38483300 | -0.29622200 |
| N | 2.10057000 | -0.62390800 | -0.96303400 |
| C | 0.60734900 | 1.08671000 | -1.14981200 |
| H | 1.18475500 | 1.60748900 | -1.92000200 |
| H | -0.04471100 | 0.35429300 | -1.63741700 |
| C | -2.63080500 | -0.59404000 | -0.28561600 |
| C | -0.21406600 | 2.05108200 | -0.33905500 |
| C | -0.25337900 | 2.00386300 | 1.05136800 |
| C | -0.99706000 | 2.98975700 | -1.01228900 |
| C | -1.06850700 | 2.88522200 | 1.75747400 |
| H | 0.34543900 | 1.26903500 | 1.57582000 |
| C | -1.81738700 | 3.86178700 | -0.30827000 |
| H | -0.96697800 | 3.03311800 | -2.09685300 |
| C | -1.85511700 | 3.81145300 | 1.08287500 |
| H | -1.09090200 | 2.84169400 | 2.84053500 |
| H | -2.42304900 | 4.58333100 | -0.84370200 |
| H | -2.49036300 | 4.49293900 | 1.63601400 |
| H | -2.33561200 | -0.92051100 | -1.28470300 |
| H | -3.61314300 | -1.02118600 | -0.05944800 |
| H | -2.74802900 | 0.49677400 | -0.29591200 |
| C | -1.99962800 | -0.66995100 | 2.16911000 |
| H | -2.35458200 | 0.36214200 | 2.24447000 |
| H | -2.82490100 | -1.31635600 | 2.48748100 |
| H | -1.17663800 | -0.80560400 | 2.87157000 |

**Vibrational frequencies**

28.50, 38.74, 39.3, 68.72, 73.45, 80.13, 112.51, 133.24, 165.06, 172.42, 191.98, 196.83, 213.04, 214.08, 240.34, 248.34, 286.49, 297.85, 307.32, 360.71, 392.37, 411.28, 417.65, 455.24, 471.61, 473.04, 479.61, 543.02, 554.54, 614.03, 631.91, 647.19, 708.58, 727.96, 748.04, 765.78, 815.28, 825.69, 827.92, 852.79, 861.01, 867.54, 906.05, 922.16, 939.76, 950.77, 969.32, 980.89, 991.72, 1000.56, 1004.08, 1014.65, 1019.2, 1021.4, 1034.95, 1043.16, 1060.55, 1064.4, 1087.89, 1094.27, 1104.44, 1115.18, 1119.93, 1133.22, 1157.46, 1177.15, 1181.6, 1195.85, 1200.53, 1203.43, 1225.2, 1245.18, 1246.35, 1267.58, 1276.69, 1298.47, 1322.42, 1330.74, 1334.57, 1349.61, 1351.03,

1373.61, 1387.98, 1397.6, 1412.55, 1415.58, 1421.28, 1470.57, 1476.04, 1476.68, 1481.2, 1488.75, 1493.88, 1496.34, 1497.4, 1502.64, 1513.12, 1547.16, 1666.86, 1689.99, 1697.33, 1762.26, 3022.04, 3032.89, 3036.47, 3037.56, 3044.79, 3060.22, 3070.22, 3072.73, 3079.28, 3085.28, 3091.59, 3094.17, 3103.91, 3122.4, 3128.79, 3135.74, 3142.63, 3169.29, 3181.61, 3189.75, 3191.88, 3202.51, 3208.25, 3235.02.

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## 19h

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.489817
Thermal correction to Energy= 0.515724
Thermal correction to Enthalpy=0.516668
Thermal correction to Gibbs Free Energy= 0.431808

Sum of electronic and zero-point Energies= -1213.000160
Sum of electronic and thermal Energies= -1212.974253
Sum of electronic and thermal Enthalpies= -1212.973309
Sum of electronic and thermal Free Energies= -1213.058169

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 4.14208100 | -1.78054200 | -0.97798300 |
| C | 5.15888700 | -0.63591700 | -0.80801000 |
| C | 4.74565600 | -0.02130600 | 0.50718500 |
| C | 3.54225300 | -0.42876300 | 0.89772800 |
| C | 2.92932800 | -1.39457700 | -0.10350200 |
| H | 4.57025900 | -2.70937000 | -0.59270200 |
| H | 5.07696800 | 0.10370200 | -1.61169300 |
| H | 6.19173500 | -0.99142600 | -0.80341300 |
| H | 5.35793600 | 0.69595200 | 1.04170900 |
| H | 3.01670400 | -0.09268000 | 1.78287400 |
| H | 3.83629500 | -1.94660500 | -2.01187600 |
| C | 2.28380800 | -2.64158700 | 0.53812000 |
| H | 2.07958600 | -3.36679700 | -0.25867400 |
| H | 3.05135100 | -3.08477800 | 1.17974000 |
| C | 1.01194600 | -2.41597600 | 1.36096900 |
| H | 0.86812400 | -3.28751300 | 2.01039300 |
| H | 1.13443000 | -1.56415400 | 2.03805000 |
| C | -0.23149700 | -2.22093900 | 0.53150200 |
| H | -0.11984100 | -2.41973500 | -0.53121700 |
| C | -1.41245900 | -1.81098100 | 1.01100600 |
| O | 1.23518900 | 0.11363100 | -0.23226400 |
| N | 1.96560700 | -0.72527500 | -0.99144200 |
| C | 0.20315000 | 0.73109600 | -1.00620900 |
| H | 0.67804900 | 1.27271200 | -1.83035100 |
| H | -0.44609900 | -0.04571000 | -1.41888500 |
| C | -2.60622400 | -1.56286800 | 0.15719900 |
| C | -3.76739100 | -1.01369200 | 0.71446700 |
| C | -2.60301800 | -1.81050300 | -1.22433900 |
| C | -4.86408200 | -0.68877400 | -0.07871500 |
| H | -3.80774000 | -0.81732700 | 1.77875800 |
| C | -3.69500800 | -1.48491300 | -2.01598600 |
| H | -1.73868700 | -2.26065600 | -1.69718500 |
| C | -4.83198500 | -0.91132600 | -1.44925500 |
| H | -5.74540400 | -0.25646200 | 0.38122200 |
| H | -3.66001900 | -1.68141600 | -3.08135000 |
| H | -5.68250000 | -0.65295900 | -2.06884600 |
| C | -0.56971800 | 1.64760400 | -0.10032100 |

| | | | |
|---|---|---|---|
| C | -1.95905200 | 1.70733000 | -0.18094300 |
| C | 0.09902400 | 2.43997900 | 0.83476400 |
| C | -2.67568800 | 2.54340800 | 0.67104500 |
| H | -2.48775300 | 1.08252500 | -0.89477300 |
| C | -0.61718900 | 3.27225300 | 1.68676000 |
| H | 1.17950100 | 2.38045900 | 0.90537300 |
| C | -2.00754900 | 3.32311000 | 1.60846400 |
| H | -3.75754200 | 2.56808400 | 0.61034000 |
| H | -0.09185200 | 3.87757700 | 2.41629400 |
| H | -2.56687400 | 3.96601200 | 2.27806100 |
| C | -1.54313300 | -1.53357600 | 2.47550500 |
| C | -1.79688300 | -2.57296600 | 3.37054500 |
| C | -1.40452400 | -0.23350300 | 2.96571100 |
| C | -1.90733100 | -2.31952700 | 4.73504000 |
| H | -1.90903000 | -3.58288800 | 2.98992700 |
| C | -1.51374700 | 0.01983200 | 4.32893500 |
| H | -1.21177900 | 0.57814400 | 2.27305800 |
| C | -1.76511600 | -1.02231900 | 5.21691000 |
| H | -2.10475500 | -3.13514200 | 5.42106500 |
| H | -1.40281400 | 1.03415900 | 4.69535900 |
| H | -1.85075100 | -0.82480900 | 6.27901500 |

**Vibrational frequencies**

14.59, 32.91, 46.46, 50.36, 55.94, 60.28, 63.02, 70.06, 87.91, 94.81, 107.01, 120.7, 128.08, 171.65, 178.59, 198.96, 218.92, 227.31, 251.48, 259.67, 267.23, 280.1, 303.34, 316.06, 350.71, 374.11, 402.74, 408.67, 412.94, 419.04, 425.73, 463.8, 481.46, 495.28, 519.61, 550.24, 589.6, 616.39, 621.18, 631.24, 631.74, 642.14, 649.53, 656.63, 706.51, 719.44, 721.98, 725.82, 744.84, 760.68, 767.42, 781.91, 801.66, 820.43, 834.99, 853.17, 857.49, 872.6, 881.3, 884.59, 894.34, 923.8, 943.4, 947.37, 948.97, 955.8, 962.35, 984.4, 996.51, 1004.41, 1008.04, 1010.63, 1013.41, 1015.61, 1016.56, 1020.8, 1022.76, 1024.4, 1024.55, 1030.21, 1056.72, 1062.36, 1065.01, 1067.25, 1074.9, 1088.89, 1109.26, 1112.65, 1118.32, 1121.83, 1123.36, 1155.51, 1177.02, 1178.32, 1179.72, 1181.64, 1192.9, 1198.42, 1202.57, 1205.66, 1207.42, 1221.27, 1234.79, 1251.1, 1260.3, 1263.61, 1278.21, 1305.45, 1316.24, 1320.48, 1328.97, 1333.91, 1337.21, 1349.54, 1355.11, 1362.4, 1363.3, 1380.61, 1389.8, 1399.75, 1416.24, 1464.63, 1477.55, 1480.9, 1484.69, 1487.37, 1495.74, 1498.99, 1507.96, 1536.55, 1546.17, 1546.55, 1651.35, 1654.56, 1663.96, 1674.19, 1679.04, 1686.77, 1698.61, 1723.27, 3029.52, 3038.92, 3055.23, 3068.64, 3072.93, 3075.55, 3088.5, 3100.51, 3117.9, 3130.12, 3158.9, 3170.67, 3177.58, 3180.78, 3183.44, 3185.02, 3187.36, 3189.57, 3191.33, 3195.65, 3199.65, 3203.54, 3205.36, 3206.83, 3209.24, 3212.51, 3213.52, 3217.82.

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## TS (19c → 21c)

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.325021 (Hartr
Thermal correction to Energy= 0.342721
Thermal correction to Enthalpy= 0.343665
Thermal correction to Gibbs Free Energy= 0.277351

Sum of electronic and zero-point Energies= -843.344654
Sum of electronic and thermal Energies= -843.326954
Sum of electronic and thermal Enthalpies= -843.326009
Sum of electronic and thermal Free Energies= -843.392324

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.19234600 | 3.52762600 | 1.60527200 |
| C | 1.30016000 | 3.66789200 | 1.25299900 |
| C | 1.30773200 | 3.46404500 | -0.24081800 |
| C | 0.16641000 | 2.94476300 | -0.67952100 |
| C | -0.81738800 | 2.70827900 | 0.45114300 |
| H | -0.66330400 | 4.51447800 | 1.61311000 |
| H | 1.90504600 | 2.89045300 | 1.73146200 |

| | | | |
|---|---|---|---|
| H | 1.70981700 | 4.63507800 | 1.55262000 |
| H | 2.16678600 | 3.68636900 | -0.86286300 |
| H | -0.04809100 | 2.68672900 | -1.71058200 |
| H | -0.37829200 | 3.05383200 | 2.57054800 |
| C | -2.26511600 | 3.04596500 | 0.11763900 |
| H | -2.83620400 | 3.07334500 | 1.04896100 |
| H | -2.33460300 | 4.02864800 | -0.35108500 |
| C | -2.79808700 | 1.92322400 | -0.79705400 |
| H | -3.83352300 | 1.67880100 | -0.55451900 |
| H | -2.78390500 | 2.23935100 | -1.84369800 |
| C | -1.93503200 | 0.67748200 | -0.67953600 |
| H | -1.02431600 | 0.66447600 | -1.27416000 |
| C | -2.51416300 | -0.56552700 | -0.47613500 |
| O | 0.27489800 | 0.72472400 | 0.90079000 |
| N | -0.95185200 | 1.29945100 | 0.88305100 |
| C | 0.27380000 | -0.42538700 | 1.76672300 |
| H | 0.01822700 | -0.08539400 | 2.77403800 |
| H | -0.48965600 | -1.12558500 | 1.42077200 |
| C | 1.64396100 | -1.03323500 | 1.71168300 |
| C | 1.91212800 | -2.08716600 | 0.84029800 |
| C | 2.66625400 | -0.52400100 | 2.51142300 |
| C | 3.19294500 | -2.62668300 | 0.77332500 |
| H | 1.11585500 | -2.48501000 | 0.21892900 |
| C | 3.94653600 | -1.06021500 | 2.44293300 |
| H | 2.45327100 | 0.29337000 | 3.19345000 |
| C | 4.20986600 | -2.11381300 | 1.57192100 |
| H | 3.39518700 | -3.44913200 | 0.09754300 |
| H | 4.73558800 | -0.66239300 | 3.07001400 |
| H | 5.20632900 | -2.53668000 | 1.51894700 |
| H | -3.51030300 | -0.66374000 | -0.06160900 |
| C | -1.79463500 | -1.75742300 | -0.72199900 |
| N | -1.19243100 | -2.72574000 | -0.91410200 |

**Vibrational frequencies**

557.01*i*, 27.63, 39.21, 41.99, 58.84, 86.66, 105.78, 109.04, 136.13, 150.62, 188.51, 216.84, 234.47, 272.85, 280.74, 319.65, 348.88, 361.95, 397.71, 413.05, 434.83, 444.5, 496.48, 506.64, 514.39, 579.13, 599.69, 628.6, 632.58, 690.2, 716.77, 730.9, 751.62, 776.43, 782.24, 801.18, 822.89, 854.28, 872.92, 879.41, 935.04, 948.5, 957.94, 973.59, 985.06, 988.17, 997.28, 1001.9, 1009.71, 1021.77, 1028.06, 1038.11, 1062.32, 1063.95, 1068.57, 1073.46, 1084.78, 1116.29, 1118.88, 1131.59, 1154.69, 1177, 1178.69, 1207.07, 1215.46, 1224.8, 1240.69, 1254.67, 1257.67, 1283.92, 1301.37, 1310.4, 1313.91, 1327.77, 1339.72, 1346.7, 1357.66, 1368.43, 1392.17, 1413.96, 1473.73, 1484.44, 1494.16, 1497.08, 1504.67, 1513.58, 1523.1, 1547.07, 1668.63, 1688.56, 1707.85, 2319.76, 3051.87, 3058.26, 3072.66, 3073.39, 3076.99, 3097.53, 3121.16, 3127.71, 3134.25, 3137.33, 3163.55, 3170.33, 3176.16, 3185.07, 3192.12, 3196.65, 3206.07, 3208.55, 3217.45.

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## TS (19d → 21d)

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.398342
Thermal correction to Energy= 0.419886
Thermal correction to Enthalpy= 0.420830
Thermal correction to Gibbs Free Energy= 0.344990
Sum of electronic and zero-point Energies= -1018.202651
Sum of electronic and thermal Energies= -1018.181107
Sum of electronic and thermal Enthalpies= -1018.180163
Sum of electronic and thermal Free Energies= -1018.256003

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -4.26684100 | -0.91509800 | -5.12526100 |
| C | -5.31655800 | -1.98933100 | -5.46269100 |
| C | -6.18129000 | -2.01667200 | -4.22737700 |
| C | -5.61872500 | -1.37764300 | -3.20742300 |
| C | -4.26780900 | -0.79877300 | -3.58018300 |
| H | -4.57696300 | 0.04880800 | -5.53832300 |
| H | -4.85185600 | -2.96927900 | -5.61551600 |
| H | -5.87919900 | -1.75104000 | -6.36847200 |
| H | -7.13128100 | -2.53659600 | -4.18237600 |
| H | -6.03489400 | -1.29910900 | -2.20926800 |
| H | -3.26853000 | -1.14670300 | -5.50310200 |
| C | -3.99940500 | 0.59552900 | -3.03010600 |
| H | -3.10500900 | 0.99135900 | -3.51900400 |
| H | -4.83132500 | 1.26694900 | -3.24861700 |
| C | -3.75123000 | 0.44469800 | -1.51633600 |
| H | -3.03199400 | 1.18504500 | -1.16250900 |
| H | -4.67960800 | 0.61124900 | -0.96303000 |
| C | -3.25842100 | -0.95690700 | -1.19314900 |
| H | -4.01674000 | -1.71722800 | -1.01483400 |
| C | -2.07754400 | -1.15795400 | -0.50295000 |
| O | -3.36656400 | -2.87165300 | -3.09308000 |
| N | -3.10561900 | -1.54018800 | -3.04960600 |
| C | -2.13772300 | -3.60194000 | -3.21416200 |
| H | -1.41533600 | -3.19780000 | -2.50207200 |
| H | -2.39367900 | -4.62266400 | -2.93052200 |
| C | -1.63327500 | -3.51289700 | -4.62947900 |
| C | -0.66064500 | -2.57992800 | -4.98265400 |
| C | -2.20835000 | -4.30622200 | -5.62229300 |
| C | -0.26522400 | -2.44275700 | -6.30986500 |
| H | -0.22557100 | -1.95139900 | -4.21316300 |
| C | -1.82033800 | -4.16804200 | -6.94997400 |
| H | -2.96876200 | -5.03141700 | -5.34911500 |
| C | -0.84713800 | -3.23426200 | -7.29505400 |
| H | 0.49358800 | -1.71610100 | -6.57564200 |
| H | -2.27257200 | -4.78914100 | -7.71427400 |
| H | -0.54098600 | -3.12655000 | -8.32893700 |
| C | -1.79092800 | -2.45481400 | 0.09716800 |
| O | -2.49462100 | -3.43953400 | 0.02903700 |
| O | -0.60942500 | -2.45208100 | 0.75440100 |
| C | -0.24481900 | -3.68596700 | 1.38261000 |
| C | 1.05800300 | -3.45184300 | 2.11401900 |
| H | -0.14960100 | -4.45939800 | 0.61612900 |
| H | -1.04658200 | -3.98979300 | 2.05939100 |
| H | 1.37937500 | -4.37182400 | 2.60584200 |
| H | 1.83859100 | -3.13854800 | 1.41911200 |
| H | 0.93755500 | -2.67656200 | 2.87218200 |
| H | -1.32122600 | -0.38624100 | -0.42413900 |

**Vibrational frequencies**

551.74*i*, 24.84, 27.19, 32.97, 44.28, 49.47, 73.39, 91.04, 102.28, 111.77, 127.36, 134.25, 162.12, 169.25, 209.95, 229.94, 251.26, 267.52, 283.62, 303.11, 321.95, 361.53, 381.77, 394.89, 411.75, 418.6, 426.63, 440.77, 494.52, 507.58, 540.39, 588.31, 626.12, 632.94, 677.9,

710.87, 712.5, 738.96, 756.29, 773.79, 780.64, 808.79, 812.19, 825.66, 836.37, 844.09, 855.06, 865.76, 905.4, 928.5, 944.14, 946.69, 976.15, 983.16, 993.76, 998.4, 1005.79, 1010.99, 1017.61, 1022.11, 1028.14, 1046.49, 1055.42, 1062.67, 1079.44, 1094.48, 1108.95, 1114.94, 1118.38, 1128.08, 1141.83, 1154.63, 1174.81, 1177.69, 1186.76, 1201.81, 1206.27, 1227.9, 1232.84, 1248.97, 1253.06, 1277.43, 1294.43, 1295.88, 1312.8, 1314.42, 1323.8, 1335.33, 1340.18, 1347.01, 1355.79, 1366.8, 1392.19, 1397.47, 1404.07, 1441, 1477.64, 1486.78, 1490.18, 1495.15, 1497.95, 1500.35, 1505.78, 1506.25, 1530.93, 1541.76, 1555.06, 1665.76, 1686.02, 1705.27, 1771.38, 3060.48, 3061.22, 3062.68, 3062.94, 3067.45, 3076.06, 3104.17, 3109.47, 3113.6, 3117.58, 3120.88, 3125, 3136.72, 3154.17, 3160.25, 3167.04, 3170.14, 3171.58, 3183.07, 3185.51, 3188.89, 3200.51, 3208.27, 3210.85.

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## TS (19e → 21e)

### M06-2X/6-311+G(*d*,*p*)

Zero-point correction= 0.358796
Thermal correction to Energy= 0.377760
Thermal correction to Enthalpy= 0.378704
Thermal correction to Gibbs Free Energy= 0.307815
Sum of electronic and zero-point Energies= -865.574061
Sum of electronic and thermal Energies= -865.555098
Sum of electronic and thermal Enthalpies= -865.554153
Sum of electronic and thermal Free Energies= -865.625042

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.49287700 | 3.34684200 | 1.90777900 |
| C | 1.02284600 | 3.61886300 | 1.87011300 |
| C | 1.32114100 | 3.62444000 | 0.39082600 |
| C | 0.32641900 | 3.10322800 | -0.31963900 |
| C | -0.82972800 | 2.66086300 | 0.56073700 |
| H | -1.03316100 | 4.29650400 | 1.95514400 |
| H | 1.58900000 | 2.81777300 | 2.35845800 |
| H | 1.29279900 | 4.55592400 | 2.36269100 |
| H | 2.25965900 | 3.97767800 | -0.02164900 |
| H | 0.33527400 | 2.95844600 | -1.39418500 |
| H | -0.80994900 | 2.72960000 | 2.74915500 |
| C | -2.20456800 | 2.99054100 | -0.00649000 |
| H | -2.95684600 | 2.74679300 | 0.74944400 |
| H | -2.28557300 | 4.05357100 | -0.24248400 |
| C | -2.39807800 | 2.10478500 | -1.24742100 |
| H | -3.45669000 | 1.93043000 | -1.44053800 |
| H | -1.98244500 | 2.60212100 | -2.12760600 |
| C | -1.68064000 | 0.77416500 | -1.06409000 |
| H | -0.69195500 | 0.67092500 | -1.50198800 |
| C | -2.39507700 | -0.40106300 | -1.00340100 |
| H | -1.93873900 | -1.37865800 | -1.12901200 |
| O | 0.34762100 | 0.68586500 | 0.79360300 |
| N | -0.93573400 | 1.20320300 | 0.74893400 |
| C | 0.32643300 | -0.58510800 | 1.40786700 |
| H | -0.10718700 | -0.49357700 | 2.41054100 |
| H | -0.31574300 | -1.26106800 | 0.82897400 |
| C | 1.73164200 | -1.12493500 | 1.47686800 |
| C | 1.93531000 | -2.42241100 | 1.94834800 |
| C | 2.82990000 | -0.36074000 | 1.08900600 |
| C | 3.21690000 | -2.95011100 | 2.03557000 |
| H | 1.08161100 | -3.02292300 | 2.24874600 |
| C | 4.11495600 | -0.89161900 | 1.17618200 |
| H | 2.67026600 | 0.64320600 | 0.71421200 |
| C | 4.31328700 | -2.18347800 | 1.64811200 |

| | | | |
|---|---|---|---|
| H | 3.36129000 | -3.95892200 | 2.40424500 |
| H | 4.96430100 | -0.29080000 | 0.87169200 |
| H | 5.31420200 | -2.59315900 | 1.71432200 |
| O | -3.69856100 | -0.38390500 | -0.64193400 |
| C | -4.31842100 | -1.65331200 | -0.57539700 |
| H | -3.83834400 | -2.27842600 | 0.18422000 |
| H | -5.35756300 | -1.48463600 | -0.30117000 |
| H | -4.27420000 | -2.15799300 | -1.54572400 |

**Vibrational frequencies**

631.79*i*, 14.8, 20.97, 36.68, 41.82, 64.03, 85.2, 89.51, 116.93, 134.06, 180.9, 192.89, 204.07, 223.4, 229.14, 237.92, 286.78, 322.36, 343.11, 382.8, 404.84, 411.11, 462.14, 464.73, 475.71, 539.26, 589.94, 607.26, 631.64, 645.09, 694.47, 712.21, 718.3, 735.74, 755.6, 771.5, 812.45, 818.19, 856.62, 860.33, 882.31, 920.09, 936.56, 944.61, 971.32, 983.35, 997.92, 1006.42, 1009.79, 1018.35, 1020.17, 1025.57, 1026.35, 1045.84, 1059.11, 1065.89, 1075.4, 1093.19, 1112.76, 1126.16, 1143.35, 1161.78, 1169.77, 1178.96, 1179.46, 1183.22, 1210.33, 1215.4, 1221.57, 1224.69, 1244.31, 1258.82, 1260.6, 1280.33, 1306.42, 1316.93, 1323.89, 1330.81, 1340.98, 1356.76, 1358.6, 1391.83, 1407.64, 1427.61, 1477.18, 1479.23, 1480.14, 1495.3, 1498.82, 1501.9, 1503.92, 1510.65, 1512.28, 1547.56, 1558.33, 1662.47, 1688.92, 1699.11, 3030.64, 3039.61, 3051.94, 3056.09, 3062.75, 3064.62, 3077.76, 3093.09, 3097.45, 3112.13, 3131.88, 3133.36, 3164.94, 3173.19, 3179.16, 3189.85, 3191.31, 3196.31, 3200.75, 3208.22, 3215.84, 3216.71.

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## TS (19f → 21f)

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.353526
Thermal correction to Energy= 0.371308
Thermal correction to Enthalpy= 0.372252
Thermal correction to Gibbs Free Energy= 0.305332
Sum of electronic and zero-point Energies= -790.372765
Sum of electronic and thermal Energies= -790.354983
Sum of electronic and thermal Enthalpies= -790.354039
Sum of electronic and thermal Free Energies= -790.420959

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.62733000 | 3.92933800 | 2.03287000 |
| C | 0.87845800 | 4.25290600 | 2.01624200 |
| C | 1.22022600 | 4.15709700 | 0.54987000 |
| C | 0.26431000 | 3.55099600 | -0.14618500 |
| C | -0.89949300 | 3.12991700 | 0.73554600 |
| H | -1.20135300 | 4.85918900 | 1.98949400 |
| H | 1.45819600 | 3.51516800 | 2.58081200 |
| H | 1.09958300 | 5.23560700 | 2.43908300 |
| H | 2.15558300 | 4.51655600 | 0.13651100 |
| H | 0.30037200 | 3.34735800 | -1.21040100 |
| H | -0.95029700 | 3.36874700 | 2.91103000 |
| C | -2.27258100 | 3.35552200 | 0.11149600 |
| H | -3.02682300 | 3.22537100 | 0.89212800 |
| H | -2.35828900 | 4.37275900 | -0.27478700 |
| C | -2.45797300 | 2.28948400 | -0.98985800 |
| H | -3.49365200 | 1.94674300 | -1.02803800 |
| H | -2.23012500 | 2.71470800 | -1.97136500 |
| C | -1.53163100 | 1.10676800 | -0.75217500 |
| H | -0.51237700 | 1.22233000 | -1.11871200 |
| O | 0.31555100 | 1.21305700 | 1.22448900 |
| N | -0.96755700 | 1.68928700 | 1.04336000 |
| C | 0.27296700 | 0.01052100 | 1.97203400 |
| H | 0.19489000 | 0.24986700 | 3.03959200 |

| | | | |
|---|---|---|---|
| H | -0.62478600 | -0.54798000 | 1.68950800 |
| C | 1.50874200 | -0.80621200 | 1.69670300 |
| C | 1.66226600 | -2.03289000 | 2.34483800 |
| C | 2.48931700 | -0.38024600 | 0.80417600 |
| C | 2.77696900 | -2.82502300 | 2.10362800 |
| H | 0.90072600 | -2.36882600 | 3.04240300 |
| C | 3.60808300 | -1.17559900 | 0.56386900 |
| H | 2.37113100 | 0.57321600 | 0.30397800 |
| C | 3.75541100 | -2.39722900 | 1.20913400 |
| H | 2.88328500 | -3.77628400 | 2.61172000 |
| H | 4.36677900 | -0.83590700 | -0.13162900 |
| H | 4.62599700 | -3.01354400 | 1.01916600 |
| H | -0.05268800 | -1.10233500 | -0.85123700 |
| H | -1.31308600 | -1.96100300 | -1.75274700 |
| H | -1.25675000 | -2.08400800 | -0.00454100 |
| C | -1.99733500 | -0.19329000 | -0.73758200 |
| C | -1.10686100 | -1.39098200 | -0.83982500 |
| H | -3.05969300 | -0.36489000 | -0.58265600 |

**Vibrational frequencies**

714.14*i*, 18.55, 21.29, 41.93, 60.2, 84.62, 112.85, 142.75, 145.82, 167.63, 188.36, 222.16, 236.13, 238.3, 261.38, 285.22, 323.4, 345.88, 382.83, 411.12, 442.89, 457.77, 470.06, 471.43, 543.38, 591.11, 613.19, 631, 684.58, 712.5, 727.47, 736.44, 749.92, 773.41, 788.23, 816.19, 851.24, 854.07, 876.16, 909.98, 931.9, 942.98, 958.63, 978.5, 990.06, 998.66, 1007.14, 1007.81, 1018.06, 1022.15, 1024.69, 1034.64, 1056.91, 1061.83, 1068.43, 1080.5, 1089.29, 1106.28, 1109.67, 1125.68, 1143.11, 1169.12, 1177.72, 1179.97, 1203.92, 1216.68, 1222.71, 1239.4, 1243.45, 1273.11, 1282.58, 1302.88, 1315.27, 1318.38, 1325.12, 1330.95, 1340.01, 1351.11, 1364.99, 1390.7, 1406.06, 1413.29, 1474.31, 1474.52, 1482.08, 1489.11, 1493.33, 1495.01, 1503.25, 1508.02, 1542.71, 1546.18, 1659.01, 1682.46, 1704.01, 3031.71, 3039.77, 3060.84, 3070.79, 3073.42, 3077.04, 3078.22, 3093.48, 3105.62, 3114.52, 3122.82, 3131.18, 3137.14, 3138.05, 3166.03, 3183.14, 3200.3, 3201.24, 3210.45, 3221.34, 3225.64, 3227.57.

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## TS (19g → 21g)

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.381632
Thermal correction to Energy= 0.400793
Thermal correction to Enthalpy= 0.401737
Thermal correction to Gibbs Free Energy= 0.332222

Sum of electronic and zero-point Energies= -829.653252
Sum of electronic and thermal Energies= -829.634091
Sum of electronic and thermal Enthalpies= -829.633147
Sum of electronic and thermal Free Energies= -829.702662

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.80647000 | 3.64818700 | 1.98029900 |
| C | 0.66722300 | 4.08844400 | 2.06879300 |
| C | 1.13402900 | 3.97689000 | 0.63875500 |
| C | 0.28474900 | 3.28222400 | -0.11038900 |
| C | -0.91628900 | 2.80394400 | 0.68711800 |
| H | -1.44547700 | 4.52917700 | 1.87252900 |
| H | 1.25439500 | 3.41415200 | 2.70128300 |
| H | 0.77923300 | 5.09658800 | 2.47470200 |
| H | 2.07569200 | 4.38614900 | 0.29076300 |
| H | 0.42999200 | 3.03883100 | -1.15686700 |
| H | -1.14956600 | 3.08030400 | 2.84605000 |
| C | -2.24208900 | 2.92096800 | -0.05615000 |
| H | -3.04964200 | 2.68694200 | 0.64441400 |

| | | | |
|---|---|---|---|
| H | -2.39491100 | 3.93603800 | -0.42796600 |
| C | -2.20140500 | 1.88365700 | -1.19071500 |
| H | -3.20611200 | 1.56686700 | -1.47127600 |
| H | -1.76130300 | 2.33465800 | -2.08441000 |
| C | -1.33473600 | 0.68941500 | -0.79990300 |
| H | -0.30191700 | 0.74914900 | -1.14122600 |
| C | -1.82182200 | -0.60417700 | -0.67912700 |
| O | 0.39279900 | 0.98929800 | 1.29103100 |
| N | -0.90907000 | 1.36800400 | 1.01503000 |
| C | 0.40682500 | -0.24159200 | 1.99026200 |
| H | 0.43935900 | -0.04358900 | 3.06898200 |
| H | -0.52248900 | -0.77817300 | 1.77707200 |
| C | -3.23231500 | -0.89867300 | -0.27384300 |
| C | 1.59648600 | -1.06500000 | 1.56556700 |
| C | 1.74987400 | -2.35108800 | 2.08530000 |
| C | 2.53302800 | -0.58259500 | 0.65471700 |
| C | 2.81951200 | -3.14749600 | 1.69696900 |
| H | 1.02201800 | -2.73273500 | 2.79572100 |
| C | 3.60566000 | -1.38222000 | 0.26583400 |
| H | 2.41359300 | 0.41687600 | 0.25386900 |
| C | 3.75198000 | -2.66416100 | 0.78197200 |
| H | 2.92506200 | -4.14599600 | 2.10500400 |
| H | 4.32928300 | -0.99874800 | -0.44445400 |
| H | 4.58657500 | -3.28404700 | 0.47663200 |
| H | -3.86233000 | -0.00985100 | -0.24761200 |
| H | -3.24189400 | -1.33575500 | 0.73354900 |
| H | -3.69363400 | -1.63690800 | -0.93917800 |
| C | -0.90744400 | -1.78947400 | -0.76662200 |
| H | 0.12844800 | -1.49689900 | -0.94871900 |
| H | -0.93077400 | -2.39042400 | 0.15203400 |
| H | -1.22407900 | -2.45846300 | -1.57600200 |

**Vibrational frequencies**

691.47*i*, 21.08, 28.62, 42.52, 58.56, 72.61, 90.86, 123.48, 133.68, 158.17, 176.11, 182.03, 192.63, 225.55, 250.54, 252.66, 288.45, 325.45, 339.14, 365.01, 396.57, 411.95, 427.14, 461.93, 467.96, 472.42, 484.08, 559.67, 593.5, 616.92, 632.51, 667.95, 712.53, 734.2, 750.94, 761.8, 768.75, 815.03, 838.82, 849.22, 880.07, 882.55, 930.42, 937.03, 945.77, 953.89, 967.41, 980.56, 985.45, 1001.22, 1003.96, 1011.23, 1018.72, 1024.27, 1031.1, 1037.91, 1050.4, 1065.43, 1068.64, 1070.21, 1092.2, 1111.56, 1115.9, 1125.97, 1130.77, 1150.02, 1175.68, 1185.34, 1212.9, 1217.96, 1221.55, 1237.79, 1242.35, 1267.91, 1275.82, 1282.65, 1308.58, 1327.63, 1331.44, 1342.22, 1353.37, 1360.98, 1371.81, 1392.39, 1402.92, 1413.64, 1417.39, 1463.82, 1473.15, 1474.07, 1483.86, 1486.26, 1489.71, 1497.67, 1499.23, 1508.56, 1519.83, 1547.48, 1549.72, 1663.25, 1688.35, 1702.41, 3009.23, 3013.59, 3033.25, 3055.18, 3057.41, 3057.72, 3060.18, 3064.45, 3066.02, 3094.38, 3104.16, 3113.32, 3118.72, 3121.76, 3127.56, 3130.69, 3153.78, 3182.47, 3186.99, 3195.86, 3207.14, 3212.24, 3214.73, 3222.87.

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## TS (19h → 21h)

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.489473 (Hartr
Thermal correction to Energy= 0.514467
Thermal correction to Enthalpy= 0.515411
Thermal correction to Gibbs Free Energy= 0.431814
Sum of electronic and zero-point Energies= -1212.978335
Sum of electronic and thermal Energies= -1212.953341
Sum of electronic and thermal Enthalpies= -1212.952397
Sum of electronic and thermal Free Energies= -1213.035994

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.75644900 | 0.63419000 | -0.29201700 |
| C | 4.26608200 | 1.00572800 | 1.11287400 |
| C | 3.69712300 | -0.08989200 | 1.97927500 |
| C | 2.76154900 | -0.79183700 | 1.34936000 |
| C | 2.53397000 | -0.29357300 | -0.06504100 |
| H | 4.52381900 | 0.06656300 | -0.82573000 |
| H | 3.87851800 | 1.97826200 | 1.43508500 |
| H | 5.35649600 | 1.05891600 | 1.16011500 |
| H | 4.00245700 | -0.24849300 | 3.00724400 |
| H | 2.19225600 | -1.60573400 | 1.78443000 |
| H | 3.48229400 | 1.50090200 | -0.89777300 |
| C | 2.36286200 | -1.39900600 | -1.10307300 |
| H | 2.41851700 | -0.94815400 | -2.09865200 |
| H | 3.17236600 | -2.12717500 | -1.02332900 |
| C | 0.98018900 | -2.04929200 | -0.88867500 |
| H | 0.55960300 | -2.38749100 | -1.83624400 |
| H | 1.08732600 | -2.93310800 | -0.25206000 |
| C | 0.02185900 | -1.10412400 | -0.18266300 |
| H | 0.10080600 | -1.11119200 | 0.90049600 |
| C | -1.20994600 | -0.70355700 | -0.67458600 |
| O | 1.07147300 | 1.26221100 | 0.83871000 |
| N | 1.30077900 | 0.48510900 | -0.26146900 |
| C | 0.32931500 | 2.42382000 | 0.44559700 |
| H | -0.54190300 | 2.11027800 | -0.13505900 |
| H | -0.00301900 | 2.87074400 | 1.38368800 |
| C | -2.22612000 | -0.15048900 | 0.23998600 |
| C | -3.08980700 | 0.87545700 | -0.18083300 |
| C | -2.34797000 | -0.60017400 | 1.56474200 |
| C | -4.01294600 | 1.44008800 | 0.68933900 |
| H | -3.01846700 | 1.24283300 | -1.19866700 |
| C | -3.27215300 | -0.03633600 | 2.43333600 |
| H | -1.73033900 | -1.42100800 | 1.90895700 |
| C | -4.10842000 | 0.98992000 | 2.00293600 |
| H | -4.65819100 | 2.23830800 | 0.34096200 |
| H | -3.34924000 | -0.40908200 | 3.44817100 |
| H | -4.83132300 | 1.42716800 | 2.68132000 |
| C | 1.20888700 | 3.35962000 | -0.33991500 |
| C | 2.13965900 | 4.16033000 | 0.32130700 |
| C | 1.17292700 | 3.36653100 | -1.73303800 |
| C | 3.02563800 | 4.95496900 | -0.39778700 |
| H | 2.17120100 | 4.15383200 | 1.40648300 |
| C | 2.05465600 | 4.16408400 | -2.45630600 |
| H | 0.45701100 | 2.73303700 | -2.24660800 |
| C | 2.98436100 | 4.95579100 | -1.78942200 |
| H | 3.74574500 | 5.57377100 | 0.12462200 |
| H | 2.01975000 | 4.16419400 | -3.53948200 |
| H | 3.67290500 | 5.57477400 | -2.35267200 |
| C | -1.47527000 | -0.67331200 | -2.12708800 |
| C | -2.71376400 | -1.07837700 | -2.64415800 |
| C | -0.49118400 | -0.23207300 | -3.02145500 |
| C | -2.95238000 | -1.06205300 | -4.01148500 |
| H | -3.48543600 | -1.41710600 | -1.96117900 |

| | | | |
|---|---|---|---|
| C | -0.73456700 | -0.20998700 | -4.39107400 |
| H | 0.45433900 | 0.11886900 | -2.62202600 |
| C | -1.96321400 | -0.62770200 | -4.89153800 |
| H | -3.91148200 | -1.39227600 | -4.39357700 |
| H | 0.03601400 | 0.14020000 | -5.06855400 |
| H | -2.15178800 | -0.61334300 | -5.95844200 |

**Vibrational frequencies**

553.36*i*, 15.14, 27.83, 33.57, 41.49, 50.21, 52.7, 65.05, 74.45, 81.37, 106.49, 113.5, 120.58, 164.69, 175.57, 201.48, 215.12, 233.69, 255.49, 272.42, 278.36, 300.59, 319.05, 363.04, 388.01, 407.48, 412.92, 416.51, 420.35, 424.66, 444.28, 471.35, 482.38, 506.62, 524.4, 567.5, 594.62, 622.86, 630.15, 630.89, 633.43, 635.86, 649.44, 682.1, 713.23, 718.9, 722.1, 728.33, 740.35, 766.9, 779.45, 782.64, 795.75, 821.2, 835.08, 845.68, 857.89, 865.86, 875.02, 885.82, 917.18, 927.63, 944.73, 947.2, 950.86, 962.74, 977.84, 983.73, 1002.12, 1003.66, 1005.24, 1007.43, 1009.16, 1014.26, 1016.62, 1018.4, 1019.45, 1021.98, 1023.44, 1026.32, 1031.28, 1044.21, 1060.49, 1064.54, 1069.74, 1072.8, 1079.13, 1106.31, 1116.3, 1118.28, 1121.77, 1124.58, 1152.36, 1166.53, 1178.8, 1180.23, 1181.57, 1189.57, 1202.21, 1211.87, 1218.33, 1223.45, 1228.18, 1247.47, 1251.93, 1276.88, 1295.23, 1299.6, 1310.84, 1313.98, 1319.76, 1326.19, 1333.25, 1347.27, 1356.03, 1359.02, 1360.16, 1360.73, 1387.66, 1400.57, 1403.4, 1478.05, 1480.56, 1484.09, 1486.16, 1492.18, 1498.35, 1501.93, 1503.09, 1518.18, 1537.06, 1542.18, 1544.16, 1643.09, 1647.69, 1668.13, 1668.26, 1675.44, 1686.06, 1702.89, 3049.9, 3055.51, 3057.17, 3067.92, 3092.05, 3097.19, 3115.25, 3125.72, 3132.67, 3150.05, 3166.79, 3170.44, 3174.06, 3176.66, 3179.56, 3180.14, 3184.48, 3186.01, 3187.19, 3194.94, 3195.02, 3197.7, 3200.93, 3202, 3206.29, 3208.99, 3212.96, 3214.39.

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## 20a

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.422034
Thermal correction to Energy= 0.443472
Thermal correction to Enthalpy= 0.444416
Thermal correction to Gibbs Free Energy= 0.368033

Sum of electronic and zero-point Energies= -982.683294
Sum of electronic and thermal Energies= -982.661856
Sum of electronic and thermal Enthalpies= -982.660912
Sum of electronic and thermal Free Energies= -982.737295

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 3.91961500 | -2.03004200 | -1.04309200 |
| C | 4.95697600 | -0.91775500 | -1.27953200 |
| C | 4.77597100 | -0.04624300 | -0.06133200 |
| C | 3.63904600 | -0.30773500 | 0.57418100 |
| C | 2.85493000 | -1.41073200 | -0.11159300 |
| H | 4.39451600 | -2.86664200 | -0.52280900 |
| H | 4.73385700 | -0.34668100 | -2.18641700 |
| H | 5.97244100 | -1.30731500 | -1.38037800 |
| H | 5.48041000 | 0.72617700 | 0.22459500 |
| H | 3.26356500 | 0.21532500 | 1.44448500 |
| H | 3.47033900 | -2.41102700 | -1.96286700 |
| C | 2.28417600 | -2.46679700 | 0.85293800 |
| H | 2.05844500 | -3.37297200 | 0.27421100 |
| H | 3.09134500 | -2.73873600 | 1.54006400 |
| C | 1.03381400 | -2.07940400 | 1.66169300 |
| H | 0.98398900 | -2.74865300 | 2.52865100 |
| H | 1.12276800 | -1.06019300 | 2.04767100 |
| C | -0.24974500 | -2.21386800 | 0.89029200 |
| H | -0.40048600 | -3.16797300 | 0.38539700 |
| C | -1.17528800 | -1.25579600 | 0.81480000 |
| H | -0.97756400 | -0.32148700 | 1.33483700 |
| O | 1.16534700 | 0.21679900 | -0.24749200 |

| | | | |
|---|---|---|---|
| N | 1.84125200 | -0.78682700 | -0.99705200 |
| C | 0.31984100 | 0.91785700 | -1.12816000 |
| H | 0.91696700 | 1.36142700 | -1.93428700 |
| H | -0.40178600 | 0.21992200 | -1.58173700 |
| C | -2.43485500 | -1.27504500 | 0.05321300 |
| C | -3.23433200 | -0.12599400 | 0.06212400 |
| C | -2.85748300 | -2.37190300 | -0.70918900 |
| C | -4.41414900 | -0.06910200 | -0.67229900 |
| H | -2.91935700 | 0.73357700 | 0.64682600 |
| C | -4.03594800 | -2.31724000 | -1.43873000 |
| H | -2.26205300 | -3.27745800 | -0.73124400 |
| C | -4.81938200 | -1.16384200 | -1.42684500 |
| H | -5.01458700 | 0.83334300 | -0.65390500 |
| H | -4.34658400 | -3.17651100 | -2.02197500 |
| H | -5.73767000 | -1.12401900 | -2.00065300 |
| C | -0.44102000 | 1.97255000 | -0.36847400 |
| C | -1.46878100 | 2.65893400 | -1.01699400 |
| C | -0.16695200 | 2.26234100 | 0.96552500 |
| C | -2.21684600 | 3.61415300 | -0.34158000 |
| H | -1.69492500 | 2.42719900 | -2.05353900 |
| C | -0.92231400 | 3.21485400 | 1.64616700 |
| H | 0.63308500 | 1.73197200 | 1.46835700 |
| C | -1.94911400 | 3.89110700 | 0.99744000 |
| H | -3.01497400 | 4.13710600 | -0.85586300 |
| H | -0.70595700 | 3.42790800 | 2.68674100 |
| H | -2.53588500 | 4.63068400 | 1.52905000 |
| H | 1.11954700 | -1.49527800 | -1.17686900 |

**Vibrational frequencies**

5.92, 15.57, 29.53, 41.55, 61.84, 72.69, 85.06, 96.28, 119.06, 141.49, 172.65, 196.62, 205.81, 224.88, 236.88, 255.19, 279.97, 298.69, 300.41, 355.55, 357.3, 409.72, 411.29, 414.68, 418.13, 470.87, 477.48, 482.01, 537.44, 547.21, 613.06, 618.63, 632.32, 633.13, 647.66, 710.54, 711.33, 725.05, 752.47, 763.81, 770.98, 812.05, 831.81, 850.86, 856.16, 867.61, 876.26, 878.64, 882.97, 931.6, 946.31, 950.73, 959.94, 975.47, 982.51, 996.56, 1008.71, 1010.81, 1013.34, 1015.94, 1019.71, 1021.17, 1026.71, 1028.24, 1049.83, 1053.82, 1061.52, 1066.04, 1068.66, 1100.4, 1104.38, 1114.5, 1116.07, 1125.8, 1161.75, 1179.03, 1181.29, 1185.17, 1188.52, 1212.25, 1212.84, 1222.19, 1237.61, 1244.01, 1246.44, 1257.22, 1274.11, 1298.72, 1313.57, 1326.67, 1332.45, 1335.28, 1341.92, 1351.11, 1360.33, 1363.92, 1378.98, 1389.88, 1397.09, 1418.56, 1474.65, 1476.11, 1479.1, 1492, 1494.15, 1498.66, 1502.78, 1520.63, 1542.35, 1549.89, 1650.38, 1660.55, 1681.05, 1690.82, 1701.59, 1743.79, 3009.47, 3025.22, 3037.74, 3060.25, 3061.58, 3071.04, 3077.07, 3098.18, 3102.11, 3123.53, 3137.28, 3161.82, 3181.53, 3181.63, 3183.14, 3189.32, 3190.89, 3200.59, 3205.84, 3210.17, 3212.2, 3217.42, 3218.57, 3226.71, 3392.92.

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## 21c

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.326166 (Hartr
Thermal correction to Energy= 0.344286
Thermal correction to Enthalpy= 0.345230
Thermal correction to Gibbs Free Energy= 0.275292

Sum of electronic and zero-point Energies= -843.371894
Sum of electronic and thermal Energies= -843.353775
Sum of electronic and thermal Enthalpies= -843.352831
Sum of electronic and thermal Free Energies= -843.422768

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.64508900 | 3.07923200 | 2.14635100 |
| C | 0.87555200 | 3.28902700 | 2.27000000 |

| | | | |
|---|---|---|---|
| C | 1.25802100 | 3.71630300 | 0.87352700 |
| C | 0.29382200 | 3.46391200 | -0.00530800 |
| C | -0.90120900 | 2.80023200 | 0.65704000 |
| H | -1.15612000 | 4.00852900 | 2.41287400 |
| H | 1.39893600 | 2.35959500 | 2.52349400 |
| H | 1.13798800 | 4.02962900 | 3.02860600 |
| H | 2.22422800 | 4.14346400 | 0.63191000 |
| H | 0.35329400 | 3.65131800 | -1.07183800 |
| H | -1.04735700 | 2.28114500 | 2.77177100 |
| C | -2.25977900 | 3.23134300 | 0.10484200 |
| H | -3.02837800 | 3.03820600 | 0.85577700 |
| H | -2.26995800 | 4.29565700 | -0.13291800 |
| C | -2.48506600 | 2.33484500 | -1.13559600 |
| H | -3.48880800 | 1.90952500 | -1.13869600 |
| H | -2.34987300 | 2.87758300 | -2.07129800 |
| C | -1.41020500 | 1.21848400 | -1.01131600 |
| H | -0.56518100 | 1.42451800 | -1.68021900 |
| C | -1.90890600 | -0.15831500 | -1.30663900 |
| H | -1.70243200 | -0.63424200 | -2.25610300 |
| O | 0.27242100 | 0.72108500 | 0.52810000 |
| N | -0.98360700 | 1.34224700 | 0.38360600 |
| C | 0.22114300 | -0.25796400 | 1.56680300 |
| H | 0.08644200 | 0.23260400 | 2.53672400 |
| H | -0.63100200 | -0.92244800 | 1.39350500 |
| C | 1.51986200 | -1.01268200 | 1.52425300 |
| C | 2.44094100 | -0.92414600 | 2.56316000 |
| C | 1.81666100 | -1.80766000 | 0.41628300 |
| C | 3.64219000 | -1.62658100 | 2.50429500 |
| H | 2.21571800 | -0.30513400 | 3.42570800 |
| C | 3.01515200 | -2.50490700 | 0.35085400 |
| H | 1.09776800 | -1.87098900 | -0.39485500 |
| C | 3.93025200 | -2.41641600 | 1.39818700 |
| H | 4.35158800 | -1.55413600 | 3.32016000 |
| H | 3.23807100 | -3.12118900 | -0.51228700 |
| H | 4.86419300 | -2.96381200 | 1.34997000 |
| C | -2.74509300 | -0.83094700 | -0.40878200 |
| N | -3.43465400 | -1.39649000 | 0.33192100 |

**Vibrational frequencies**

7.73, 22.65, 23.89, 42.12, 56.91, 81.62, 102.75, 111.65, 141.58, 172.26, 216.92, 239.22, 264.29, 283.39, 332.16, 366.73, 367.28, 390.74, 410.27, 411.26, 441.74, 471.62, 507.51, 560.05, 575.05, 598.48, 634.41, 643.16, 674.62, 689.63, 710.11, 750.31, 760.52, 771.61, 778.96, 833.8, 856.95, 865.66, 868.78, 910.89, 937.23, 939.98, 952.76, 975.33, 987.25, 993.85, 998.32, 1001.43, 1012.96, 1017.39, 1022.77, 1030.69, 1046.48, 1065.35, 1085.93, 1107.38, 1118.85, 1122.37, 1133.42, 1145.38, 1185.5, 1186.49, 1198.56, 1208.17, 1218.87, 1228.98, 1242.77, 1251.32, 1255.58, 1279.37, 1304.12, 1310.61, 1325.45, 1331.55, 1343.88, 1350.42, 1358.49, 1383.35, 1393.15, 1409.1, 1413.74, 1474.24, 1485.08, 1493.33, 1503.23, 1506.85, 1525.48, 1548.97, 1668.52, 1691.48, 1701.41, 2238.63, 3036.69, 3043.33, 3056.06, 3062.24, 3079.48, 3086.57, 3089.31, 3105.27, 3123.05, 3125.17, 3143.37, 3172.26, 3179.67, 3180.1, 3189.61, 3200.62, 3204.57, 3210.06, 3221.84.

## 21d

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.400514
Thermal correction to Energy= 0.422107
Thermal correction to Enthalpy= 0.423052
Thermal correction to Gibbs Free Energy= 0.346498

Sum of electronic and zero-point Energies= -1018.224410
Sum of electronic and thermal Energies= -1018.202816
Sum of electronic and thermal Enthalpies= -1018.201872
Sum of electronic and thermal Free Energies= -1018.278426

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.87718000 | 2.84644200 | 2.30478300 |
| C | 0.60408500 | 3.14635800 | 2.60422900 |
| C | 1.13680800 | 3.54028900 | 1.24733800 |
| C | 0.30362800 | 3.20137300 | 0.26912000 |
| C | -0.93077900 | 2.50055000 | 0.80881200 |
| H | -1.46558100 | 3.75330200 | 2.46991400 |
| H | 1.13809200 | 2.25748600 | 2.96106500 |
| H | 0.73236500 | 3.92796400 | 3.35638600 |
| H | 2.10513000 | 4.00672700 | 1.10700300 |
| H | 0.48996000 | 3.34218100 | -0.79011700 |
| H | -1.31063300 | 2.04723500 | 2.90757300 |
| C | -2.22559300 | 2.82238300 | 0.06728600 |
| H | -3.07351900 | 2.49631600 | 0.67337000 |
| H | -2.31825400 | 3.88989000 | -0.13719300 |
| C | -2.13988200 | 1.96787500 | -1.21299100 |
| H | -3.11704600 | 1.59603100 | -1.51344900 |
| H | -1.71978000 | 2.53846700 | -2.04286900 |
| C | -1.16468900 | 0.81452900 | -0.84312600 |
| H | -0.22058700 | 0.92648100 | -1.38828900 |
| C | -1.67377600 | -0.56856400 | -1.05780800 |
| H | -1.10890400 | -1.29388500 | -1.62865200 |
| O | 0.35266000 | 0.48033300 | 0.90630900 |
| N | -0.90682300 | 1.03307800 | 0.59416300 |
| C | 0.21862500 | -0.47300500 | 1.95690700 |
| H | 0.02013300 | 0.03663100 | 2.90670900 |
| H | -0.62840200 | -1.13027700 | 1.73230500 |
| C | -2.93826500 | -1.00180300 | -0.47744700 |
| C | 1.50253400 | -1.25232800 | 2.02012900 |
| C | 2.38291000 | -1.12297300 | 3.08964400 |
| C | 1.82860700 | -2.11189700 | 0.97028200 |
| C | 3.57207200 | -1.84813200 | 3.11682100 |
| H | 2.13749100 | -0.45241800 | 3.90687400 |
| C | 3.01428500 | -2.83268400 | 0.99058300 |
| H | 1.14127000 | -2.20678300 | 0.13534200 |
| C | 3.88888100 | -2.70229300 | 2.06772400 |
| H | 4.25075400 | -1.74289600 | 3.95498600 |
| H | 3.25849900 | -3.49842900 | 0.17116800 |
| H | 4.81370600 | -3.26671700 | 2.08689700 |
| O | -3.74262900 | -0.28429300 | 0.07213600 |
| O | -3.12223500 | -2.33081600 | -0.63479500 |
| C | -4.34616300 | -2.85546900 | -0.10375400 |
| H | -5.18513100 | -2.35254400 | -0.59062600 |
| H | -4.39513400 | -2.62411400 | 0.96281600 |

| | | | |
|---|---|---|---|
| C | -4.34862300 | -4.34504500 | -0.36259100 |
| H | -3.49991600 | -4.82231600 | 0.12944500 |
| H | -5.26822200 | -4.78678900 | 0.02543200 |
| H | -4.28985000 | -4.54974600 | -1.43253000 |

**Vibrational frequencies**

16.2, 23.7, 26.06, 39.87, 65.59, 67.57, 91.12, 99.97, 107.21, 130.98, 146.75, 158.87, 178.45, 215.4, 235.86, 245.57, 265.59, 287.87, 299.52, 328.22, 344.78, 370.71, 395, 402.91, 411.17, 432.95, 468.44, 507.48, 536.62, 556.74, 573.06, 608.13, 635.71, 650.73, 679.51, 711.99, 729.34, 755.8, 765.67, 774.87, 776.08, 798.48, 820.17, 835.8, 861.57, 865.52, 869.63, 908.74, 925.02, 936.96, 941.86, 954.62, 981, 988.23, 997.9, 998.36, 1002.77, 1015.19, 1020.01, 1023.78, 1036.69, 1045.29, 1066.72, 1085.81, 1089.42, 1115.91, 1120, 1123.82, 1132.04, 1142.01, 1152.27, 1167.87, 1184.49, 1188.33, 1194.6, 1209.7, 1213.59, 1221.92, 1230.99, 1253.62, 1253.86, 1258.48, 1275.74, 1308.96, 1310.32, 1318.33, 1324.22, 1336.11, 1347.86, 1353.69, 1358.43, 1394.3, 1397.66, 1405.98, 1411.84, 1428.19, 1461.2, 1479.21, 1482.25, 1492.16, 1499.93, 1505.48, 1505.83, 1507.57, 1527.38, 1532.26, 1549.81, 1670.99, 1691.96, 1697.76, 1773.62, 3042.34, 3044.74, 3045.45, 3059.4, 3064.26, 3079.61, 3082.09, 3085.11, 3089.21, 3109.25, 3124.74, 3125.37, 3133.67, 3144.95, 3152.16, 3152.78, 3172.85, 3174.43, 3187.89, 3189.52, 3196.02, 3210.88, 3218.06, 3220.4.

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## 21e

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.360878
Thermal correction to Energy= 0.379931
Thermal correction to Enthalpy= 0.380876
Thermal correction to Gibbs Free Energy= 0.309874
Sum of electronic and zero-point Energies= -865.602650
Sum of electronic and thermal Energies= -865.583597
Sum of electronic and thermal Enthalpies= -865.582653
Sum of electronic and thermal Free Energies= -865.653654

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.66754400 | 3.33104700 | 2.08809700 |
| C | 0.83754000 | 3.61860600 | 2.24345700 |
| C | 1.24419600 | 3.99646500 | 0.83962300 |
| C | 0.31698400 | 3.66559200 | -0.05294900 |
| C | -0.87591500 | 2.99018100 | 0.60383900 |
| H | -1.23241600 | 4.23894100 | 2.31823900 |
| H | 1.39211500 | 2.72754700 | 2.55839600 |
| H | 1.04217300 | 4.40710300 | 2.97139900 |
| H | 2.20035600 | 4.44998000 | 0.60530400 |
| H | 0.40122300 | 3.80746100 | -1.12482000 |
| H | -1.03974200 | 2.52813900 | 2.72641500 |
| C | -2.23080900 | 3.36553600 | -0.00339000 |
| H | -3.01021000 | 3.21240500 | 0.74587000 |
| H | -2.24794900 | 4.41373700 | -0.30550400 |
| C | -2.42220700 | 2.38636600 | -1.18800200 |
| H | -3.39551000 | 1.89910300 | -1.14125700 |
| H | -2.33541100 | 2.88206300 | -2.15542200 |
| C | -1.29495200 | 1.33369400 | -1.02226100 |
| H | -0.43952400 | 1.57737000 | -1.66735800 |
| C | -1.66641600 | -0.07622900 | -1.30088200 |
| H | -1.40052600 | -0.56364200 | -2.23542400 |
| O | 0.34615900 | 0.94502500 | 0.61560700 |
| N | -0.91644300 | 1.52807400 | 0.38750100 |
| C | 0.21329900 | -0.12727800 | 1.54129600 |
| H | 0.12434000 | 0.26334300 | 2.56237200 |
| H | -0.70138100 | -0.68061900 | 1.30369000 |

| | | | |
|---|---|---|---|
| C | 1.42034200 | -1.01530500 | 1.40717000 |
| C | 2.17703700 | -1.38323100 | 2.51547300 |
| C | 1.77523800 | -1.50249100 | 0.14781300 |
| C | 3.26800200 | -2.23808200 | 2.37467400 |
| H | 1.91297000 | -0.99901900 | 3.49536900 |
| C | 2.86626700 | -2.34849700 | 0.00347400 |
| H | 1.18770400 | -1.20106400 | -0.71352800 |
| C | 3.61469600 | -2.72090700 | 1.11905400 |
| H | 3.84986200 | -2.51882700 | 3.24496200 |
| H | 3.13704500 | -2.71981700 | -0.97810800 |
| H | 4.46562000 | -3.38246000 | 1.00695100 |
| O | -2.75562900 | -0.54320800 | -0.65203400 |
| C | -3.01454800 | -1.91875600 | -0.85736100 |
| H | -2.18645500 | -2.52282100 | -0.47289200 |
| H | -3.92756100 | -2.15749400 | -0.31597400 |
| H | -3.15389200 | -2.13084600 | -1.92295900 |

**Vibrational frequencies**

18.28, 20.1, 33.13, 51.28, 57.4, 66.93, 85.56, 103.24, 147.84, 159.18, 187.34, 198.58, 224.33, 234.94, 278.27, 297.95, 322.08, 345.34, 372.14, 395.86, 412.15, 438.89, 463.58, 497.13, 550.2, 570.8, 578.16, 631.26, 645.72, 677.51, 695.38, 711.5, 751.51, 764.6, 769.11, 786.76, 834.31, 858, 864.97, 876.58, 920.24, 937.77, 942.89, 956.84, 978.2, 993.21, 1000.05, 1008.22, 1008.7, 1018.54, 1021.49, 1027.38, 1037.44, 1048.47, 1063.41, 1089.78, 1107.48, 1116.27, 1124.51, 1134.45, 1153.81, 1166.13, 1175.66, 1183.69, 1201.6, 1202.67, 1207.95, 1222.27, 1231.48, 1247.32, 1250.18, 1262.95, 1283.8, 1295.82, 1304.75, 1313.14, 1328.1, 1331.89, 1337.2, 1351.25, 1352.08, 1391.02, 1409.12, 1412.93, 1433.65, 1476.5, 1488.54, 1495.67, 1497.54, 1503.03, 1503.85, 1509.73, 1513, 1516.15, 1544.53, 1664.12, 1688.98, 1694.86, 3029.19, 3031.98, 3036.91, 3055.29, 3066.14, 3084.01, 3087.7, 3090.88, 3095.21, 3098.97, 3123.36, 3128.85, 3145.93, 3160.72, 3165.07, 3171.88, 3178.53, 3178.93, 3192.44, 3203.43, 3205.38, 3216.3.

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## 21f

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.354951
Thermal correction to Energy= 0.373035
Thermal correction to Enthalpy= 0.373980
Thermal correction to Gibbs Free Energy= 0.306247

Sum of electronic and zero-point Energies= -790.401443
Sum of electronic and thermal Energies= -790.383359
Sum of electronic and thermal Enthalpies= -790.382415
Sum of electronic and thermal Free Energies= -790.450147

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.63197600 | 3.14744700 | 2.13729600 |
| C | 0.88219400 | 3.40649800 | 2.24761300 |
| C | 1.25055300 | 3.78716600 | 0.83391700 |
| C | 0.29089700 | 3.47614500 | -0.03097400 |
| C | -0.88992800 | 2.81389500 | 0.65886100 |
| H | -1.17166400 | 4.06633700 | 2.38364700 |
| H | 1.43104700 | 2.50354200 | 2.53908300 |
| H | 1.12364700 | 4.18588100 | 2.97407100 |
| H | 2.20624000 | 4.22608000 | 0.57197500 |
| H | 0.34401800 | 3.62007900 | -1.10442400 |
| H | -1.00123300 | 2.35270000 | 2.78743000 |
| C | -2.25532100 | 3.20919100 | 0.09493800 |
| H | -3.01851300 | 3.03445700 | 0.85705400 |
| H | -2.27977000 | 4.26576900 | -0.17587900 |
| C | -2.46888900 | 2.26452900 | -1.11133900 |

| | | | |
|---|---|---|---|
| H | -3.46975700 | 1.83132300 | -1.09930600 |
| H | -2.34652600 | 2.77961900 | -2.06477000 |
| C | -1.38394700 | 1.16040400 | -0.96355800 |
| H | -0.53634900 | 1.37649200 | -1.62585300 |
| C | -1.85144100 | -0.23511700 | -1.20478500 |
| H | -1.49026700 | -0.76352200 | -2.07873500 |
| O | 0.31719100 | 0.76504500 | 0.60749400 |
| N | -0.95434400 | 1.35086000 | 0.43582300 |
| C | 0.24176100 | -0.27430500 | 1.57579700 |
| H | 0.07295800 | 0.15026800 | 2.57240600 |
| H | -0.60009300 | -0.93007200 | 1.32847100 |
| C | -2.97519500 | -0.81169200 | -0.41215600 |
| C | 1.53975300 | -1.03070400 | 1.52357700 |
| C | 2.41047100 | -1.05548400 | 2.60780900 |
| C | 1.88383000 | -1.71373700 | 0.35589900 |
| C | 3.60904500 | -1.76204400 | 2.53526700 |
| H | 2.15078900 | -0.51861000 | 3.51440900 |
| C | 3.07952000 | -2.41458700 | 0.27783600 |
| H | 1.20449000 | -1.67924600 | -0.49055300 |
| C | 3.94445000 | -2.44125300 | 1.37061800 |
| H | 4.27985600 | -1.77714800 | 3.38620200 |
| H | 3.33999900 | -2.94281000 | -0.63190500 |
| H | 4.87695500 | -2.99014900 | 1.31134900 |
| H | -3.06996500 | -0.29847700 | 0.54810800 |
| H | -2.82495600 | -1.87779900 | -0.22067100 |
| H | -3.93654700 | -0.72165200 | -0.93703600 |

**Vibrational frequencies**

22.20, 27.90, 37.80, 58.80, 80.06, 85.25, 101.57, 125.53, 140.08, 166.26, 219.13, 226.46, 240.46, 260.59, 291.08, 325.52, 369.05, 379.26, 410.44, 413.23, 432.93, 488.85, 511, 554.88, 567.88, 602.14, 633.26, 651.77, 688.66, 713.88, 742.6, 763.13, 773.14, 778.59, 826.6, 854.53, 869.80, 877.04, 898.46, 934.16, 944.31, 952.88, 963.21, 977.62, 987.56, 997.74, 1005.51, 1007.38, 1016.17, 1021.02, 1022.8, 1030.4, 1043.01, 1062.63, 1065.09, 1089.66, 1109.59, 1117.21, 1127.38, 1148.88, 1157.96, 1181.42, 1184.73, 1198, 1200.43, 1221.56, 1227.95, 1246, 1254.44, 1255.95, 1279.65, 1305.70, 1309.64, 1327.97, 1331.22, 1342.87, 1350.65, 1352.21, 1380.31, 1392.6, 1404.33, 1414.50, 1421.74, 1476.66, 1483, 1489.3, 1494.07, 1496.65, 1500.58, 1508.53, 1521.18, 1545.62, 1668.42, 1690.05, 1695.31, 3001.64, 3040.98, 3045.94, 3048.26, 3063.36, 3073.63, 3075.8, 3083.95, 3091.12, 3092.91, 3118.91, 3120.32, 3122.32, 3138.59, 3176.83, 3179.03, 3182.44, 3189.74, 3195.68, 3203.20, 3204.47, 3211.26.

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## 21g

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.383469
Thermal correction to Energy= 0.402906
Thermal correction to Enthalpy= 0.403850
Thermal correction to Gibbs Free Energy= 0.333316

Sum of electronic and zero-point Energies= -829.682621
Sum of electronic and thermal Energies= -829.663184
Sum of electronic and thermal Enthalpies= -829.662240
Sum of electronic and thermal Free Energies= -829.732774

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | -0.66123500 | 3.14812800 | 2.13571000 |
| C | 0.84606100 | 3.43624400 | 2.26762700 |
| C | 1.22975800 | 3.81454600 | 0.85733100 |
| C | 0.28970100 | 3.48006400 | -0.02029900 |
| C | -0.88990200 | 2.80164400 | 0.65572200 |

| | | | |
|---|---|---|---|
| H | -1.22173400 | 4.05784900 | 2.36942600 |
| H | 1.40667600 | 2.54531600 | 2.57333800 |
| H | 1.06163100 | 4.22425500 | 2.99289000 |
| H | 2.18148400 | 4.26894800 | 0.60762000 |
| H | 0.35741200 | 3.61615400 | -1.09404800 |
| H | -1.02478400 | 2.34969600 | 2.78454000 |
| C | -2.25189400 | 3.16849100 | 0.06643700 |
| H | -3.02670700 | 2.96101500 | 0.80851800 |
| H | -2.30034900 | 4.22726300 | -0.19222800 |
| C | -2.40786700 | 2.23345400 | -1.15572600 |
| H | -3.40966000 | 1.80390300 | -1.20120600 |
| H | -2.23360800 | 2.75954000 | -2.09527600 |
| C | -1.32985700 | 1.12662400 | -0.96041400 |
| H | -0.46709200 | 1.33048200 | -1.60950500 |
| C | -1.79063900 | -0.27661700 | -1.19758400 |
| O | 0.34916400 | 0.77062900 | 0.63713400 |
| N | -0.92740900 | 1.33734500 | 0.44065900 |
| C | 0.27486600 | -0.26265100 | 1.61217900 |
| H | 0.11580600 | 0.16801600 | 2.60791400 |
| H | -0.57180500 | -0.91493700 | 1.37383800 |
| C | -2.91593500 | -0.81371100 | -0.37350200 |
| C | 1.56769100 | -1.02727900 | 1.55344800 |
| C | 2.44623000 | -1.05545100 | 2.63105600 |
| C | 1.89809000 | -1.71496700 | 0.38442400 |
| C | 3.63968500 | -1.76989600 | 2.55079600 |
| H | 2.19691400 | -0.51484100 | 3.53833400 |
| C | 3.08845500 | -2.42394700 | 0.29884400 |
| H | 1.21152000 | -1.67721300 | -0.45640900 |
| C | 3.96169700 | -2.45363400 | 1.38504000 |
| H | 4.31706300 | -1.78740000 | 3.39645900 |
| H | 3.33869900 | -2.95594700 | -0.61159200 |
| H | 4.89034300 | -3.00838600 | 1.31985600 |
| H | -2.99353200 | -0.28418600 | 0.57835300 |
| H | -2.77996800 | -1.88070000 | -0.16802800 |
| H | -3.88001400 | -0.72000900 | -0.89634000 |
| C | -1.49401000 | -0.93188400 | -2.50536700 |
| H | -1.51537200 | -2.02208800 | -2.41523400 |
| H | -2.24136900 | -0.66762800 | -3.27069600 |
| H | -0.51613300 | -0.63460100 | -2.89244800 |

**Vibrational frequencies**

24.41, 29.72, 44.12, 53.23, 62.71, 82.56, 88.43, 113.44, 132.42, 154.88, 178.41, 192.17, 225.71, 234.15, 246.74, 291.83, 300.45, 330.34, 363.66, 369.91, 404.23, 413.8, 428.91, 490.48, 494.5, 537.39, 569.53, 588.62, 632.67, 660.63, 686.73, 714.6, 735.29, 763.44, 772.18, 773.87, 823, 840.17, 863.43, 870.64, 878.68, 937.5, 943.1, 944.95, 947.88, 957.19, 976.2, 984.03, 986.65, 996.26, 1008.33, 1017.6, 1021.58, 1023.3, 1026.32, 1035.41, 1055.73, 1060.44, 1062.15, 1090.82, 1110.5, 1117.74, 1127, 1148.96, 1160.58, 1180.28, 1196.97, 1199.2, 1219.81, 1224.85, 1238.85, 1253.87, 1254.96, 1265.19, 1278.77, 1304.23, 1311.32, 1324.93, 1330.78, 1332.38, 1342.07, 1348.95, 1351.38, 1392.46, 1397.54, 1413.36, 1414.06, 1431.13, 1477.2, 1479.05, 1479.83, 1483.54, 1493.26, 1499.52, 1501.17, 1503.27, 1507.66, 1521.62, 1544.58, 1668.67, 1689.32, 1694.64, 2970.66, 2987.01, 3028.21, 3049.06, 3054.64, 3061.65, 3064.09, 3065.86, 3070.24, 3078.4, 3094.71, 3097.71, 3113.08, 3115.89, 3121.07, 3123.19, 3132.45, 3173.91, 3179.62, 3182.06, 3189.66, 3202.52, 3204.28, 3210.49.

## 21h

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.491558
Thermal correction to Energy= 0.516526
Thermal correction to Enthalpy= 0.517470
Thermal correction to Gibbs Free Energy= 0.434696

Sum of electronic and zero-point Energies= -1213.010631
Sum of electronic and thermal Energies= -1212.985663
Sum of electronic and thermal Enthalpies= -1212.984719
Sum of electronic and thermal Free Energies= -1213.067493

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.53352800 | 2.78039700 | 1.49158100 |
| C | 1.97010600 | 3.08364600 | 1.02436100 |
| C | 1.75802000 | 3.56708400 | -0.38964800 |
| C | 0.53915600 | 3.28355100 | -0.83610400 |
| C | -0.27979900 | 2.54481900 | 0.20832900 |
| H | 0.12719100 | 3.65817200 | 2.00205400 |
| H | 2.59307600 | 2.18240300 | 1.01429400 |
| H | 2.47037400 | 3.82226100 | 1.65471000 |
| H | 2.53496100 | 4.05366100 | -0.96790600 |
| H | 0.17053800 | 3.50200200 | -1.83240200 |
| H | 0.45425300 | 1.92661900 | 2.16680400 |
| C | -1.75674500 | 2.94245500 | 0.24418300 |
| H | -2.18006100 | 2.66011500 | 1.21200100 |
| H | -1.88069500 | 4.01904000 | 0.12059700 |
| C | -2.40594500 | 2.12045900 | -0.89308900 |
| H | -3.36928100 | 1.70896600 | -0.59462700 |
| H | -2.57099200 | 2.73125700 | -1.78198600 |
| C | -1.37851400 | 1.00940500 | -1.21644700 |
| H | -0.81957600 | 1.28575300 | -2.11539600 |
| C | -1.88308300 | -0.40048400 | -1.38897800 |
| O | 0.79907700 | 0.52999500 | -0.45931800 |
| N | -0.43327400 | 1.09786500 | -0.07609500 |
| C | 1.03808700 | -0.64503700 | 0.30566900 |
| H | 1.22553300 | -0.37938500 | 1.35270000 |
| H | 0.14514000 | -1.28186600 | 0.26968900 |
| C | -2.86805700 | -0.95446300 | -0.47237700 |
| C | -3.75365500 | -1.96642400 | -0.89793400 |
| C | -3.01102900 | -0.47669400 | 0.84653100 |
| C | -4.72838500 | -2.47147400 | -0.05161000 |
| H | -3.68406500 | -2.33436100 | -1.91498400 |
| C | -3.98624700 | -0.98968700 | 1.68985900 |
| H | -2.32067000 | 0.27388700 | 1.21001700 |
| C | -4.85085800 | -1.98822100 | 1.24942600 |
| H | -5.40286700 | -3.23991200 | -0.41122200 |
| H | -4.06710800 | -0.61269300 | 2.70296800 |
| H | -5.61154000 | -2.38452800 | 1.91128400 |
| C | 2.22006500 | -1.36557900 | -0.28428900 |
| C | 3.21007800 | -1.89517100 | 0.53970900 |
| C | 2.31181900 | -1.55003400 | -1.66490200 |
| C | 4.27256200 | -2.61388700 | -0.00151200 |
| H | 3.15101400 | -1.74475900 | 1.61296400 |
| C | 3.37458600 | -2.26210600 | -2.20622900 |

| | | | |
|---|---|---|---|
| H | 1.54982200 | -1.12891200 | -2.31102700 |
| C | 4.35620800 | -2.79910300 | -1.37665900 |
| H | 5.03610800 | -3.02121800 | 0.65083900 |
| H | 3.43395300 | -2.39999100 | -3.27999800 |
| H | 5.18434300 | -3.35427200 | -1.80159600 |
| C | -1.26253000 | -1.23888700 | -2.40825200 |
| C | -0.83381900 | -0.71905400 | -3.64579100 |
| C | -1.00729800 | -2.60292000 | -2.15662700 |
| C | -0.18254200 | -1.51801300 | -4.57467600 |
| H | -1.03357800 | 0.31633000 | -3.89361700 |
| C | -0.34442100 | -3.39463200 | -3.08172300 |
| H | -1.30178500 | -3.02647400 | -1.20323900 |
| C | 0.07288500 | -2.85898500 | -4.29747300 |
| H | 0.12714900 | -1.09152600 | -5.52186500 |
| H | -0.13506100 | -4.43138700 | -2.84522200 |
| H | 0.59268300 | -3.47770900 | -5.01903100 |

**Vibrational frequencies**

16.77, 29.03, 38.76, 43.33, 58.58, 66.19, 72.08, 83.13, 86.64, 104.72, 113.5, 134.67, 151.7, 183.6, 209.11, 215.96, 235.36, 237.66, 266.95, 278.38, 296.77, 310.19, 331.54, 377.31, 388.36, 411.94, 412.96, 421.59, 435.03, 444.37, 479.86, 489.89, 499.37, 548.63, 572.2, 594.8, 610, 628.48, 629.82, 633.29, 649.9, 669.97, 683.42, 707.96, 712.97, 714.66, 727.93, 748.3, 759.89, 771.45, 776.03, 782.61, 813.94, 826.8, 853.45, 862.46, 868.07, 873.62, 876.1, 916.18, 936.14, 938.19, 942.05, 952.19, 954.04, 955.3, 985.21, 999.37, 1000.55, 1003.97, 1007.23, 1009.22, 1010.39, 1013.86, 1016.77, 1017.64, 1020.35, 1022.71, 1030.99, 1036.46, 1050.41, 1062.95, 1064.86, 1068.73, 1087.13, 1108.43, 1109.97, 1114.83, 1120.65, 1125.95, 1136.3, 1146.93, 1154.39, 1174.16, 1177.09, 1182.3, 1192.5, 1199.82, 1210.09, 1212.7, 1217.15, 1226.49, 1244.26, 1246.32, 1268.65, 1275.87, 1281.96, 1299.42, 1309.28, 1312.55, 1327, 1327.86, 1332.23, 1335.66, 1343.53, 1348.6, 1351.36, 1361.08, 1364.69, 1391.88, 1412.92, 1445.4, 1469.65, 1482.74, 1488.31, 1490.45, 1493.76, 1494.07, 1513.19, 1524.79, 1526.02, 1529.31, 1543.84, 1628.69, 1634.24, 1654.81, 1659.95, 1663.25, 1687.58, 1699.09, 3041.83, 3056.92, 3058.96, 3061.64, 3073.31, 3081.78, 3083.51, 3095.99, 3120.69, 3121.02, 3135.37, 3172.19, 3178.23, 3180.41, 3181.25, 3184.32, 3185.72, 3191.12, 3191.42, 3196.22, 3201.38, 3202.64, 3208.38, 3208.55, 3209.4, 3211.68, 3213.28, 3223.03.

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## 22

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.311548
Thermal correction to Energy= 0.327608
Thermal correction to Enthalpy= 0.328552
Thermal correction to Gibbs Free Energy= 0.266900

Sum of electronic and zero-point Energies= -788.097017
Sum of electronic and thermal Energies= -788.080958
Sum of electronic and thermal Enthalpies= -788.080013
Sum of electronic and thermal Free Energies= -788.141665

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.26041000 | 0.49495600 | 0.54656500 |
| C | 1.45401800 | 1.50390200 | -0.39506500 |
| C | 0.71601300 | 2.67882400 | -0.32260400 |
| C | -0.22600600 | 2.82319300 | 0.69368000 |
| C | -0.43264400 | 1.80239000 | 1.62059400 |
| C | 0.30986000 | 0.62600100 | 1.55068400 |
| C | 2.12007900 | -0.71771200 | 0.20802400 |
| C | 3.16280900 | -0.12268600 | -0.75877600 |
| C | 2.47347200 | 1.08261600 | -1.42728200 |
| C | 2.73264900 | -1.43550700 | 1.40654900 |
| N | 1.26441700 | -1.59964800 | -0.60348200 |
| O | 0.38862000 | -2.19018100 | 0.23694700 |

| | | | |
|---|---|---|---|
| C | -0.81597800 | -2.55713200 | -0.45194200 |
| C | -1.76027500 | -1.38345800 | -0.45252700 |
| C | -1.52489900 | -0.30140000 | -1.30328800 |
| C | -2.33291800 | 0.82568600 | -1.24368700 |
| C | -3.39116300 | 0.87955100 | -0.33954500 |
| C | -3.63463600 | -0.19555200 | 0.50666500 |
| C | -2.81651700 | -1.32126200 | 0.45245000 |
| H | 0.86615900 | 3.47130100 | -1.04846400 |
| H | -0.80973800 | 3.73442500 | 0.76054800 |
| H | -1.18227700 | 1.92214300 | 2.39415500 |
| H | 0.14046900 | -0.17691300 | 2.25957900 |
| H | 3.51190900 | -0.87363600 | -1.46934400 |
| H | 4.01826800 | 0.22167700 | -0.17188900 |
| H | 1.96195000 | 0.77674000 | -2.34599100 |
| H | 3.17154300 | 1.88054200 | -1.68775000 |
| H | 3.35538400 | -0.73836200 | 1.97026300 |
| H | 3.35361600 | -2.26840400 | 1.06712500 |
| H | 1.96004000 | -1.82905000 | 2.06697900 |
| H | -1.22871300 | -3.39953300 | 0.10365500 |
| H | -0.54613000 | -2.87016800 | -1.46260100 |
| H | -0.68983900 | -0.34069400 | -1.99473000 |
| H | -2.13192000 | 1.66743800 | -1.89585800 |
| H | -4.02113500 | 1.76045200 | -0.29416300 |
| H | -4.45685100 | -0.15802500 | 1.21167500 |
| H | -2.99826600 | -2.15541800 | 1.12263400 |

**Vibrational frequencies**

28.07, 34.49, 71.62, 77.09, 88.66, 149.41, 169.23, 203.84, 213.82, 234.89, 260.12, 291.43, 317, 346.26, 369.2, 384.5, 408.59, 440.39, 460.9, 472.39, 511.63, 561.32, 567.11, 593.27, 613.87, 630.77, 649.04, 707.68, 731.02, 745.02, 774.22, 780.52, 809.45, 837.3, 855.65, 861.94, 895.08, 928.81, 933.49, 942.66, 973.11, 990.46, 991.9, 1002.49, 1014.21, 1014.89, 1016, 1020.85, 1048.76, 1060.57, 1066.72, 1082.37, 1116.12, 1122.95, 1128.23, 1160.49, 1180.93, 1181.38, 1192.12, 1208.49, 1210.48, 1231.72, 1244.8, 1245.82, 1282.7, 1295.27, 1302.32, 1328.25, 1345.05, 1352.29, 1360.05, 1361.14, 1389.39, 1401.49, 1474.63, 1489.49, 1492.12, 1493.01, 1499.18, 1505.32, 1507.74, 1526.54, 1546.29, 1663.3, 1667.22, 1680.78, 1684.94, 3049.03, 3053.55, 3072.6, 3085.8, 3099.48, 3128.81, 3132.22, 3147.93, 3149.09, 3169.35, 3179.96, 3180.16, 3189.69, 3191.93, 3195.81, 3196.74, 3209.61, 3216.01.

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## 23

**M06-2X/6-311+G(*d*,*p*)–LANL2DZ**

Zero-point correction= 0.373888 (Hartr
Thermal correction to Energy= 0.394359
Thermal correction to Enthalpy= 0.395303
Thermal correction to Gibbs Free Energy= 0.321031

Sum of electronic and zero-point Energies= -476.996300
Sum of electronic and thermal Energies= -476.975829
Sum of electronic and thermal Enthalpies= -476.974885
Sum of electronic and thermal Free Energies= -477.049157

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 5.50001400 | -0.03124200 | 0.18744000 |
| C | 4.29596400 | -0.66581100 | 0.87899400 |
| C | 3.02690300 | -0.60087200 | 0.02789100 |
| C | 1.80568700 | -1.22515100 | 0.71126500 |
| Sn | 0.03140600 | -1.06117600 | -0.48418700 |
| C | -0.04201100 | 0.96790900 | -1.17501400 |
| H | 0.08846400 | -2.16363300 | -1.79393800 |
| C | -1.75507200 | -1.35733200 | 0.66886600 |

| | | | |
|---|---|---|---|
| C | -2.98560800 | -0.74283000 | -0.00726500 |
| C | -0.05050900 | 1.94052000 | 0.01003400 |
| C | -0.14470500 | 3.40877700 | -0.40662900 |
| C | -0.13560700 | 4.36041700 | 0.78746900 |
| C | -4.26896900 | -0.89706400 | 0.80961600 |
| C | -5.47927200 | -0.26840100 | 0.12336200 |
| H | 6.39553600 | -0.08206000 | 0.81003300 |
| H | 5.30850500 | 1.02127500 | -0.03835900 |
| H | 5.71853700 | -0.53822000 | -0.75617400 |
| H | 4.10820100 | -0.16483300 | 1.83487200 |
| H | 4.51204600 | -1.71307200 | 1.11629200 |
| H | 3.21915600 | -1.10117200 | -0.92983400 |
| H | 2.82132300 | 0.44938900 | -0.21741700 |
| H | 1.61383200 | -0.72155200 | 1.66508500 |
| H | 1.99990500 | -2.27548500 | 0.94821800 |
| H | -0.93792000 | 1.11086200 | -1.78773300 |
| H | 0.81551900 | 1.17084500 | -1.82416400 |
| H | -1.60166900 | -0.89873600 | 1.65185400 |
| H | -1.91310100 | -2.42525800 | 0.84582200 |
| H | -3.13955500 | -1.19850100 | -0.99398200 |
| H | -2.81437100 | 0.32535100 | -0.19379800 |
| H | 0.85766400 | 1.80334700 | 0.61269100 |
| H | -0.89135600 | 1.71120000 | 0.67900200 |
| H | -1.05949800 | 3.55309200 | -0.99161400 |
| H | 0.69046100 | 3.64230000 | -1.07569800 |
| H | -0.97379900 | 4.15163500 | 1.45764500 |
| H | -0.21037200 | 5.40297200 | 0.47193900 |
| H | 0.78628200 | 4.25045700 | 1.36478000 |
| H | -4.12010200 | -0.44056600 | 1.79430000 |
| H | -4.45294200 | -1.96198300 | 0.98754700 |
| H | -5.32149700 | 0.80107400 | -0.04018400 |
| H | -6.38691500 | -0.38561800 | 0.71877300 |
| H | -5.65631400 | -0.72978700 | -0.85193600 |

**Vibrational frequencies**

20.66, 23.58, 27.67, 36.67, 60.85, 69.65, 85.26, 95.59, 103.97, 132.05, 135.99, 141.81, 153.29, 177.76, 188.66, 232.37, 233.56, 239.82, 242.75, 245.61, 254.8, 377.94, 379.59, 399.21, 529.67, 555.36, 606.32, 611.81, 621.02, 666.79, 691.76, 694.23, 741.5, 753.58, 758.99, 859.69, 879.94, 883.56, 899.49, 901.01, 904.67, 1017.38, 1031.09, 1032.31, 1036.52, 1037.64, 1042.92, 1079.07, 1083.04, 1083.78, 1091.95, 1095.12, 1105.73, 1181.6, 1191.3, 1195.42, 1221.15, 1228.56, 1231.25, 1298.15, 1308.94, 1311.77, 1315.9, 1326.06, 1327.38, 1336.77, 1344.56, 1349.87, 1385.69, 1394.72, 1395.85, 1406.84, 1415.36, 1418.17, 1457.95, 1464.61, 1467.85, 1482.74, 1489.22, 1491.93, 1496.01, 1499.29, 1501.03, 1502.01, 1502.11, 1506.22, 1510.41, 1512.23, 1513.94, 1913.92, 3006.67, 3021.23, 3024.5, 3033.66, 3037.48, 3039.66, 3041.17, 3043.56, 3044.2, 3046.93, 3048.2, 3048.85, 3053.94, 3055.49, 3056.99, 3073.68, 3086.54, 3087.8, 3091.01, 3102.39, 3103.89, 3111.36, 3116.58, 3119.52, 3120.36, 3122.27, 3127.91.

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## 24

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.324958
Thermal correction to Energy= 0.340948
Thermal correction to Enthalpy= 0.341892
Thermal correction to Gibbs Free Energy= 0.281911
Sum of electronic and zero-point Energies= -788.721294
Sum of electronic and thermal Energies= -788.705304
Sum of electronic and thermal Enthalpies= -788.704359
Sum of electronic and thermal Free Energies= -788.764341

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 1.20758500 | 0.36633400 | 0.48209900 |
| C | 1.40633400 | 1.40069700 | -0.43024700 |
| C | 0.67993100 | 2.57965400 | -0.32603000 |
| C | -0.25632600 | 2.70504400 | 0.69781500 |
| C | -0.46878000 | 1.66124100 | 1.59642400 |
| C | 0.26602700 | 0.48189900 | 1.49487500 |
| C | 2.11013000 | -0.81209600 | 0.16515600 |
| C | 3.15330500 | -0.17466900 | -0.78076400 |
| C | 2.43798900 | 1.00778800 | -1.45930500 |
| C | 2.73700300 | -1.46008200 | 1.39711500 |
| N | 1.35953300 | -1.78610400 | -0.65926700 |
| O | 0.43441400 | -2.47242300 | 0.17416100 |
| C | -0.81096300 | -2.63517600 | -0.50149200 |
| C | -1.67603400 | -1.40214500 | -0.46955900 |
| C | -1.46386200 | -0.35931500 | -1.37295900 |
| C | -2.24371900 | 0.78863500 | -1.31705300 |
| C | -3.25454100 | 0.90175000 | -0.36601700 |
| C | -3.47649500 | -0.13362700 | 0.53433700 |
| C | -2.68564400 | -1.27805700 | 0.48296900 |
| H | 0.83820400 | 3.39106700 | -1.02876800 |
| H | -0.83034700 | 3.61994400 | 0.79303900 |
| H | -1.21489400 | 1.76662800 | 2.37543200 |
| H | 0.09645600 | -0.33677800 | 2.18563400 |
| H | 3.56015200 | -0.90087700 | -1.48971300 |
| H | 3.98174700 | 0.19676600 | -0.17210900 |
| H | 1.93875100 | 0.68333600 | -2.37850200 |
| H | 3.11699000 | 1.82228000 | -1.71851100 |
| H | 3.25366700 | -0.70793500 | 1.99674800 |
| H | 3.46226200 | -2.22285600 | 1.09582000 |
| H | 1.97382500 | -1.93758900 | 2.01260000 |
| H | -1.30319700 | -3.45382500 | 0.02788200 |
| H | -0.61799000 | -2.94872000 | -1.53186000 |
| H | -0.66975100 | -0.45018400 | -2.10624900 |
| H | -2.06176500 | 1.59880700 | -2.01355200 |
| H | -3.86490000 | 1.79683800 | -0.32718000 |
| H | -4.26261600 | -0.05051200 | 1.27604400 |
| H | -2.85494600 | -2.08474400 | 1.18939700 |
| H | 2.02604800 | -2.51364500 | -0.92544200 |

**Vibrational frequencies**

41.94, 57.5, 75.42, 78.75, 104.26, 141.36, 165.36, 208.78, 213.7, 235.81, 276.61, 281.02, 330.32, 351.2, 363.38, 392.58, 410.12, 436.78, 460.73, 469.92, 501.98, 556.75, 573.78, 592.1, 616.03, 632.26, 639.95, 707.75, 730.56, 740.41, 767.99, 776.63, 803.18, 840.05, 858.22, 861.32, 883.79, 909.17, 921.45, 942.27, 964.3, 976.58, 992.52, 998.56, 1008.63, 1009.76, 1012.3, 1015.21, 1021.05, 1041.31, 1059.93, 1066.57, 1089.7, 1115.75, 1122.66, 1130.47, 1154.82, 1177.05, 1184.11, 1200.49, 1204.01, 1210.84, 1222.76, 1247.1, 1250.92, 1297.24, 1299.3, 1318.03, 1332.12, 1349.31, 1354.08, 1362.76, 1366.65, 1400.79, 1405.79, 1473.75, 1484.33, 1488.85, 1490.25, 1500.95, 1501.92, 1504.2, 1515.02, 1532.98, 1545.9, 1665.69, 1666.18, 1683.85, 1687.93, 3037.42, 3047.88, 3067.59, 3069.83, 3101.26, 3113.7, 3121.75, 3138.1, 3140.93, 3172.5, 3173.45, 3183.81, 3185.23, 3189.06, 3194.12, 3201.36, 3211.1, 3211.27, 3423.21.

## TS3

**M06-2X/6-311+G(*d*,*p*)–LANL2DZ**

Zero-point correction= 0.684723 (Hartr
Thermal correction to Energy= 0.722294
Thermal correction to Enthalpy= 0.723238
Thermal correction to Gibbs Free Energy= 0.609258

Sum of electronic and zero-point Energies= -1265.082221
Sum of electronic and thermal Energies= -1265.044650
Sum of electronic and thermal Enthalpies= -1265.043705
Sum of electronic and thermal Free Energies= -1265.157685

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 0.04207100 | -0.01019300 | -0.03963200 |
| C | 0.05379900 | 0.02896700 | 1.35316400 |
| C | 1.26029700 | 0.00501100 | 2.04168000 |
| C | 2.44878700 | -0.07265500 | 1.31854700 |
| C | 2.43114400 | -0.13318000 | -0.07420500 |
| C | 1.22252000 | -0.10271800 | -0.76505900 |
| C | -1.38817700 | -0.02524800 | -0.56306900 |
| C | -2.18915100 | 0.45754500 | 0.66388900 |
| C | -1.35508900 | 0.05851100 | 1.89627600 |
| C | -1.60863300 | 0.82517000 | -1.81166200 |
| N | -1.72278600 | -1.45381000 | -0.73435500 |
| O | -1.09469300 | -1.89323600 | -1.88598600 |
| C | -0.75972300 | -3.27860500 | -1.76599400 |
| C | 0.55975300 | -3.45303600 | -1.06062900 |
| C | 0.63672800 | -3.34998300 | 0.32969500 |
| C | 1.86531600 | -3.43660600 | 0.97135100 |
| C | 3.02828300 | -3.63487400 | 0.23120800 |
| C | 2.95917900 | -3.73991200 | -1.15290900 |
| C | 1.72741600 | -3.64542400 | -1.79479000 |
| H | 1.27937300 | 0.04480000 | 3.12582500 |
| H | 3.39706600 | -0.09348400 | 1.84375400 |
| H | 3.36353700 | -0.21199200 | -0.62094100 |
| H | 1.20109300 | -0.16508800 | -1.84748400 |
| H | -3.19964900 | 0.04288400 | 0.66837400 |
| H | -2.26902400 | 1.54653700 | 0.60945900 |
| H | -1.63704400 | -0.93882200 | 2.24918200 |
| H | -1.47542200 | 0.75218400 | 2.73063900 |
| H | -1.19173300 | 1.82234000 | -1.65432100 |
| H | -2.67661900 | 0.92553200 | -2.02168800 |
| H | -1.12430000 | 0.37808900 | -2.68125200 |
| H | -0.70837600 | -3.65212300 | -2.79171200 |
| H | -1.57038800 | -3.78597300 | -1.23522700 |
| H | -0.27056000 | -3.17767500 | 0.89899200 |
| H | 1.91788700 | -3.33870900 | 2.04947900 |
| H | 3.98622700 | -3.70349100 | 0.73386200 |
| H | 3.86189300 | -3.89454400 | -1.73241500 |
| H | 1.67258900 | -3.71932700 | -2.87655500 |
| C | -9.01903500 | 0.02172600 | 0.42775700 |
| C | -8.39831800 | -1.23053600 | -0.18698100 |
| C | -7.03956700 | -0.95591700 | -0.83254900 |
| C | -6.39672600 | -2.19763500 | -1.45838900 |
| Sn | -4.50467400 | -1.72776600 | -2.37380700 |
| C | -4.88552800 | -0.00233800 | -3.60700700 |
| H | -3.11994500 | -1.46422500 | -1.14935600 |

| | | | |
|---|---|---|---|
| C | -3.80760300 | -3.27084000 | -3.70865900 |
| C | -2.82601500 | -2.71274000 | -4.74539200 |
| C | -6.00889900 | -0.28670200 | -4.60995900 |
| C | -6.30479700 | 0.89101400 | -5.54025600 |
| C | -7.42006800 | 0.58728800 | -6.53774800 |
| C | -2.21460200 | -3.79061200 | -5.64197900 |
| C | -1.21237600 | -3.21986700 | -6.64243200 |
| H | -9.98601300 | -0.19122500 | 0.88788500 |
| H | -9.17217200 | 0.79330800 | -0.33164000 |
| H | -8.36611800 | 0.44044500 | 1.19831100 |
| H | -9.07285400 | -1.64865000 | -0.94193700 |
| H | -8.27759400 | -2.00213500 | 0.58097800 |
| H | -6.36970900 | -0.53016600 | -0.07364800 |
| H | -7.16336600 | -0.17505900 | -1.59469300 |
| H | -7.05372400 | -2.61352600 | -2.23075800 |
| H | -6.26463200 | -2.97925700 | -0.70470800 |
| H | -3.96482800 | 0.26710000 | -4.13486900 |
| H | -5.14872100 | 0.85295900 | -2.97557900 |
| H | -4.66757400 | -3.73097000 | -4.20783600 |
| H | -3.32900800 | -4.06309400 | -3.12395700 |
| H | -2.01693800 | -2.16802700 | -4.24198900 |
| H | -3.33498400 | -1.97407300 | -5.37771500 |
| H | -6.93037200 | -0.55433400 | -4.07556100 |
| H | -5.75155200 | -1.16154800 | -5.22249900 |
| H | -5.38767000 | 1.15747700 | -6.07644400 |
| H | -6.57308300 | 1.76319600 | -4.93438600 |
| H | -7.15689400 | -0.26783300 | -7.16620400 |
| H | -7.61626300 | 1.43736000 | -7.19433400 |
| H | -8.35092900 | 0.34321200 | -6.01886500 |
| H | -3.01697200 | -4.31509400 | -6.17228000 |
| H | -1.72405500 | -4.54171800 | -5.01170700 |
| H | -1.68974500 | -2.48254700 | -7.29331500 |
| H | -0.78522500 | -3.99932900 | -7.27663500 |
| H | -0.38977100 | -2.71867400 | -6.12435300 |

**Vibrational frequencies**

1396.46*i*, 11.12, 16.71, 20.41, 23.25, 28.31, 33.24, 41.61, 49.69, 53.32, 57.02, 76.74, 79.68, 87.72, 89.77, 95.45, 96.85, 102.48, 116.18, 118.53, 126.11, 142.34, 143.59, 148.6, 166.14, 175.65, 189.68, 192.87, 200.24, 213.58, 220.13, 229.31, 238.83, 242.42, 244.3, 248.66, 256.57, 258.56, 281.44, 296.02, 340.09, 363.25, 380.96, 388.93, 393.93, 399.27, 416, 432.14, 460.32, 473.94, 494.75, 517.82, 562.3, 589.9, 593.84, 596.24, 601.87, 603.67, 620.56, 631.94, 640.94, 646.87, 670.73, 681.9, 712.26, 731.74, 743.37, 745.96, 753.16, 757.32, 774.57, 777.92, 807.9, 841.12, 856.79, 862.91, 865.29, 867.65, 877.18, 890.39, 895.6, 898.02, 903.13, 908.34, 925.14, 926.95, 944.95, 969.91, 983.75, 999.25, 1000.15, 1008.24, 1013.8, 1014.97, 1019.75, 1022.93, 1031.25, 1031.49, 1031.92, 1034.05, 1037, 1043.67, 1059.04, 1063.55, 1080.64, 1081.93, 1082.51, 1087.34, 1088.04, 1091.62, 1099.45, 1101.13, 1119.7, 1122.87, 1127.51, 1162.3, 1176.37, 1177.4, 1178.05, 1181.57, 1188.7, 1191.24, 1203.36, 1208.96, 1223.17, 1227.1, 1228.23, 1228.64, 1242.9, 1247.88, 1288.6, 1298.03, 1299.21, 1299.5, 1305.45, 1307.18, 1316.7, 1321.16, 1325.06, 1325.74, 1336.2, 1340.5, 1346.31, 1346.48, 1351.73, 1359.23, 1361.92, 1388.82, 1390.42, 1393.36, 1398.62, 1402.68, 1411.21, 1415.61, 1417.4, 1459.89, 1463, 1470.84, 1472.49, 1486.89, 1488.15, 1490.89, 1491.81, 1493.64, 1497.19, 1499.27, 1499.79, 1500.55, 1501.13, 1502.03, 1502.5, 1504.19, 1505.3, 1506.06, 1513.62, 1514.57, 1515.66, 1525.98, 1541.66, 1664.32, 1664.63, 1682.93, 1684.16, 3016.6, 3018.26, 3022.73, 3035.16, 3042.26, 3042.99, 3044.64, 3044.98, 3046.69, 3046.82, 3050.05, 3050.47, 3050.9, 3051.24, 3052.61, 3053.71, 3062.67, 3065.99, 3077.86, 3084.9, 3088.05, 3089.66, 3095.33, 3100.97, 3101.95, 3106.6, 3115.69, 3117.27, 3118.27, 3118.97, 3123.92, 3125.46, 3127.55, 3127.95, 3133.57, 3142.16, 3169.54, 3171.83, 3178.06, 3183.36, 3183.42, 3191.21, 3192.35, 3202.81, 3204.53.

**25**

**M06-2X/6-311+G(*d*,*p*)–LANL2DZ**

Zero-point correction= 0.365727 (Hartr
Thermal correction to Energy= 0.385934
Thermal correction to Enthalpy= 0.386879
Thermal correction to Gibbs Free Energy= 0.312724

Sum of electronic and zero-point Energies= -476.387514
Sum of electronic and thermal Energies= -476.367307
Sum of electronic and thermal Enthalpies= -476.366363
Sum of electronic and thermal Free Energies= -476.440518

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| C | 5.51927800 | -0.25998400 | 0.22018700 |
| C | 4.25918000 | -0.73681600 | 0.93721800 |
| C | 3.01613900 | -0.67813300 | 0.04656400 |
| C | 1.74552300 | -1.16372100 | 0.74622200 |
| Sn | -0.01989700 | -0.99596000 | -0.50120100 |
| C | -0.01596800 | 1.04834500 | -1.22192400 |
| C | -1.79709400 | -1.18197900 | 0.72847700 |
| C | -3.04207700 | -0.59250900 | 0.06332200 |
| C | 0.05673700 | 2.02748200 | -0.04479100 |
| C | 0.04463900 | 3.49562500 | -0.47886900 |
| C | 0.15512300 | 4.45719100 | 0.70092300 |
| C | -4.30149200 | -0.70334800 | 0.92547500 |
| C | -5.53311800 | -0.11538100 | 0.24238800 |
| H | 6.39571000 | -0.30864200 | 0.87063100 |
| H | 5.41147400 | 0.77501700 | -0.11647900 |
| H | 5.72417500 | -0.87520200 | -0.66057200 |
| H | 4.08668300 | -0.12732300 | 1.83118200 |
| H | 4.39850500 | -1.76604700 | 1.28556500 |
| H | 3.19874600 | -1.27844100 | -0.85372600 |
| H | 2.88200700 | 0.35440400 | -0.30186100 |
| H | 1.54910700 | -0.56582100 | 1.64527700 |
| H | 1.85947200 | -2.20002200 | 1.07704300 |
| H | -0.92056400 | 1.22049900 | -1.81326000 |
| H | 0.83443400 | 1.19278600 | -1.89504200 |
| H | -1.58423300 | -0.66803000 | 1.67412300 |
| H | -1.95603200 | -2.23617600 | 0.97320500 |
| H | -3.22664900 | -1.09512000 | -0.89469600 |
| H | -2.87342700 | 0.46480400 | -0.17871500 |
| H | 0.96688100 | 1.84222100 | 0.54061200 |
| H | -0.78411300 | 1.85709900 | 0.64065800 |
| H | -0.87735800 | 3.69428700 | -1.03593200 |
| H | 0.87224000 | 3.66562800 | -1.17572700 |
| H | -0.67323500 | 4.31563800 | 1.40094500 |
| H | 0.13930100 | 5.49932600 | 0.37312200 |
| H | 1.08594000 | 4.29534100 | 1.25202400 |
| H | -4.12776100 | -0.19396100 | 1.87961000 |
| H | -4.47794700 | -1.75783200 | 1.16420800 |
| H | -5.38914400 | 0.94615600 | 0.02192800 |
| H | -6.42384700 | -0.20772400 | 0.86814600 |
| H | -5.73677100 | -0.62552200 | -0.70337100 |

**Vibrational frequencies**

21.56, 26.13, 31.7, 41.58, 61.13, 83.34, 88.43, 96.32, 107.03, 125.88, 131.84, 135.34, 150.84, 175.71, 182.97, 224.82, 237.69, 239.82, 242.26, 247.38, 254.72, 375.17, 382.65, 395.98, 578.73, 581.01, 591.83, 620.11, 663.14, 665.27, 738.77, 744.28, 745.49, 853.03, 863, 865.35, 897.66, 899.46, 901.16, 1011.02, 1019.21, 1021.3, 1027, 1033.99, 1037.11, 1075.62, 1077.68, 1079.99, 1082.92, 1083.3, 1094.43, 1161.19, 1164.11, 1174.44, 1218.89, 1220.66, 1221.89, 1294.94, 1296.91, 1300.65, 1310.08, 1311.49, 1314.84, 1331.86, 1334.9, 1337.77, 1377.18, 1381.92, 1385.15, 1405.68, 1408.23, 1408.64, 1449.24, 1452.47, 1456.11, 1474.44, 1477.79, 1480.36, 1487.9, 1488.96, 1491.19, 1493.47, 1494.07, 1496.11, 1503.37, 1504.48, 1505.9, 3019.74, 3023, 3023.81, 3040.37, 3042.27, 3046.89, 3048.16, 3049.28, 3050.78, 3053.34, 3053.93, 3054.05, 3054.4, 3054.6, 3062.69, 3084.48, 3085.48, 3087.11, 3102.33, 3103.22, 3110.83, 3122.75, 3123.08, 3123.3, 3126.8, 3129.28, 3130.38.

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## 26

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.019177
Thermal correction to Energy= 0.022014
Thermal correction to Enthalpy= 0.022959
Thermal correction to Gibbs Free Energy= 0.000212

Sum of electronic and zero-point Energies= -55.845793
Sum of electronic and thermal Energies= -55.842956
Sum of electronic and thermal Enthalpies= -55.842011
Sum of electronic and thermal Free Energies= -55.864758

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| H | 1.06203900 | -0.11221200 | -0.03178300 |
| N | 2.08669500 | -0.05942600 | -0.01679100 |
| H | 2.37626700 | -1.00736200 | -0.28242500 |

**Vibrational frequencies**

1509.83, 3406.44, 3501.52.

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## 27

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.034623 (Hartr
Thermal correction to Energy= 0.037494
Thermal correction to Enthalpy= 0.038439
Thermal correction to Gibbs Free Energy= 0.015559

Sum of electronic and zero-point Energies= -56.511226
Sum of electronic and thermal Energies= -56.508355
Sum of electronic and thermal Enthalpies= -56.507410
Sum of electronic and thermal Free Energies= -56.530290

**Cartesian coordinates**

| | | | |
|---|---|---|---|
| H | 1.06129500 | 0.09448200 | 0.00481300 |
| N | 2.07375100 | 0.07596000 | 0.02744600 |
| H | 2.39791500 | -0.24231300 | -0.87790500 |
| H | 2.39803900 | 1.02687100 | 0.15564600 |

**Vibrational frequencies**

1018.35, 1664.52, 1666.4, 3526.11, 3660.6, 3661.63.

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**H**

**M06-2X/6-311+G(*d*,*p*)**

Zero-point correction= 0.000000
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.497821
Sum of electronic and thermal Energies= -0.496405
Sum of electronic and thermal Enthalpies= -0.495461
Sum of electronic and thermal Free Energies= -0.508475

**B3LYP/6-311+G(*d*,*p*)**

Zero-point correction= 0.000000
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.501829
Sum of electronic and thermal Energies= -0.500413
Sum of electronic and thermal Enthalpies= -0.499469
Sum of electronic and thermal Free Energies= -0.512483

**mPWPW91/6-311+G(*d*,*p*)**

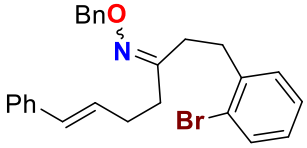
Zero-point correction= 0.000000
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.502552
Sum of electronic and thermal Energies= -0.501136
Sum of electronic and thermal Enthalpies= -0.500192
Sum of electronic and thermal Free Energies= -0.513206

**TPSSh/6-311+G(*d*,*p*)**

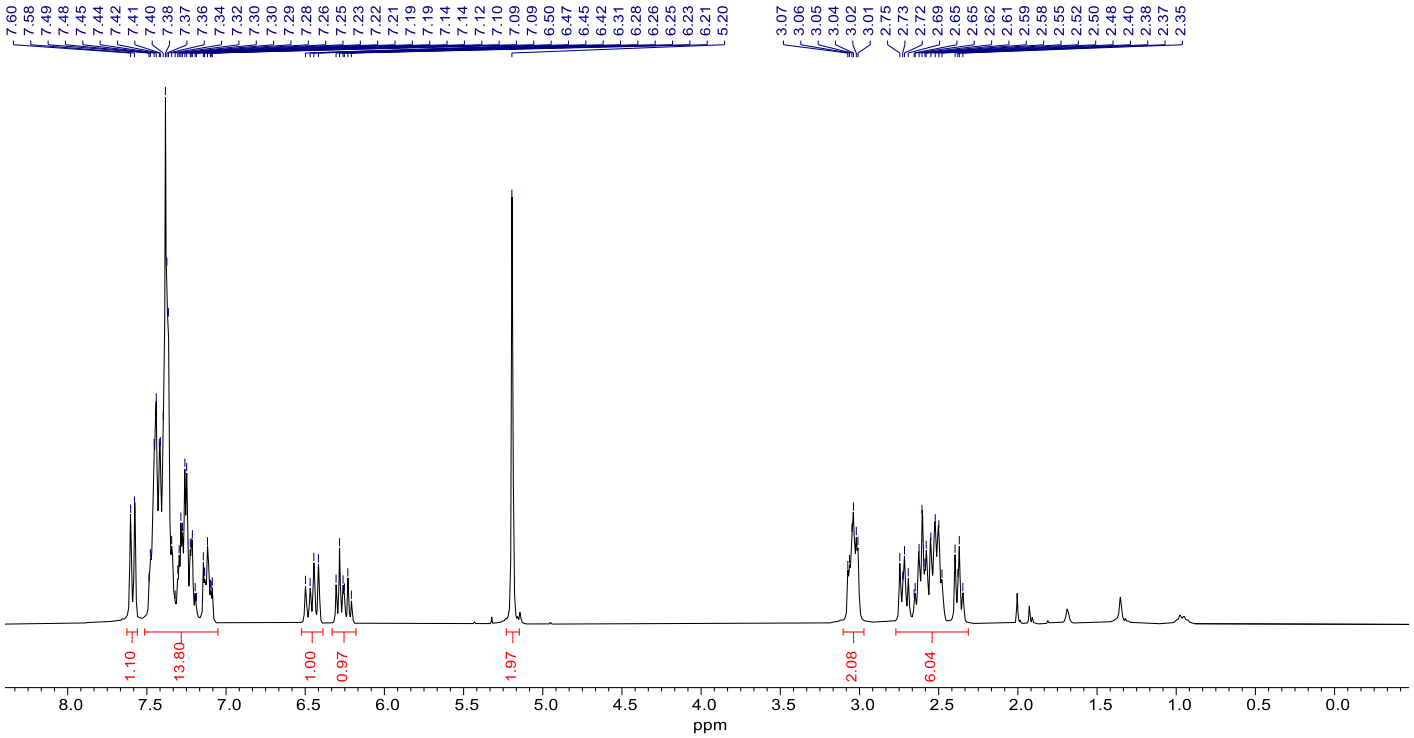
Zero-point correction= 0.000000
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.499508
Sum of electronic and thermal Energies= -0.498092
Sum of electronic and thermal Enthalpies= -0.497148
Sum of electronic and thermal Free Energies= -0.510162

## 7. Copies of NMR spectra

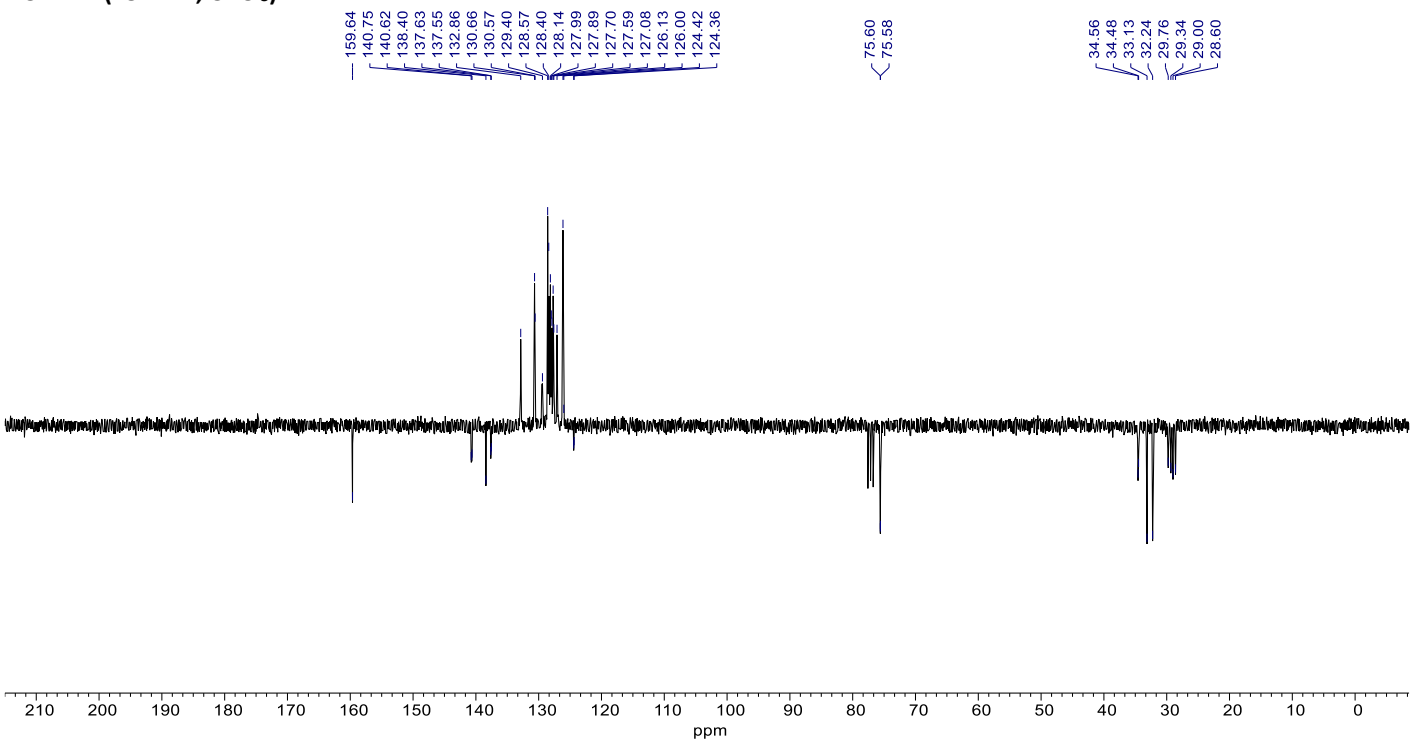
**(3*EZ*,6*E*)-1-(2-Bromophenyl)-7-phenylhept-6-en-3-one *O*-benzyl oxime (5c)**



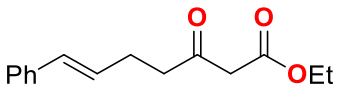

**$^{1}$H NMR (300 MHz, $CDCl_3$)**



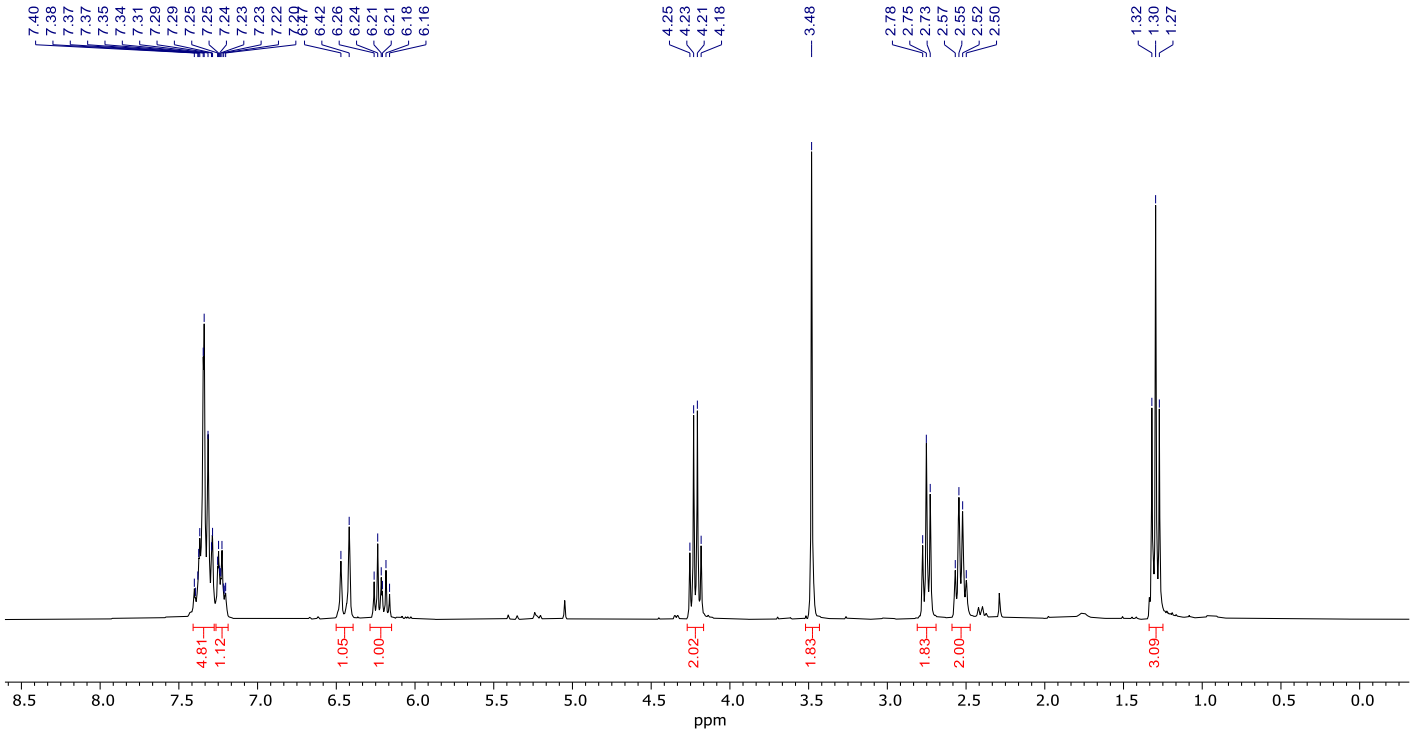

**$^{13}$C NMR (75 MHz, $CDCl_3$)**



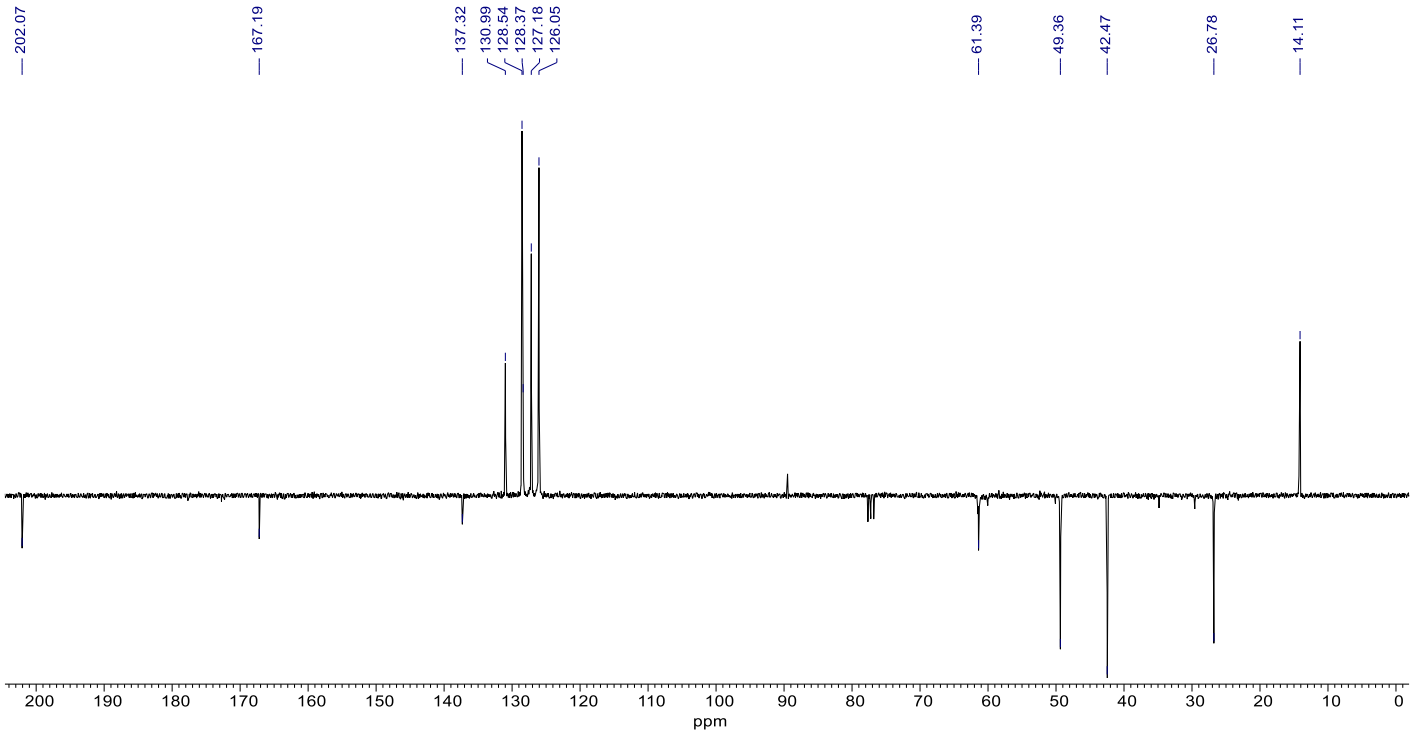
**Ethyl (*E*)-3-oxo-7-phenylhept-6-enoate (11)**



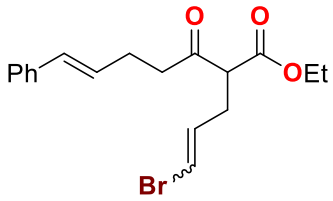

**$^{1}$H NMR (300 MHz, $CDCl_3$)**



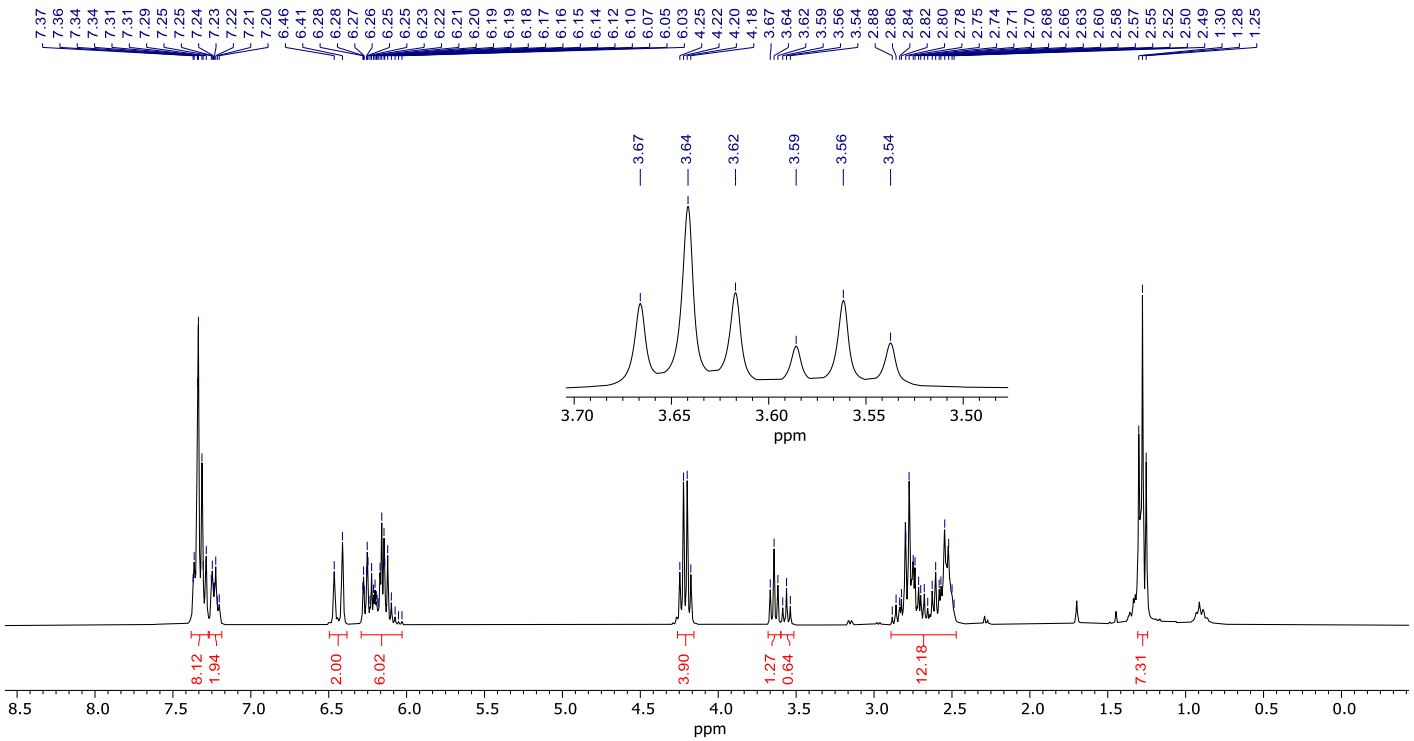

**$^{13}$C NMR (75 MHz, $CDCl_3$)**



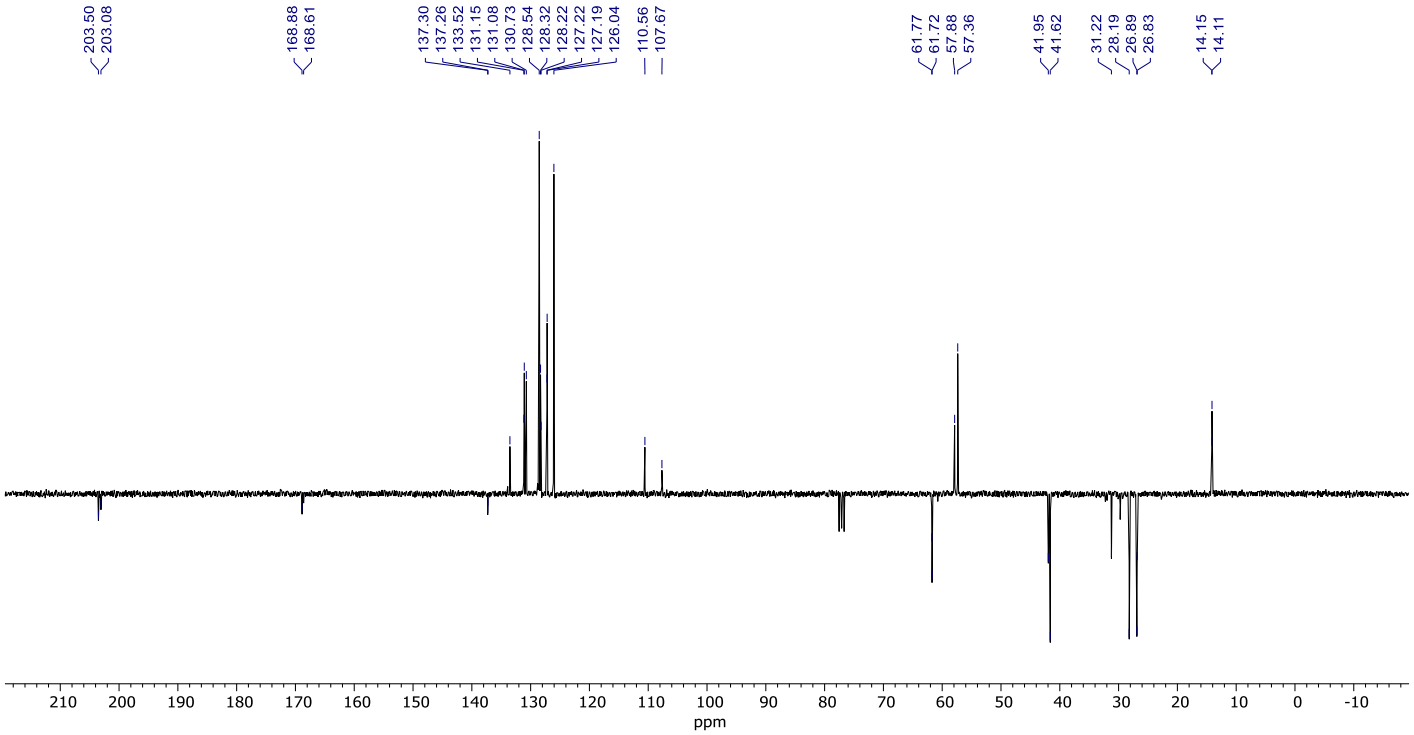
**Ethyl (6*E*)-2-(3-bromoallyl)-3-oxo-7-phenylhept-6-enoate (13)**



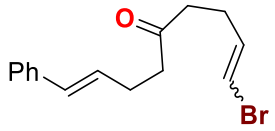

**$^{1}$H NMR (300 MHz, $CDCl_3$)**



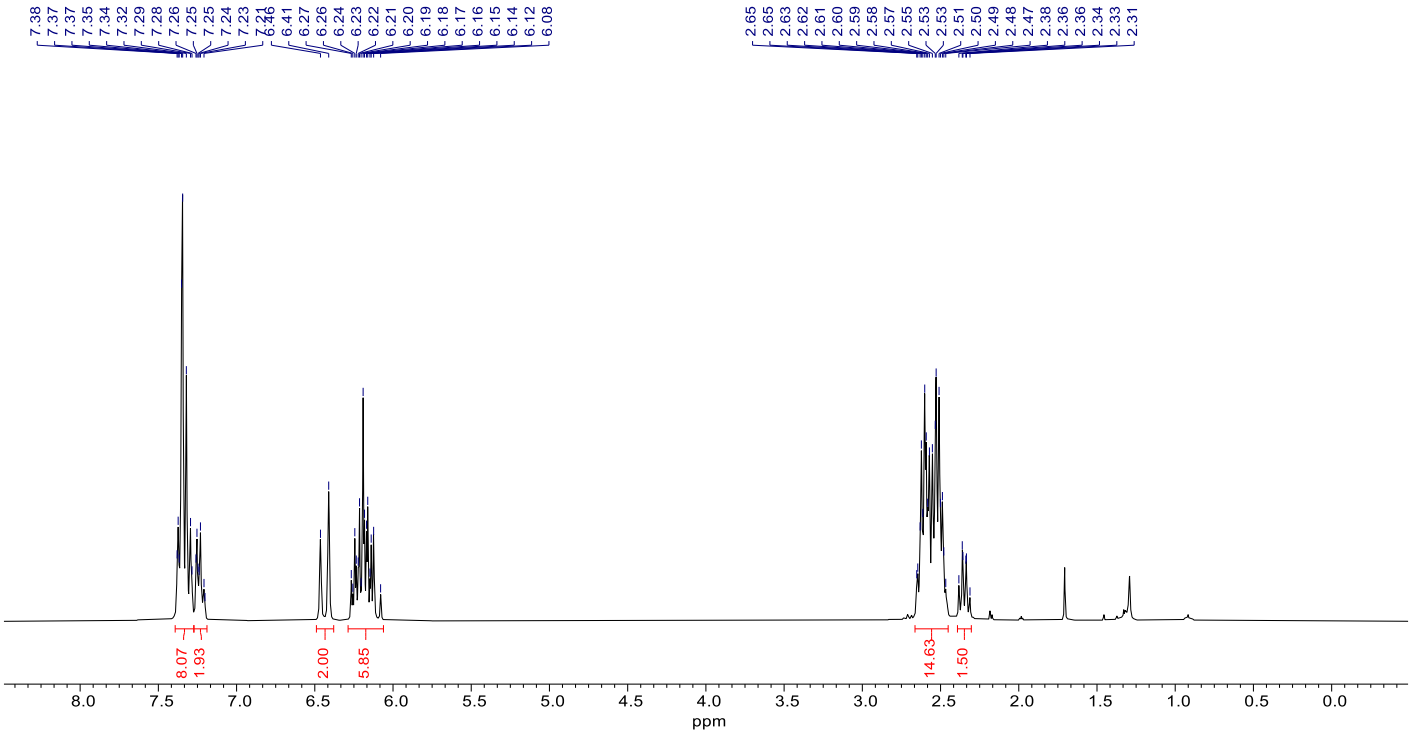

**$^{13}$C NMR (75 MHz, $CDCl_3$)**



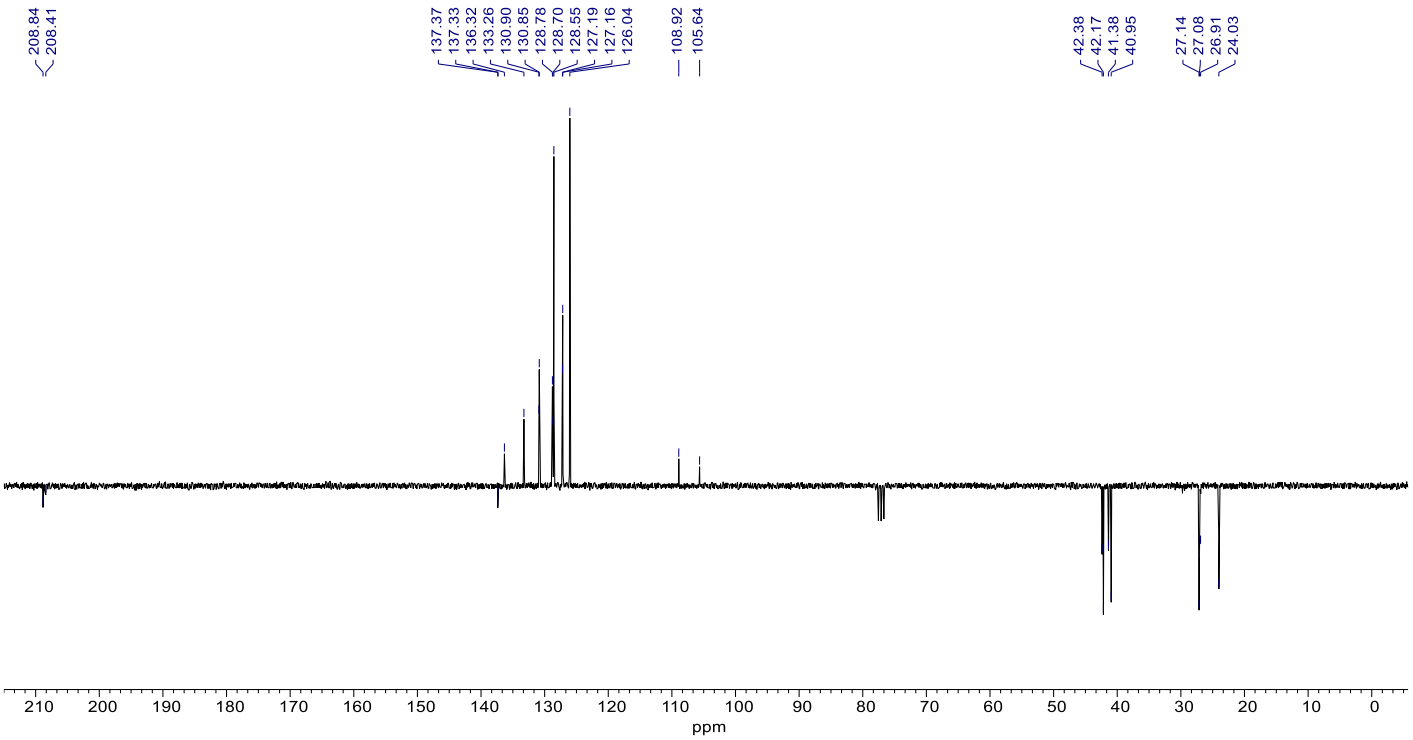
**(1*EZ*,8*E*)-1-Bromo-9-phenylnona-1,8-dien-5-one (14)**



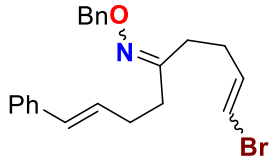

**$^{1}$H NMR (300 MHz, $CDCl_3$)**



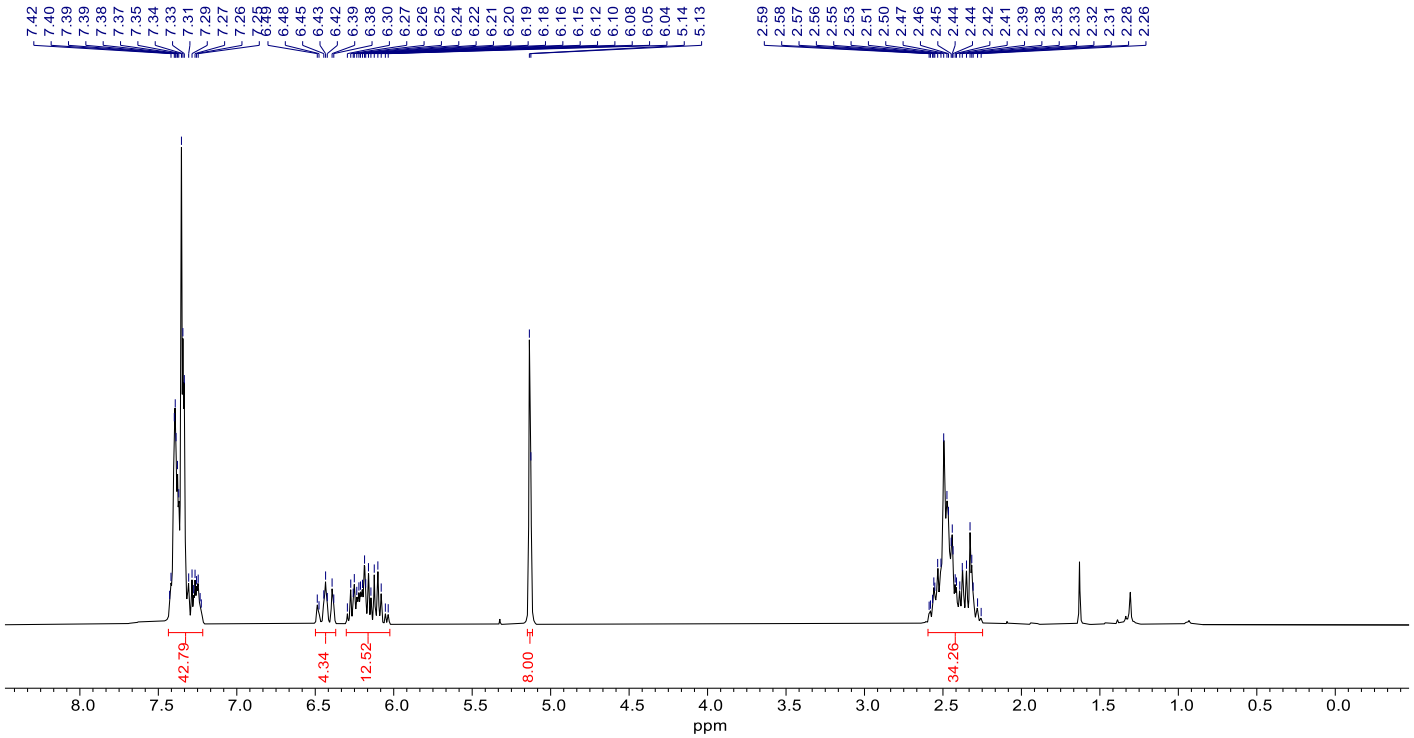

**$^{13}$C NMR (75 MHz, $CDCl_3$)**



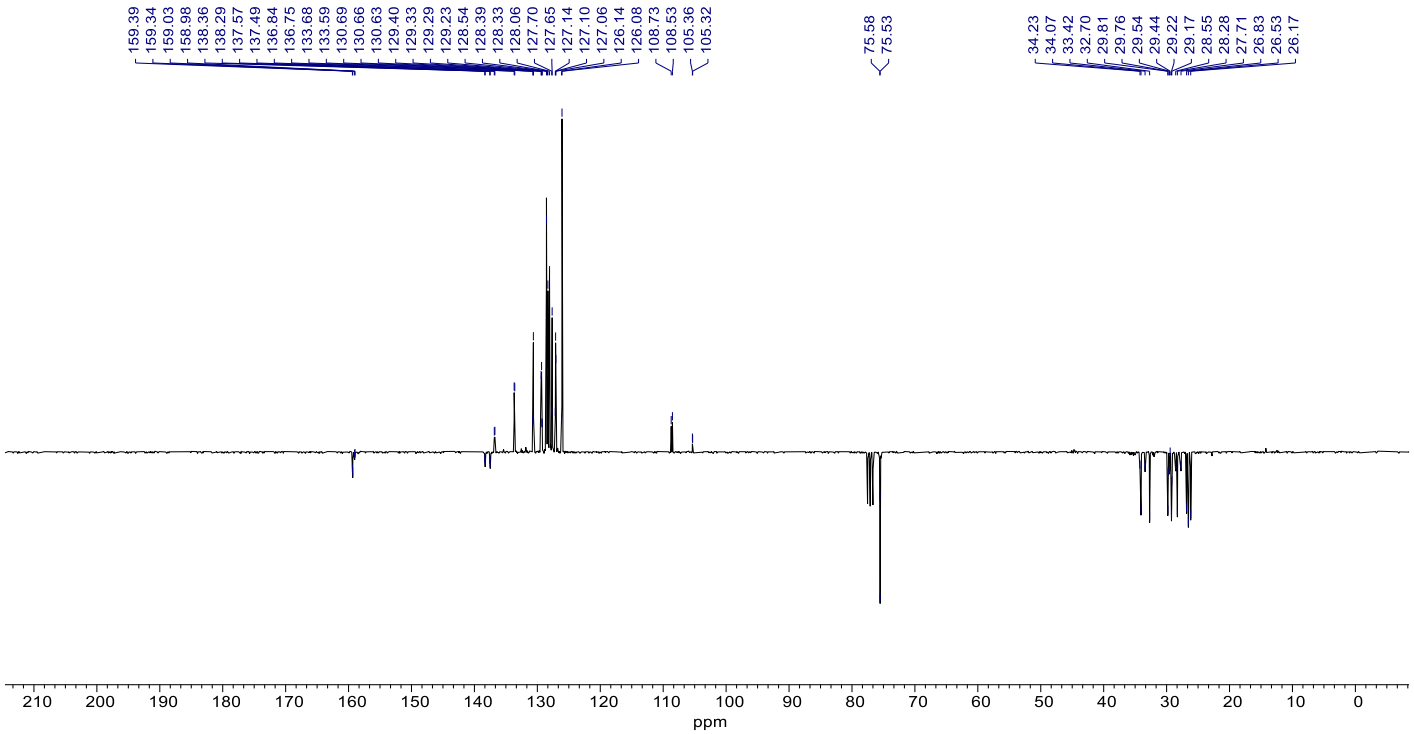
**(1*EZ*,5*EZ*,8*E*)-1-Bromo-9-phenylnona-1,8-dien-5-one *O*-benzyl oxime (15)**



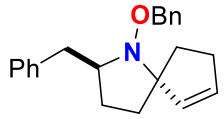

**$^{1}$H NMR (300 MHz, $CDCl_3$)**



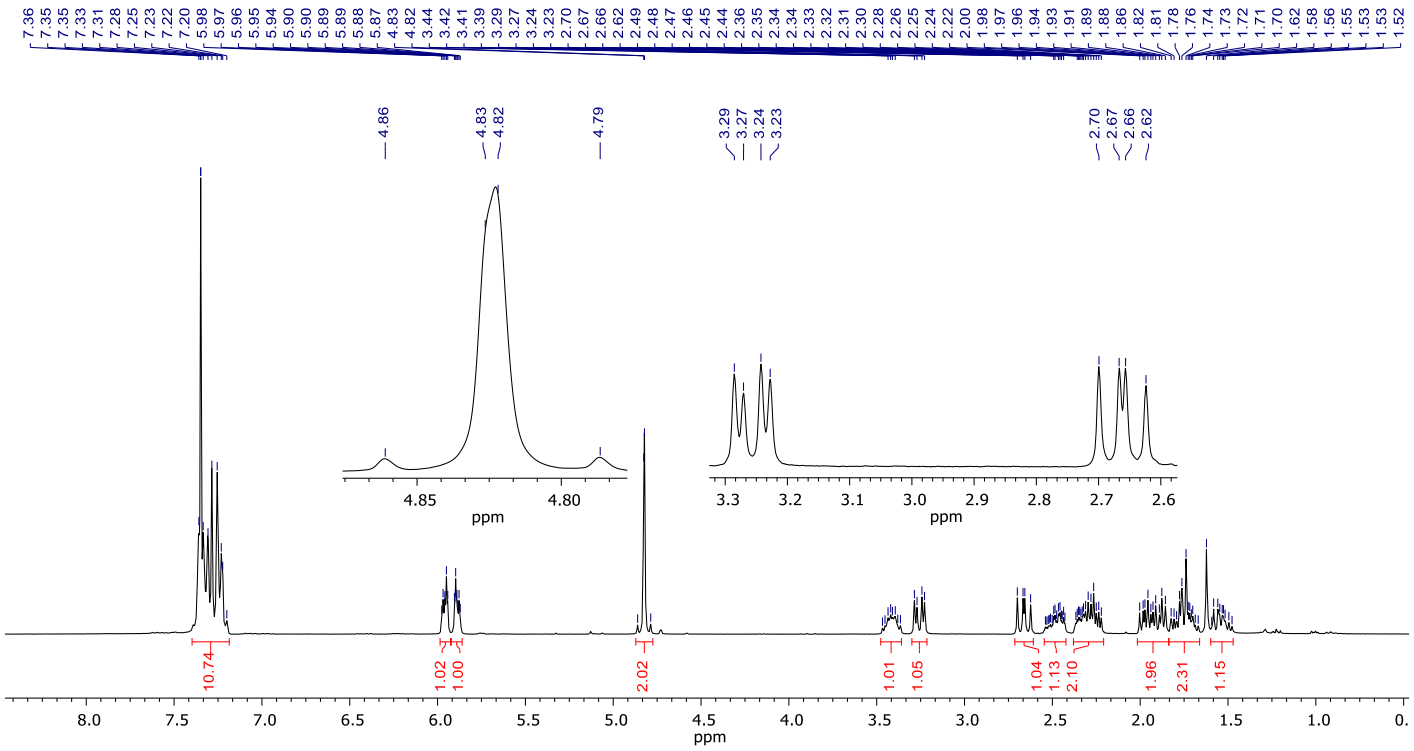

**$^{13}$C NMR (75 MHz, $CDCl_3$)**



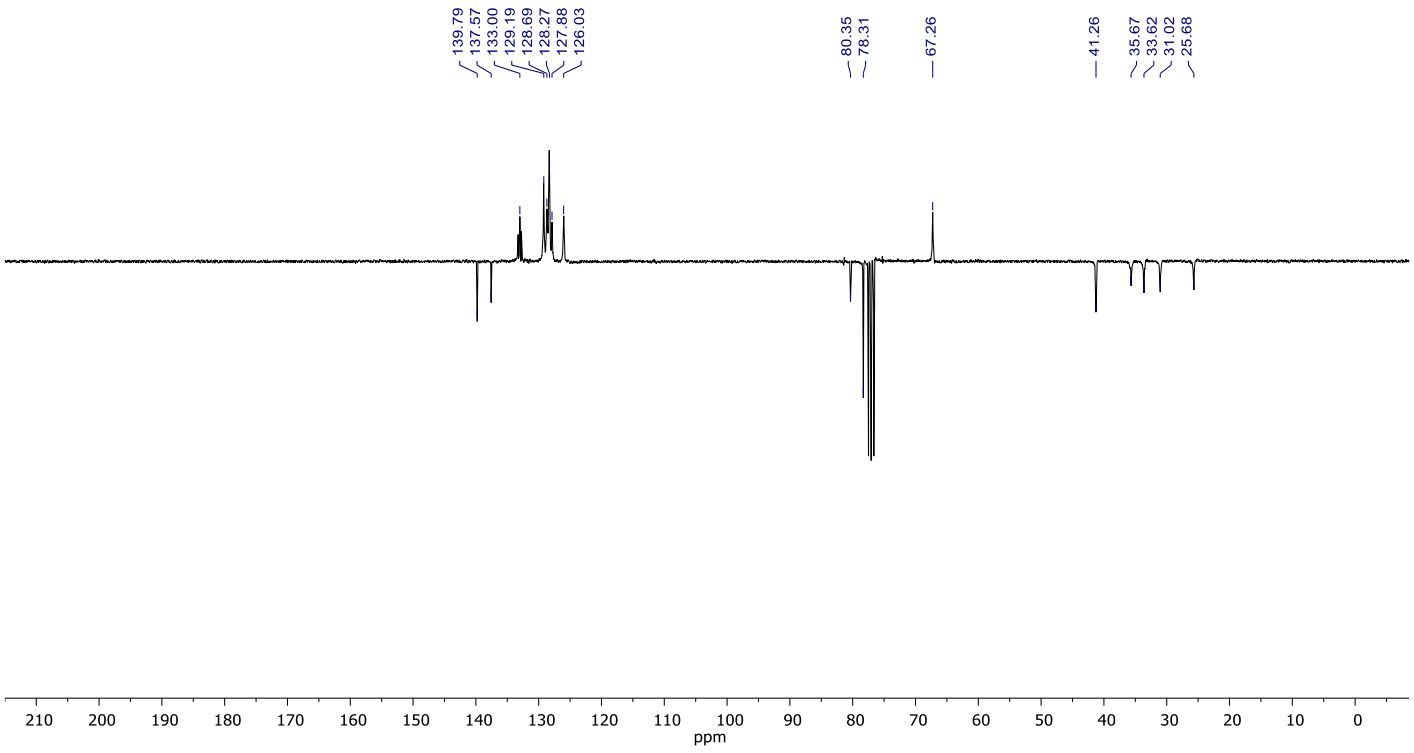
***trans*-2-Benzyl-1-(benzyloxy)-1-azaspiro[4.4]non-6-ene (16)**



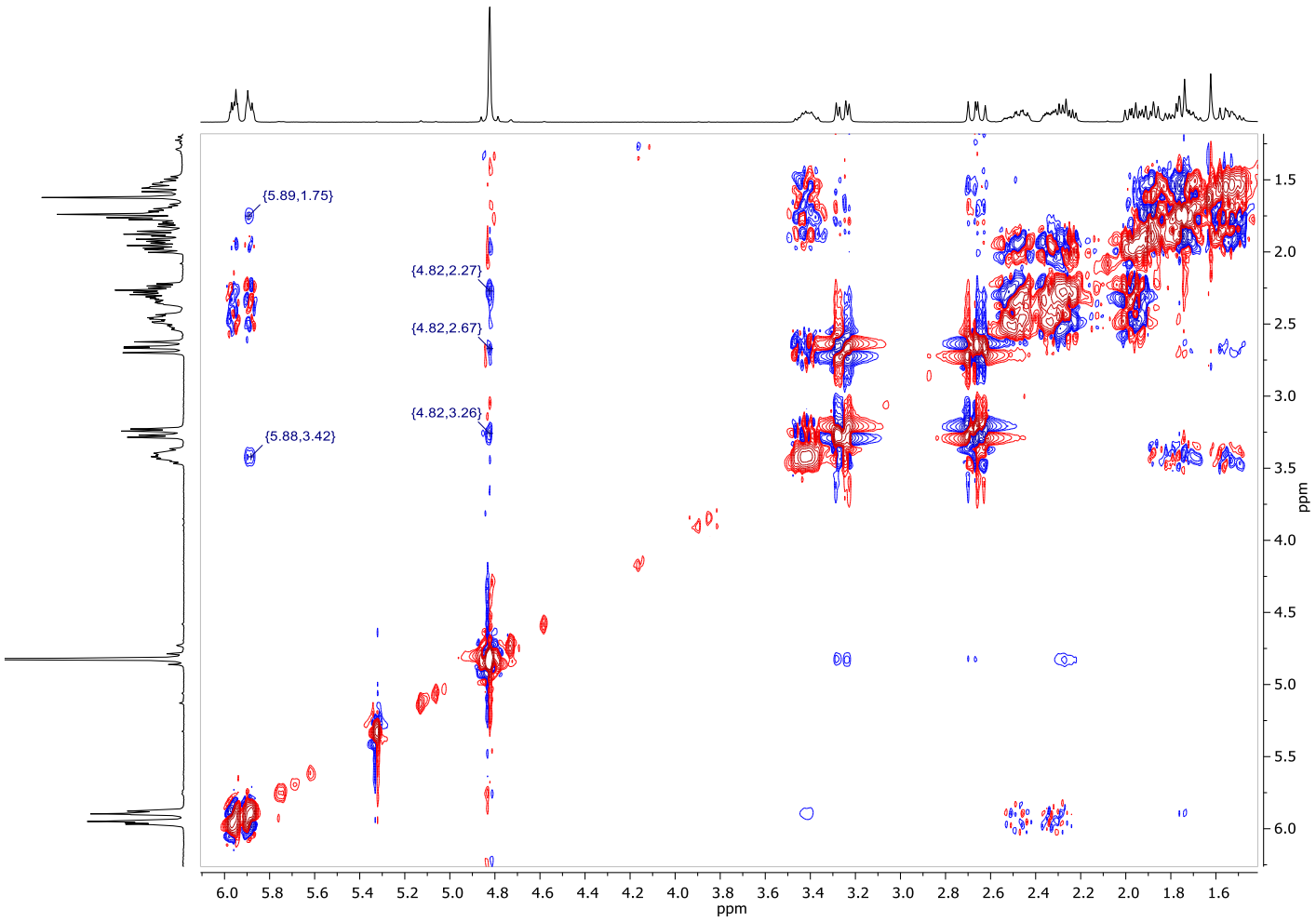

**$^{1}$H NMR (300 MHz, $CDCl_3$)**

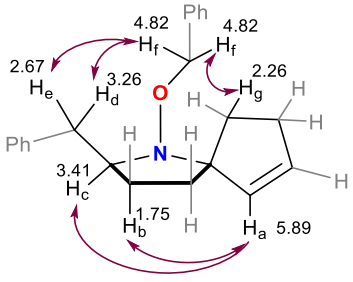



**$^{13}$C NMR (75 MHz, $CDCl_3$)**



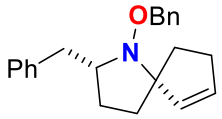
**1H-1H 2D NOESY NMR**



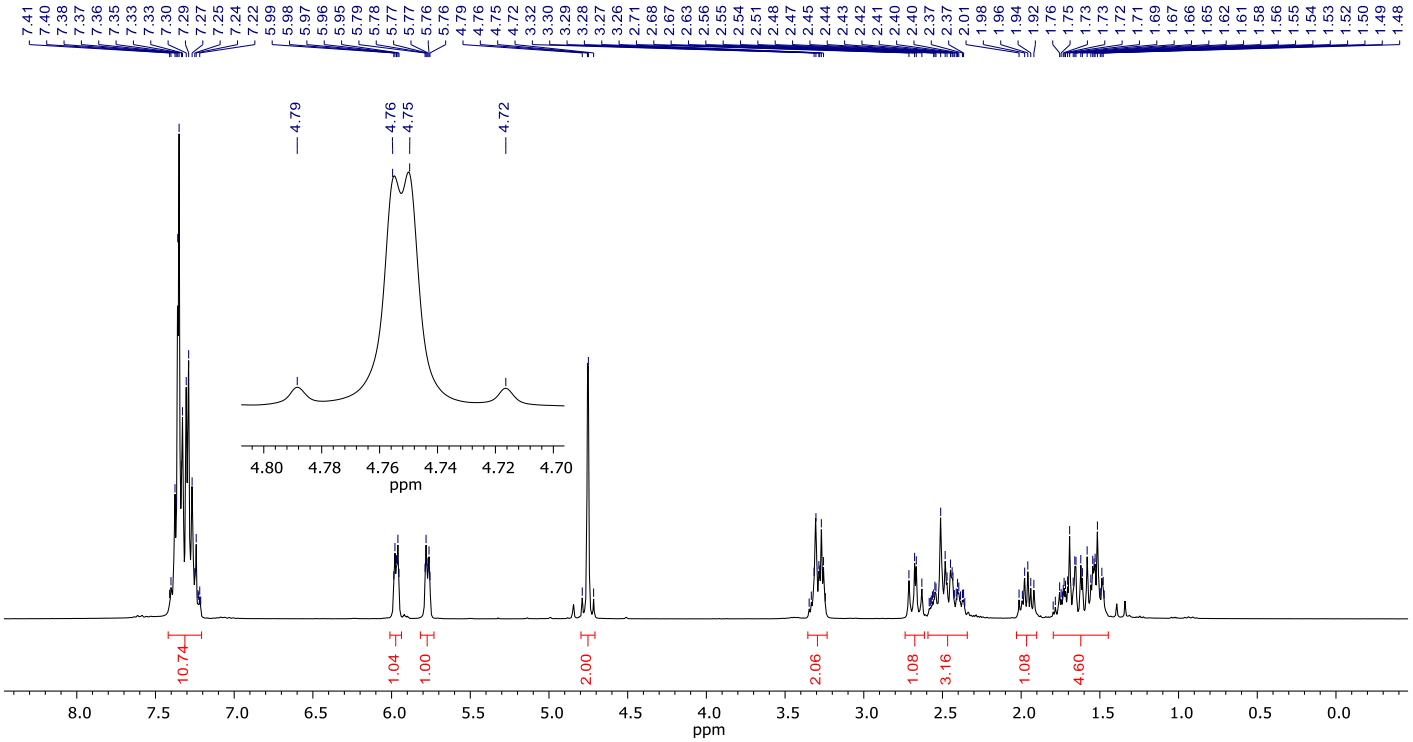




**16** *Trans*

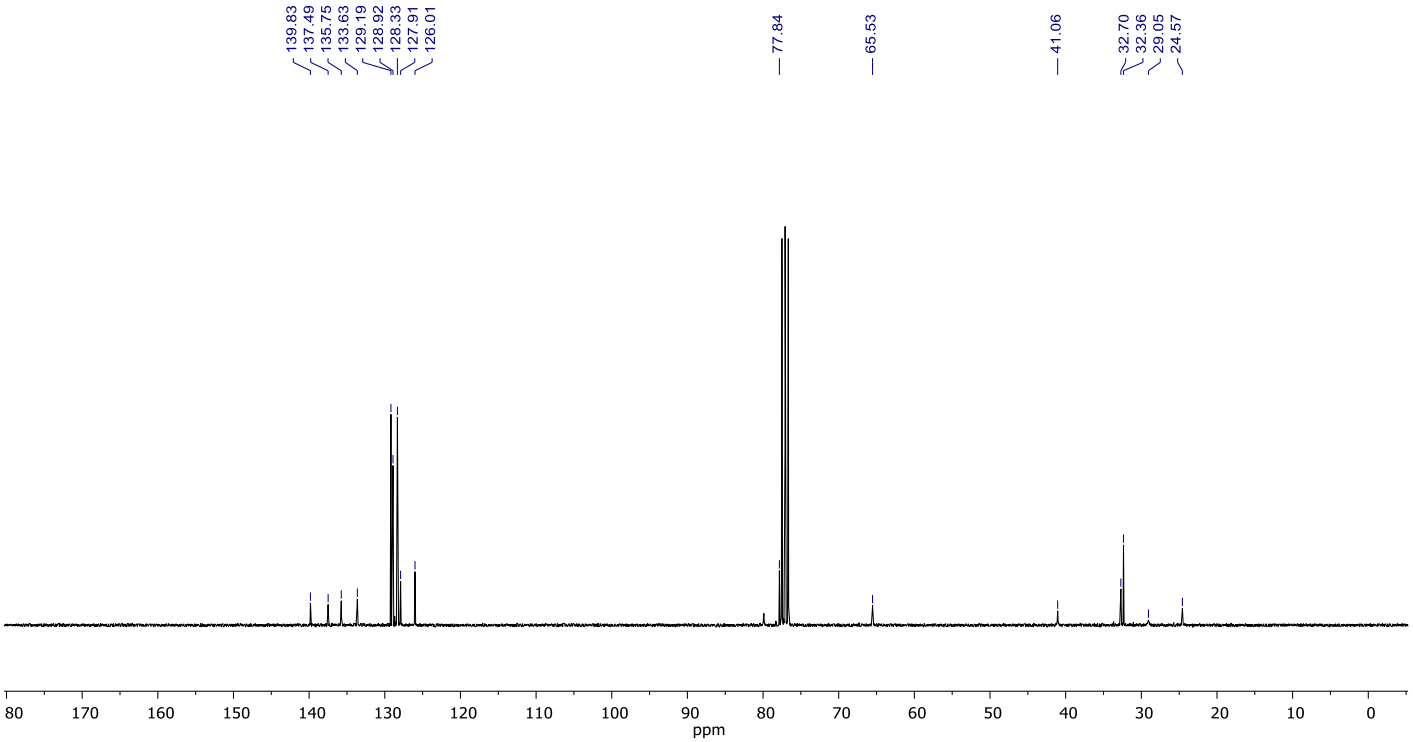
***cis*-2-Benzyl-1-(benzyloxy)-1-azaspiro[4.4]non-6-ene (16)**



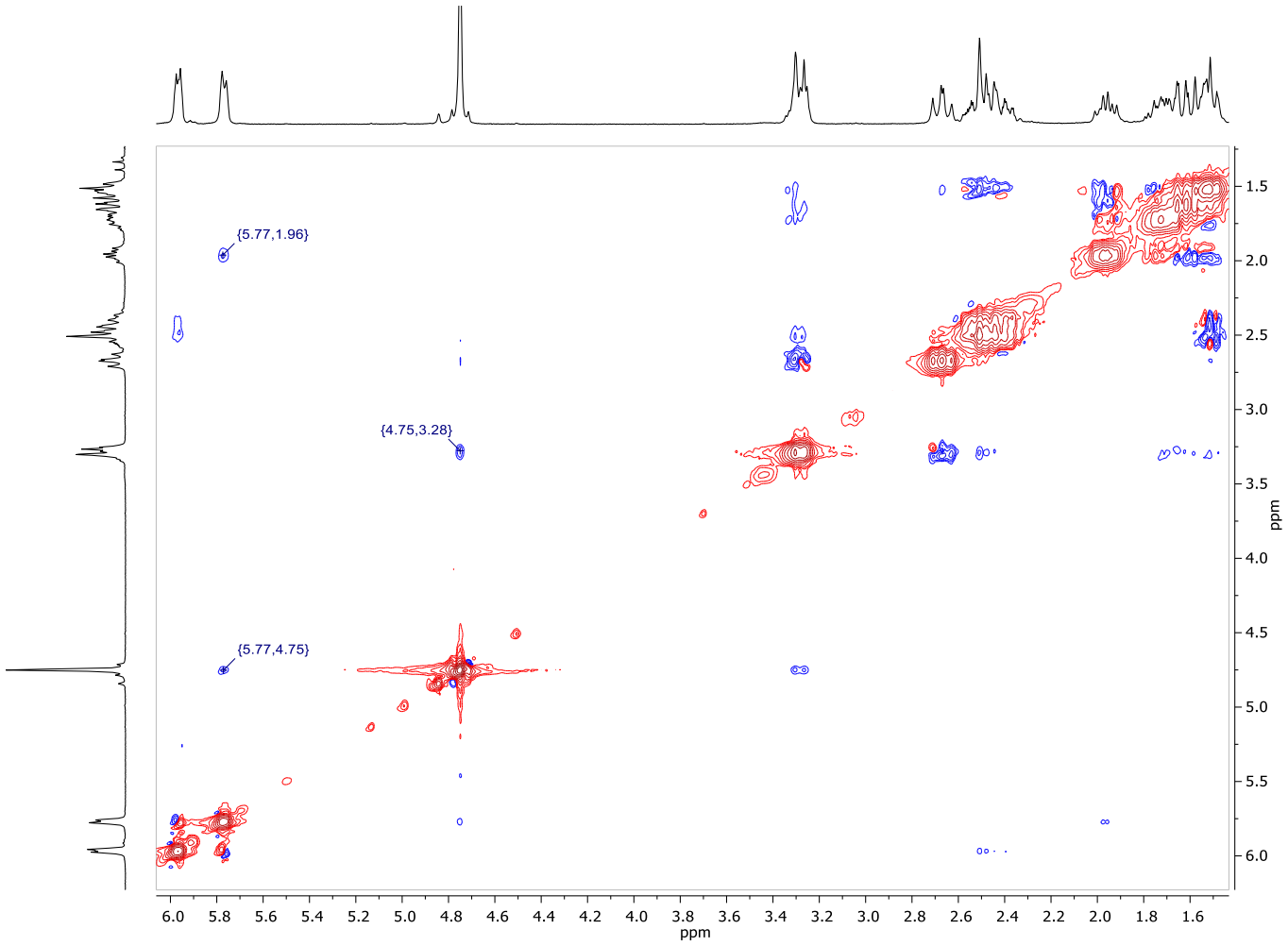

**$^{1}$H NMR (300 MHz, $CDCl_3$)**

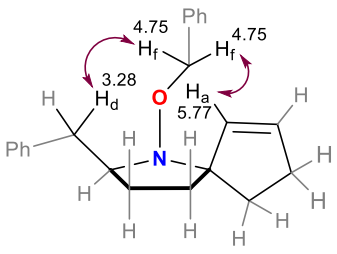



**$^{13}$C NMR (75 MHz, $CDCl_3$)**



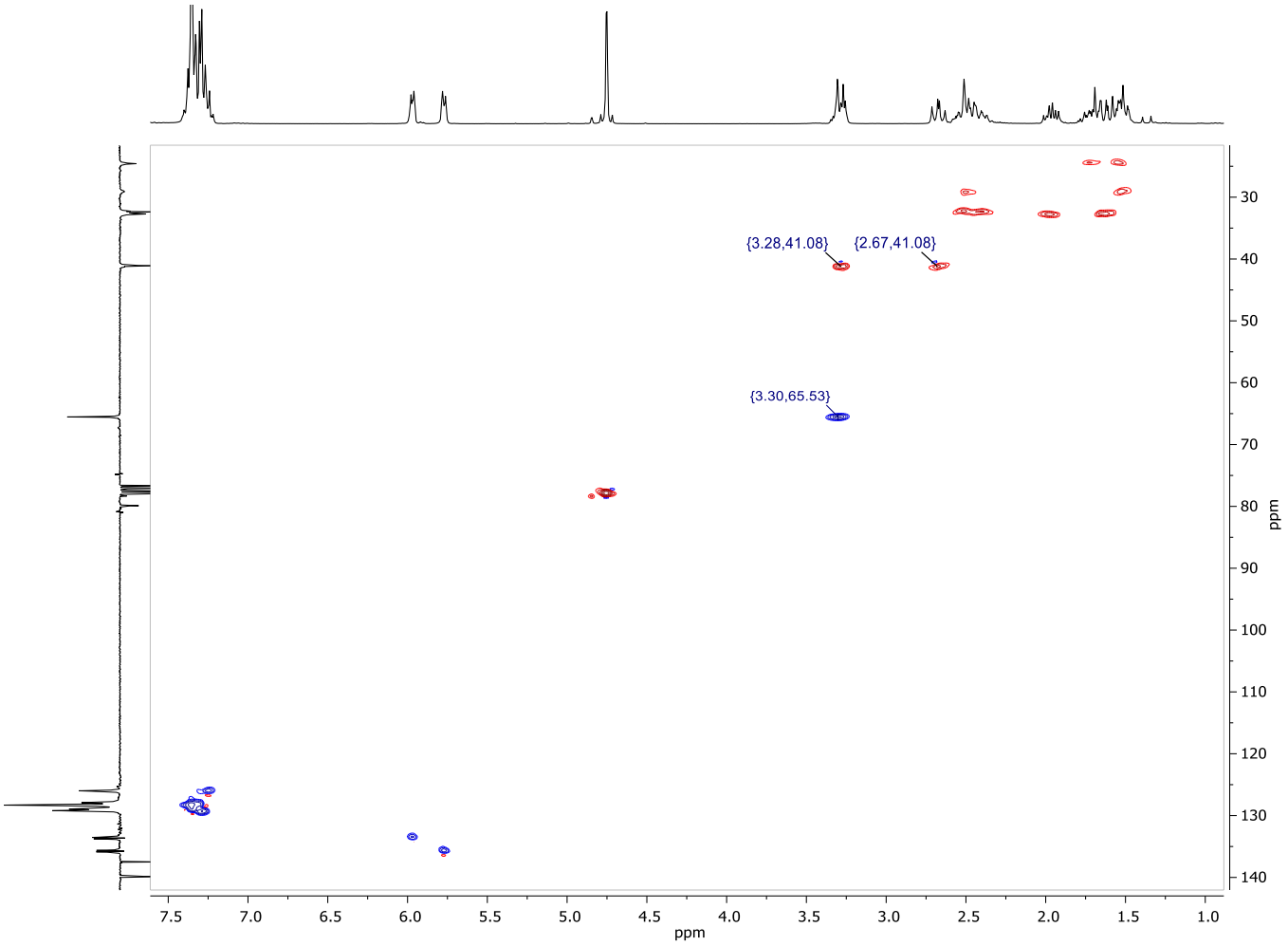
**1H-1H 2D NOESY NMR**

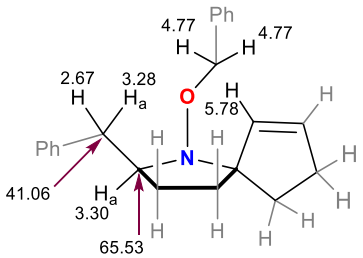



**16**$_{cis}$

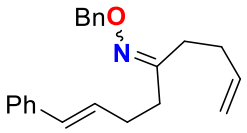
**1H-13C 2D HSQC NMR**



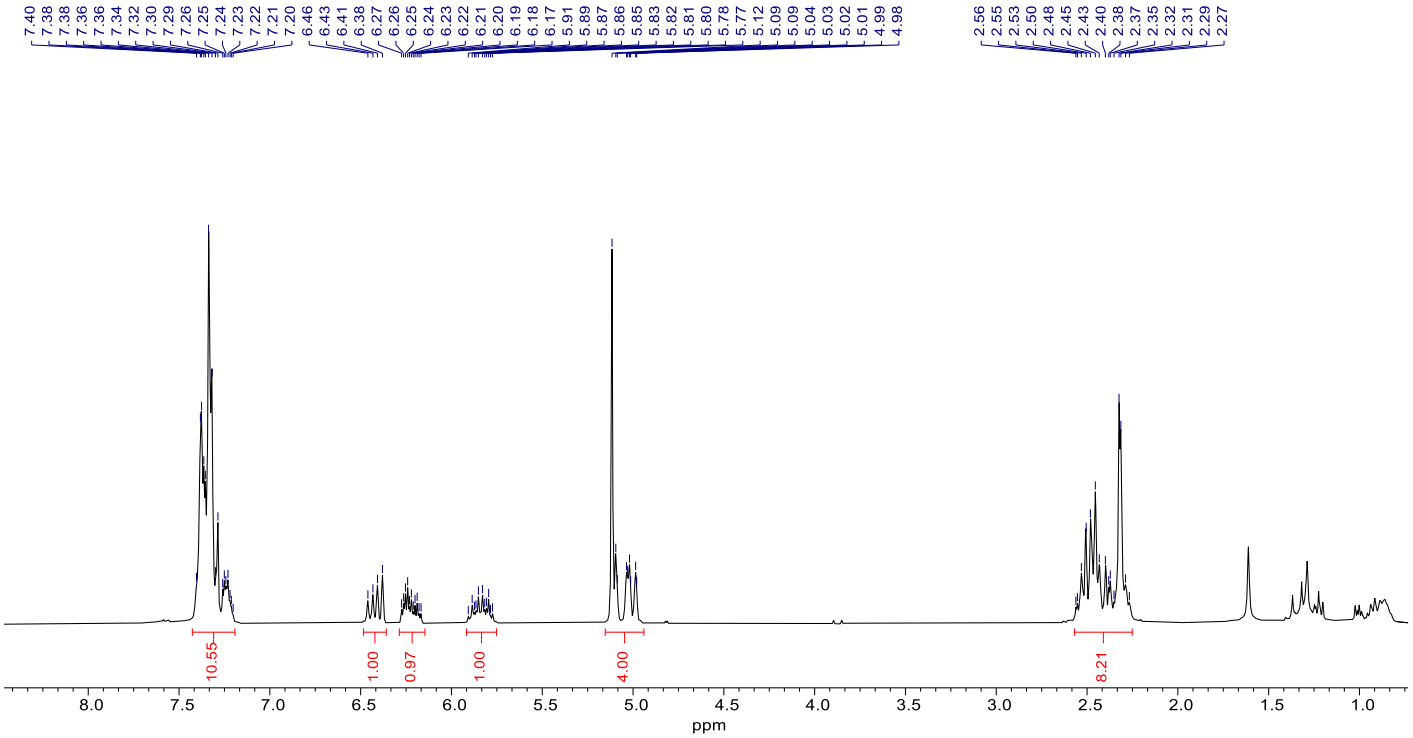




**16**$_{cis}$

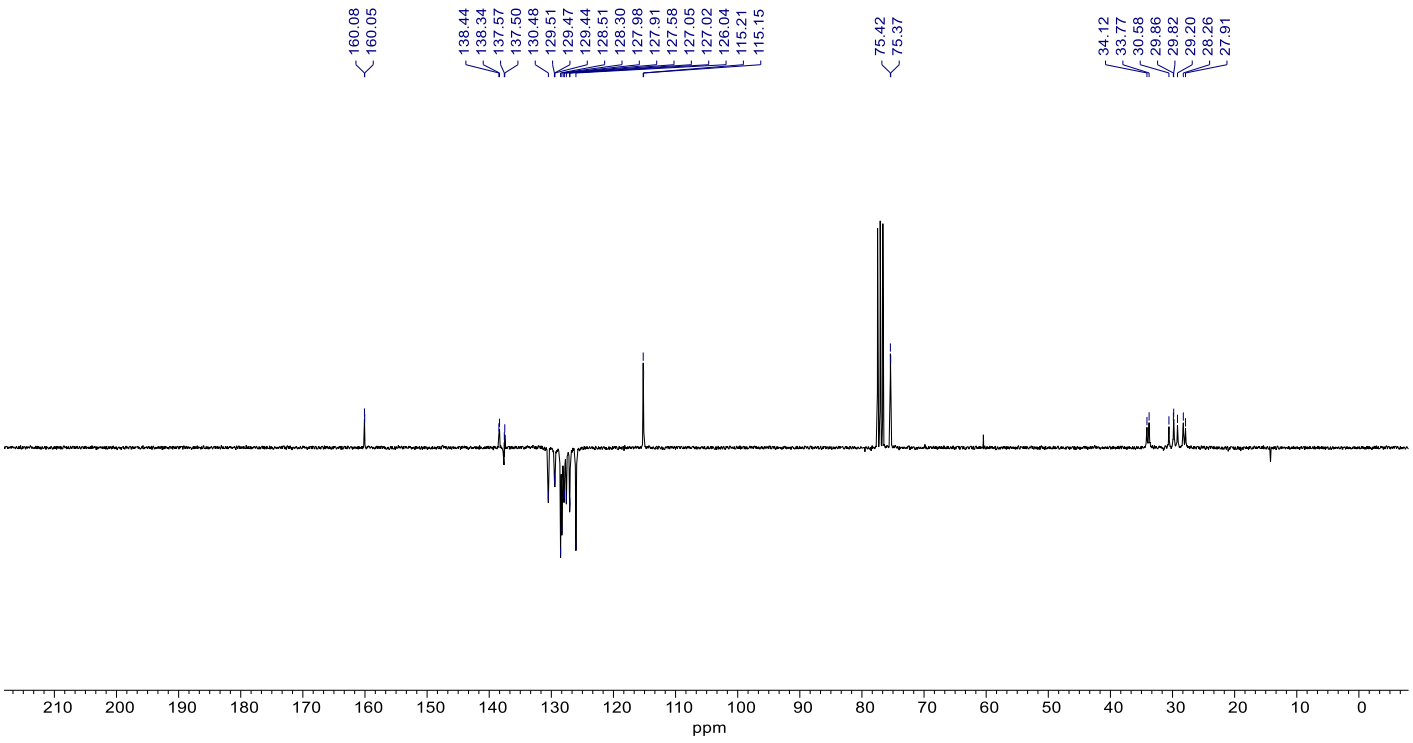
**(1*E*, 5*EZ*)-1-Phenylnona-1,8-dien-5-one O-benzyl oxime (17)**




**$^{1}$H NMR (300 MHz, $CDCl_3$)**



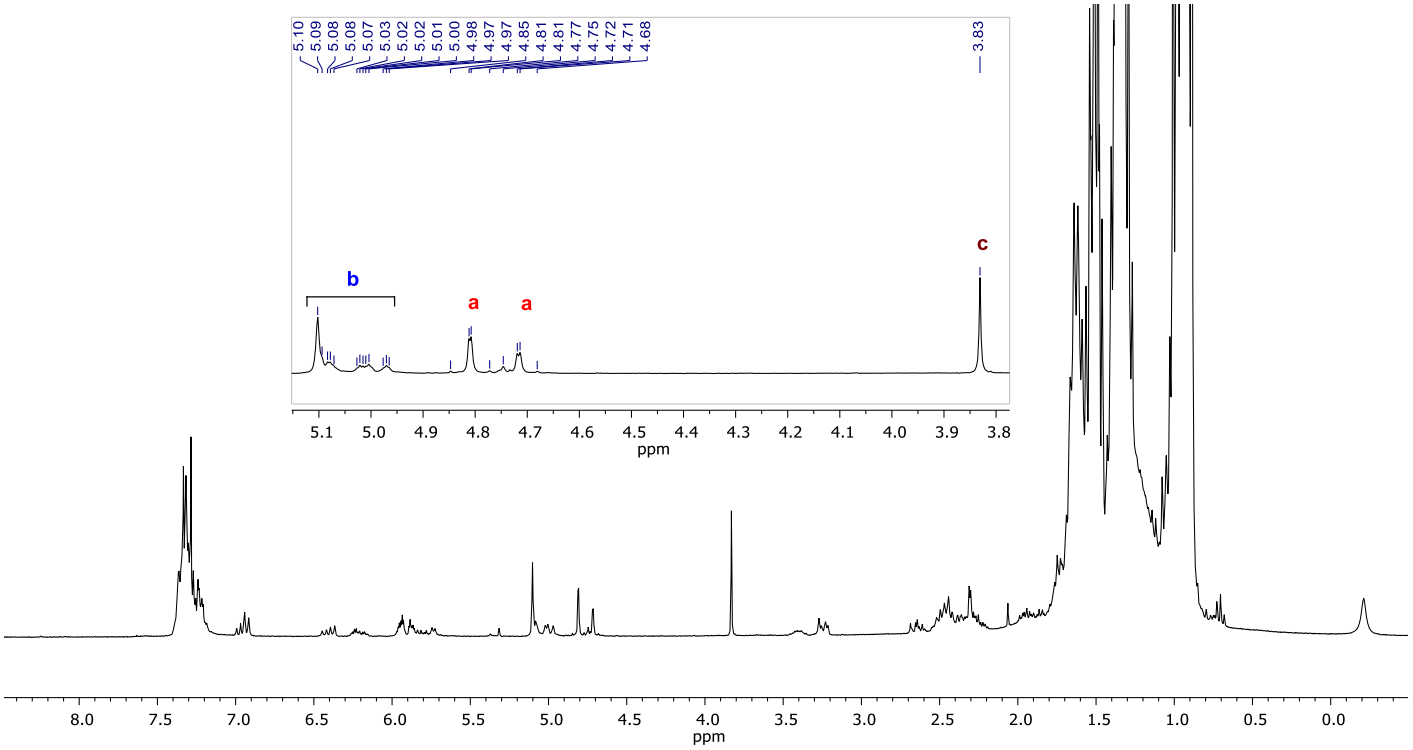

**$^{13}$C NMR (75 MHz, $CDCl_3$)**

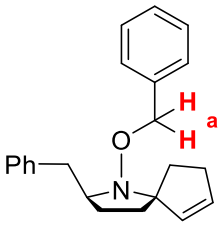


## Selected $^1$H NMR spectra from competition experiments

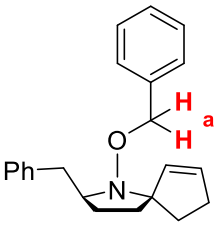
### Competition experiment of oxime ether 15

**$^1$H NMR (300 MHz, $CDCl_3$)**

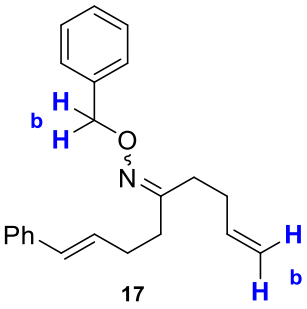


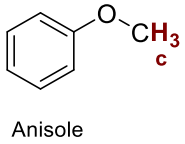

**16$_{trans}$**




**16$_{cis}$**



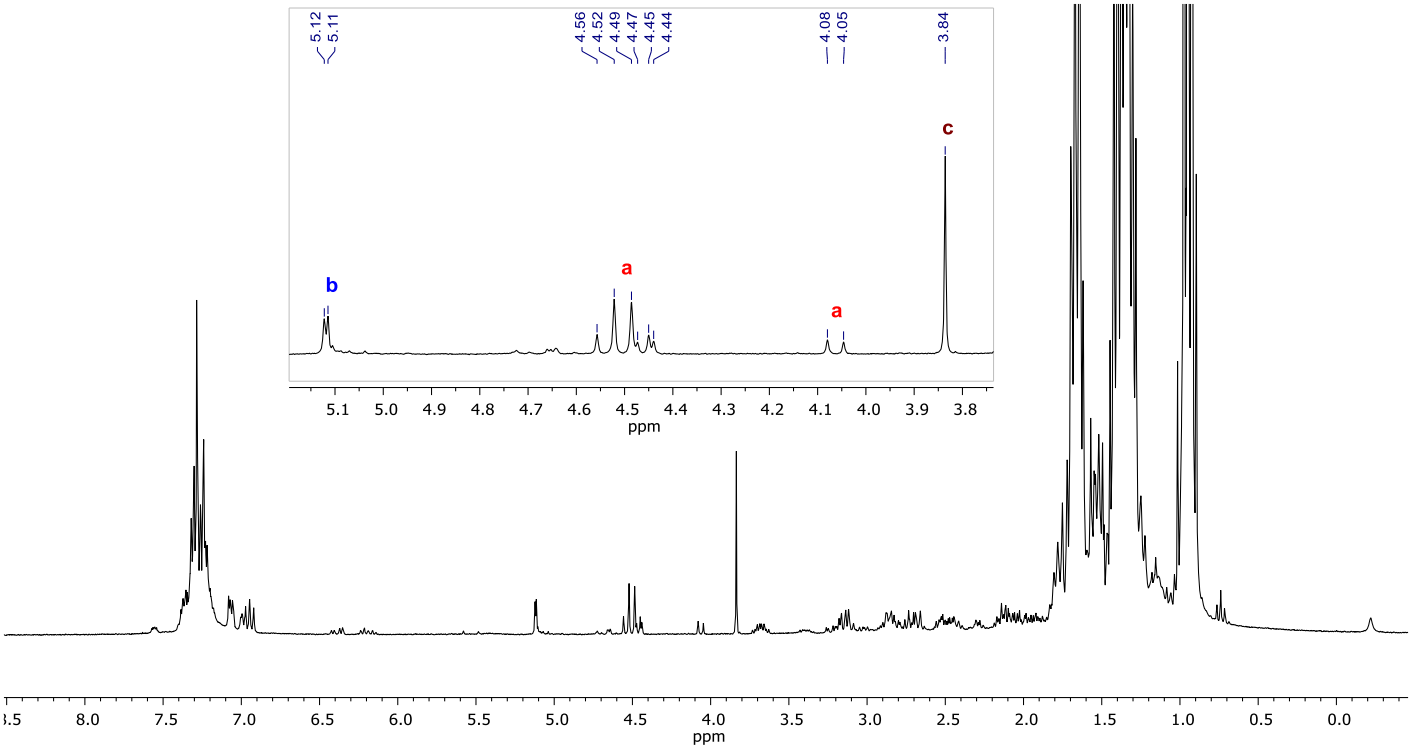

**17**

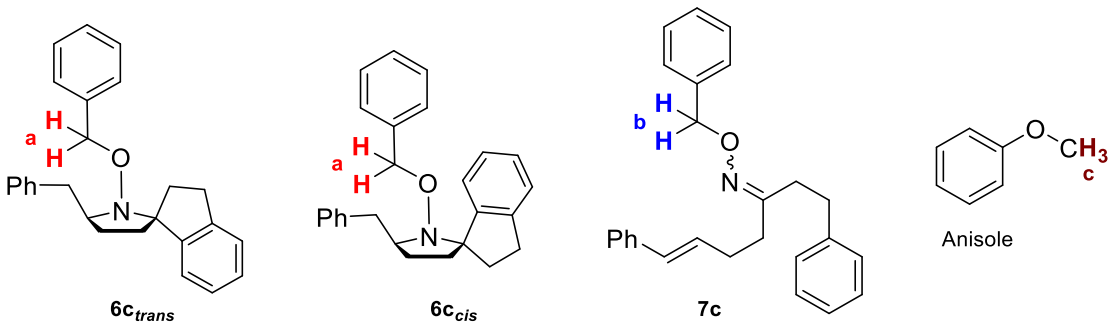



Anisole

**Competition experiment of oxime ether 5c**

**$^1$H NMR (300 MHz, $CDCl_3$)**

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