Supporting Information

Organocatalytic Reductive Coupling of Aldehydes with 1,1-Diarylethylenes Using the *in situ* Generated Pyridine-Boryl Radical

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1. Computational Investigations

1.1 Computational Details

All calculations were performed with the Gaussian 09 package.[1] Geometry optimizations and vibrational frequencies of all the stationary points were calculated by using the M06-2X[2]/6-31G(d,p) method. A "broken-symmetry" guess was used for calculations on open-shell systems. Each of the species was identified to be a minimum (number of imaginary frequencies, NIMAG=0) or a transition state (NIMAG=1). To confirm that each transition state connects the desired reactants and products along the reaction path, we performed intrinsic reaction coordinate (IRC)[3] calculations at the M06-2X/6-31G(d,p) level of theory. In order to obtain reliable energies, single point energies (Esol) were computed at the M06-2X/cc-PVTZ level. The solvent effect was treated with the polarizable continuum model (PCM) with benzene as the solvent.[4] The 3D structures were generated with CLY view.[5]

1.2 Revisit on the pathway for the reaction of 4-cyanopyridine and $B_2(pin)_2$.

Recently, Tang and co-workers reported that the reaction between isoquinolines and $B_2(pin)_2$ was proposed through a [3,3]-sigmatropic rearrangement mechanism.[6] In this work, we reinvestigated the possible pathway for the formation of the pyridine-boryl radical using 4-cyanopyrdine and $B_2(pin)_2$. Surprisingly, an intermediate, IntA3, was located along the pathway (Figure S1). Then, two transition states, one for the [3,3]-simatropic rearrangement process, another for the homolytic cleavage of C-C bond (to generate two pyridine-boryl radicals), were successfully determined. IRC calculations for the first transition state indicate that a [3,3]-simatropic rearrangement process is involved, in which the breaking of the B-B bond is concomitant with the formation of the C-C bond **(**Figure S2**)**. This step-wise picture is different from the concerted step reported in our previous study, in which the key intermediate IntA3, was not found.[7] Thus, the formation of the pyridine-boryl radical proceed through a [3,3]-sigmatropic rearrangement/homolytic C-C bond cleavage pathway (as shown in Figure S1 and Scheme S1).

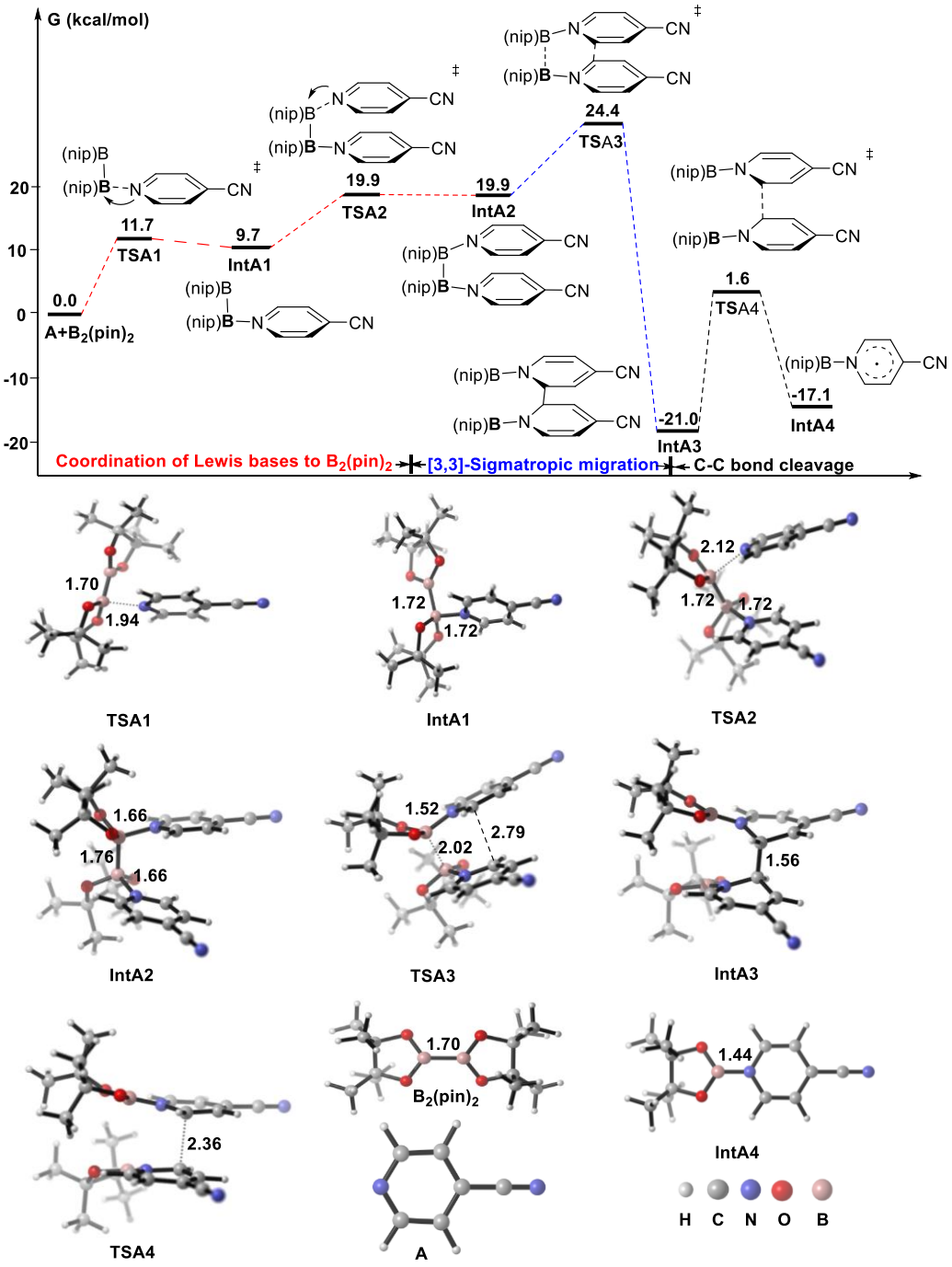


Figure S1. Computed Gibbs energy profile for 4-cyanopyridine (**A**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

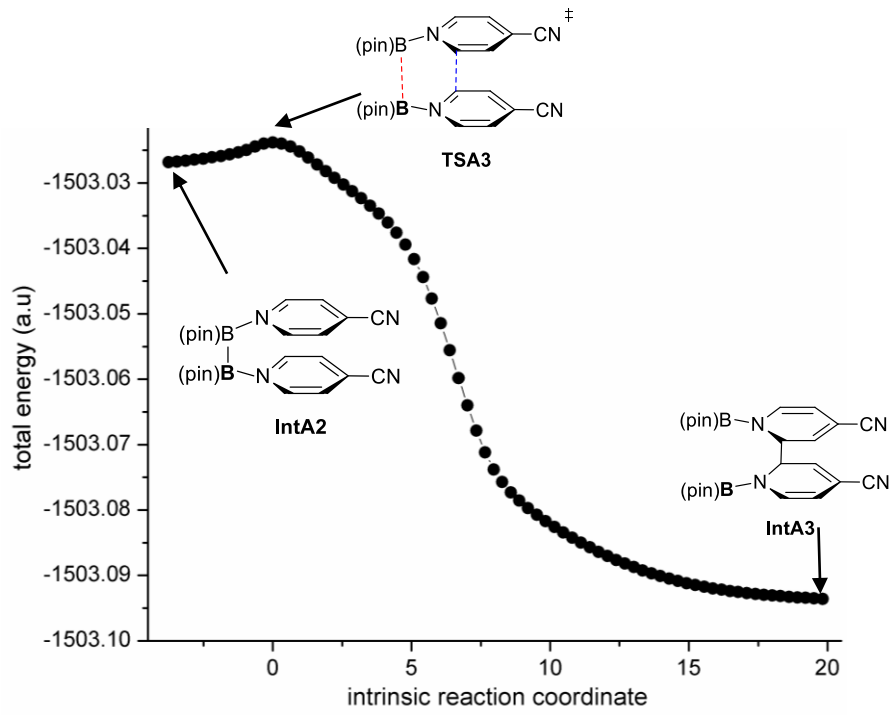
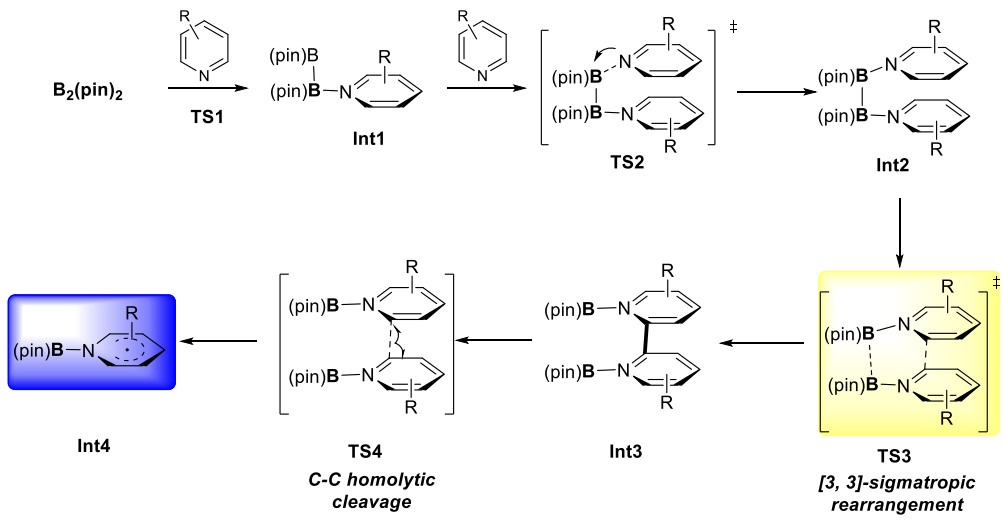


Figure S2. IRC analysis starting from the [3,3]-sigmatropic rearrangement transition state (TSA3).



Scheme S1. Proposed pathway for the formation of the pyridine–boryl radical via a [3,3]-sigmatropic rearrangement/ homolytic cleavage of the C-C bond mechanism..

1.3 Catalyst selection for the formation of the pyridine-boryl radical using pyridine and $B_2(pin)_2$

Then, we performed density functional theory (DFT) calculations to search the suitable substituted pyridine for the formation of pyridine-boryl radical using $B_2(pin)_2$. As shown in Figure S2 and Figure S3-S12, the [3,3]-sigmatropic rearrangement (*via* TS3) is the rate-determining step (*r.d.s.*) for the formation of the corresponding pyridine-boryl radical. As shown in Figure S1, five pyridines (**A**, **B**, **C**, **D**, **E**) with free energy barriers (*r.d.s.*) of no more than 28.5 kcal/mol are possible candidates for the formation of the pyridine-boryl radical.

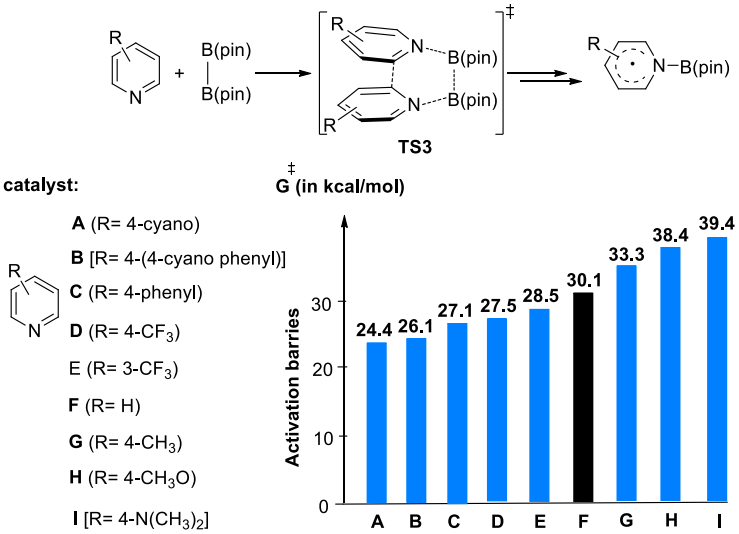


Figure S3. Activation barrier for rate-determining step (TS3) for the formation of pyridine-boryl radical.

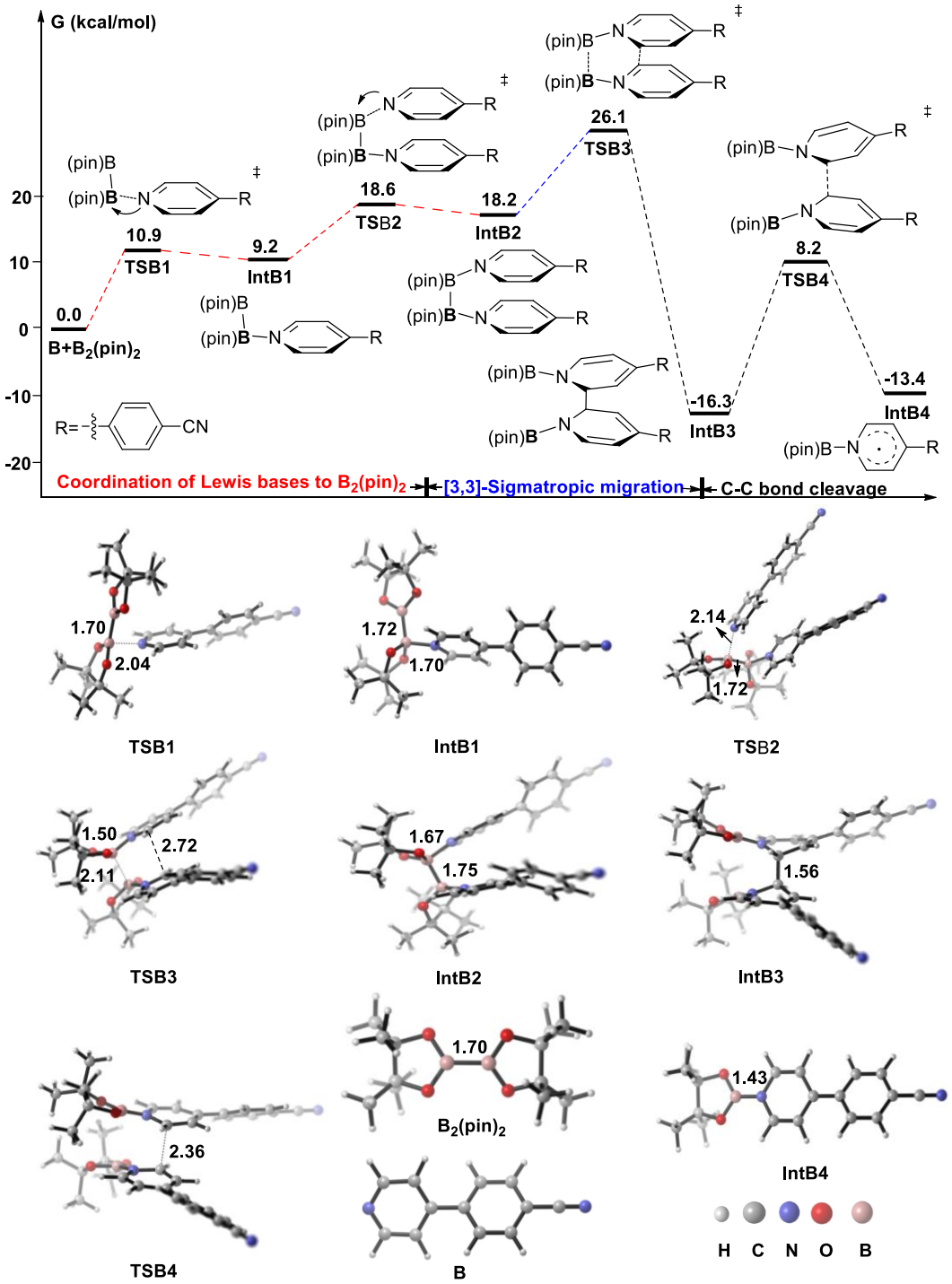


Figure S4. Computed Gibbs energy profile for 4-(4-pyridinyl)benzonitrile (**B**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

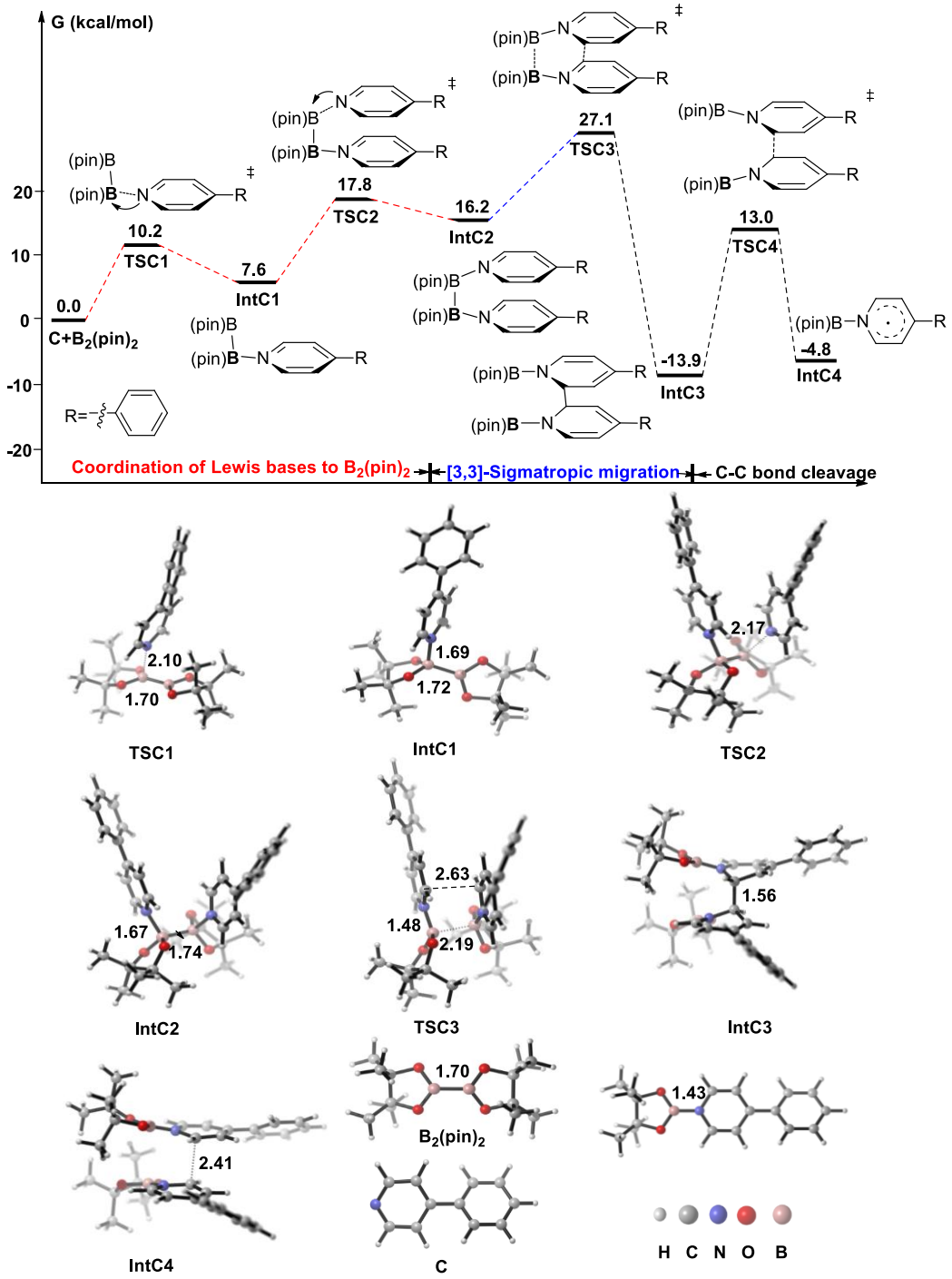


Figure S5. Computed Gibbs energy profile for 4-phenylpyridine (**C**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

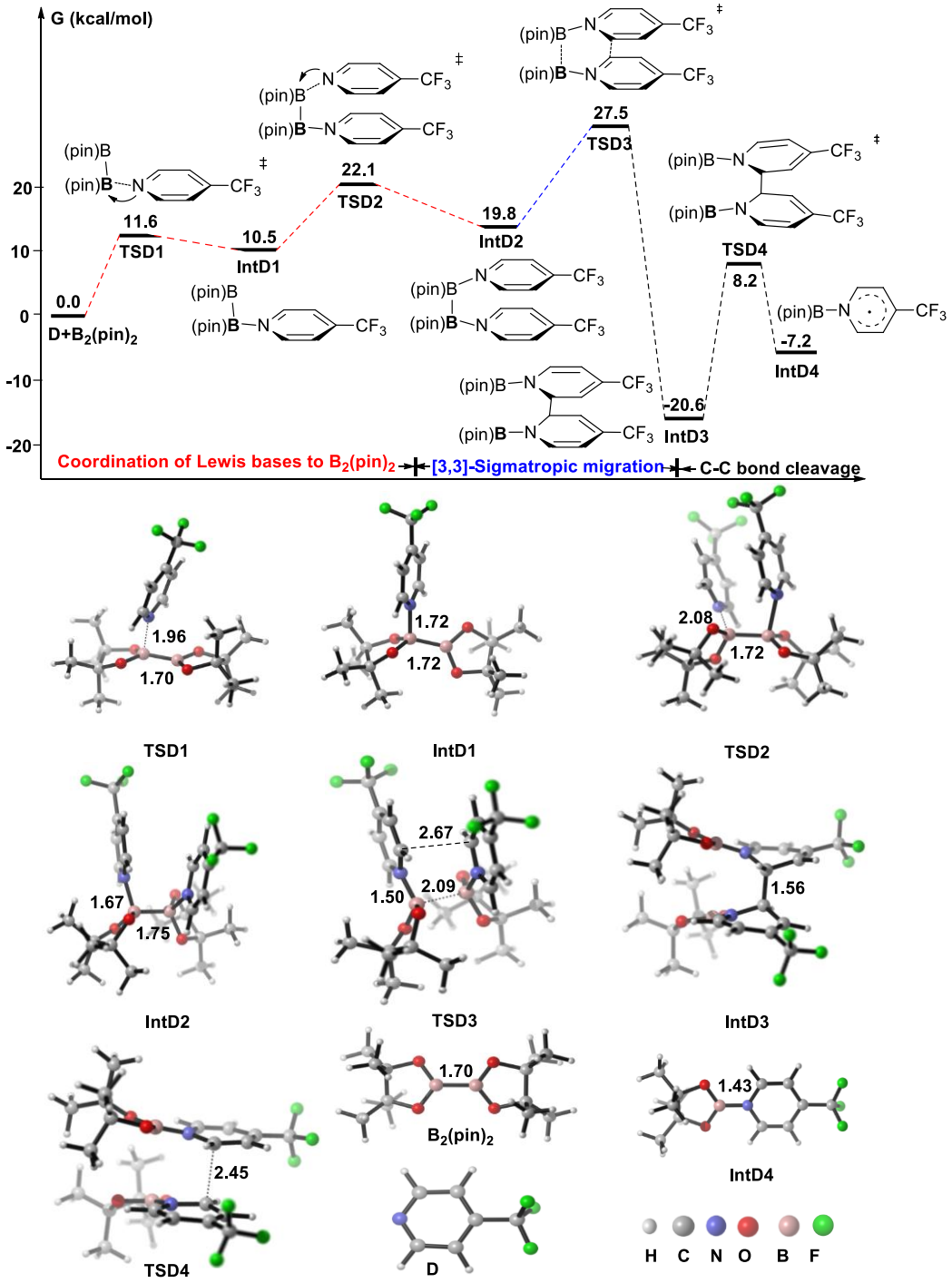


Figure S6. Computed Gibbs energy profile for 4-(trifluoromethyl)pyridine (**D**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

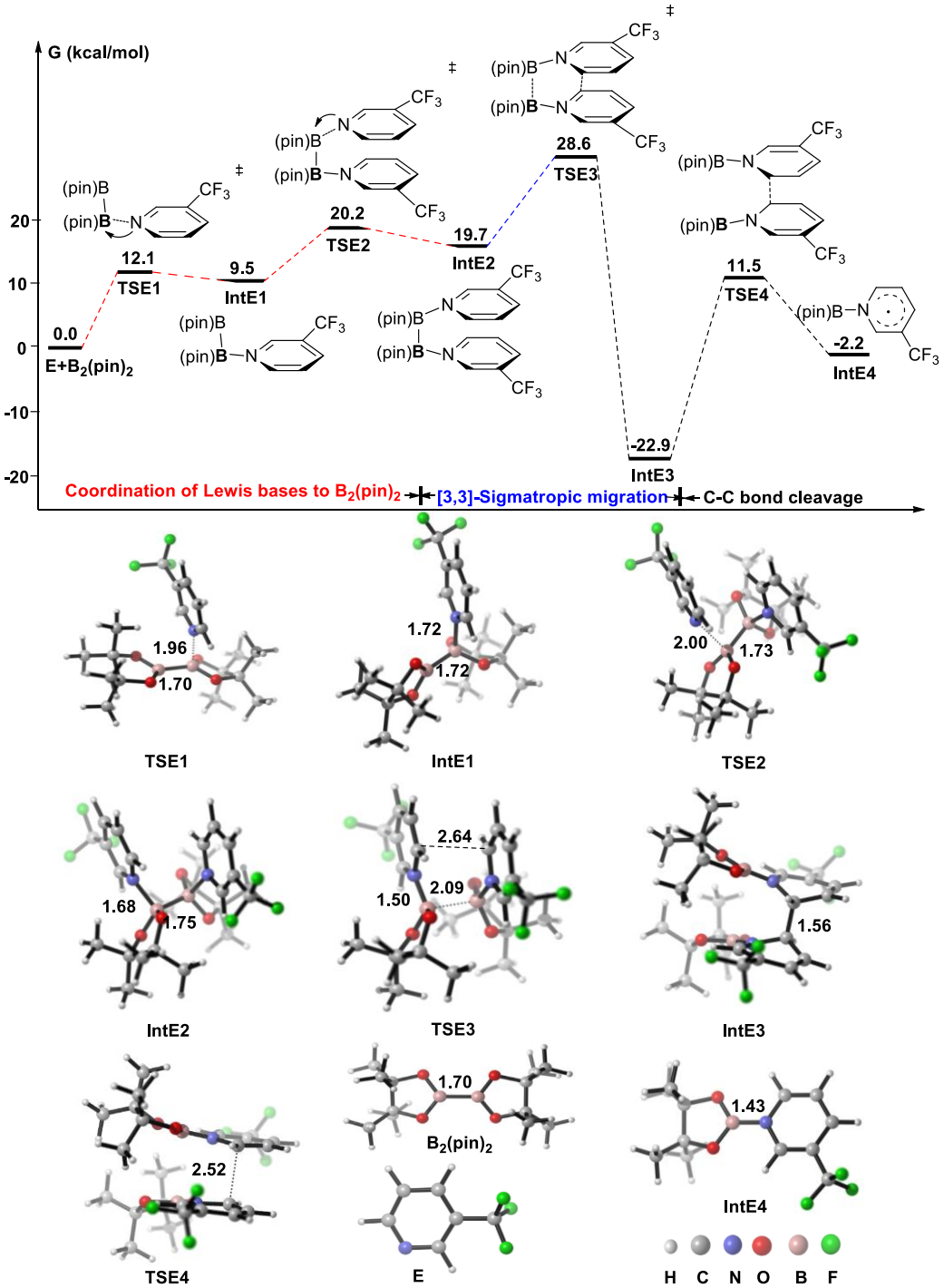


Figure S7. Computed Gibbs energy profile for 3-(trifluoromethyl)pyridine (**E**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

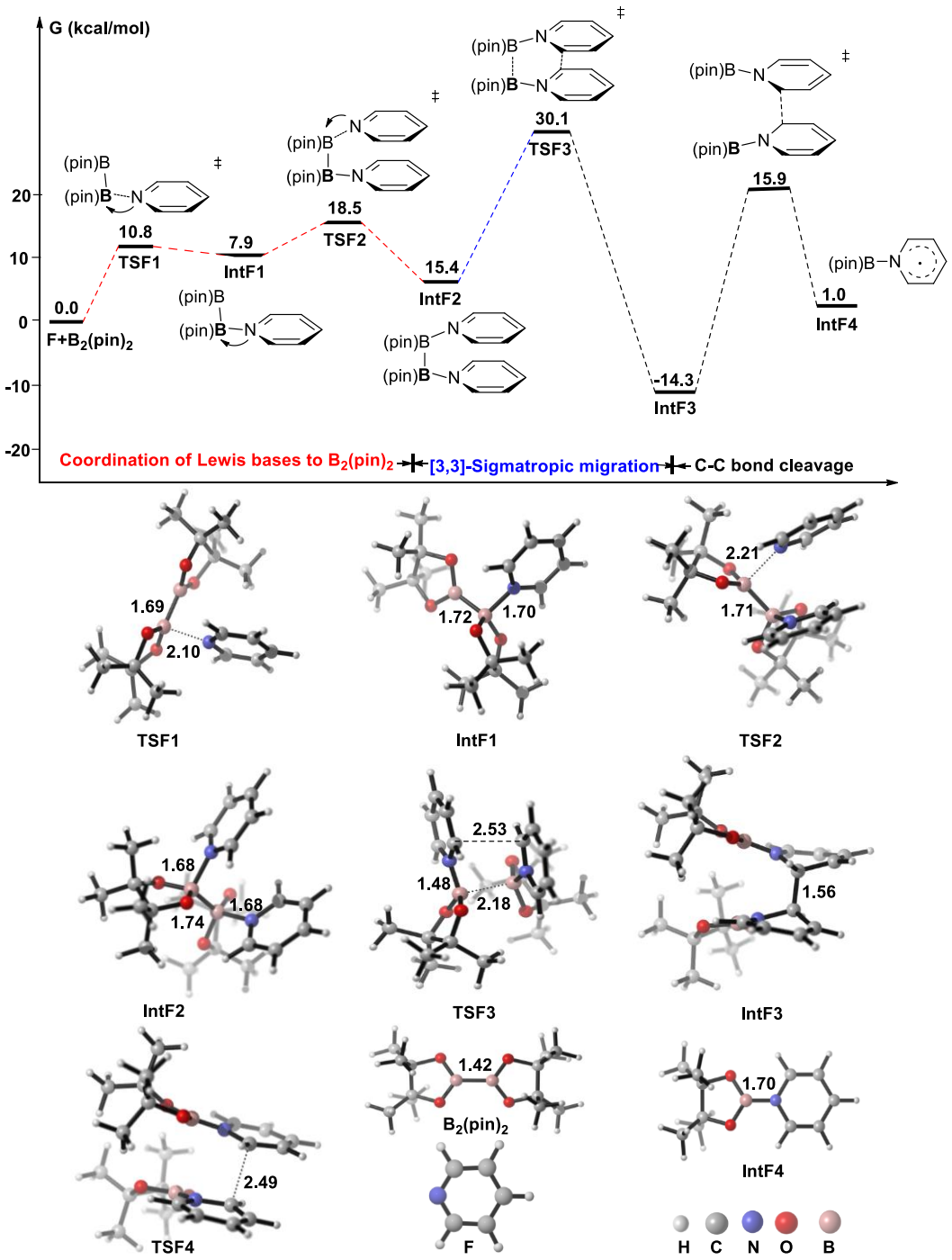


Figure S8. Computed Gibbs energy profile for pyridine (**F**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

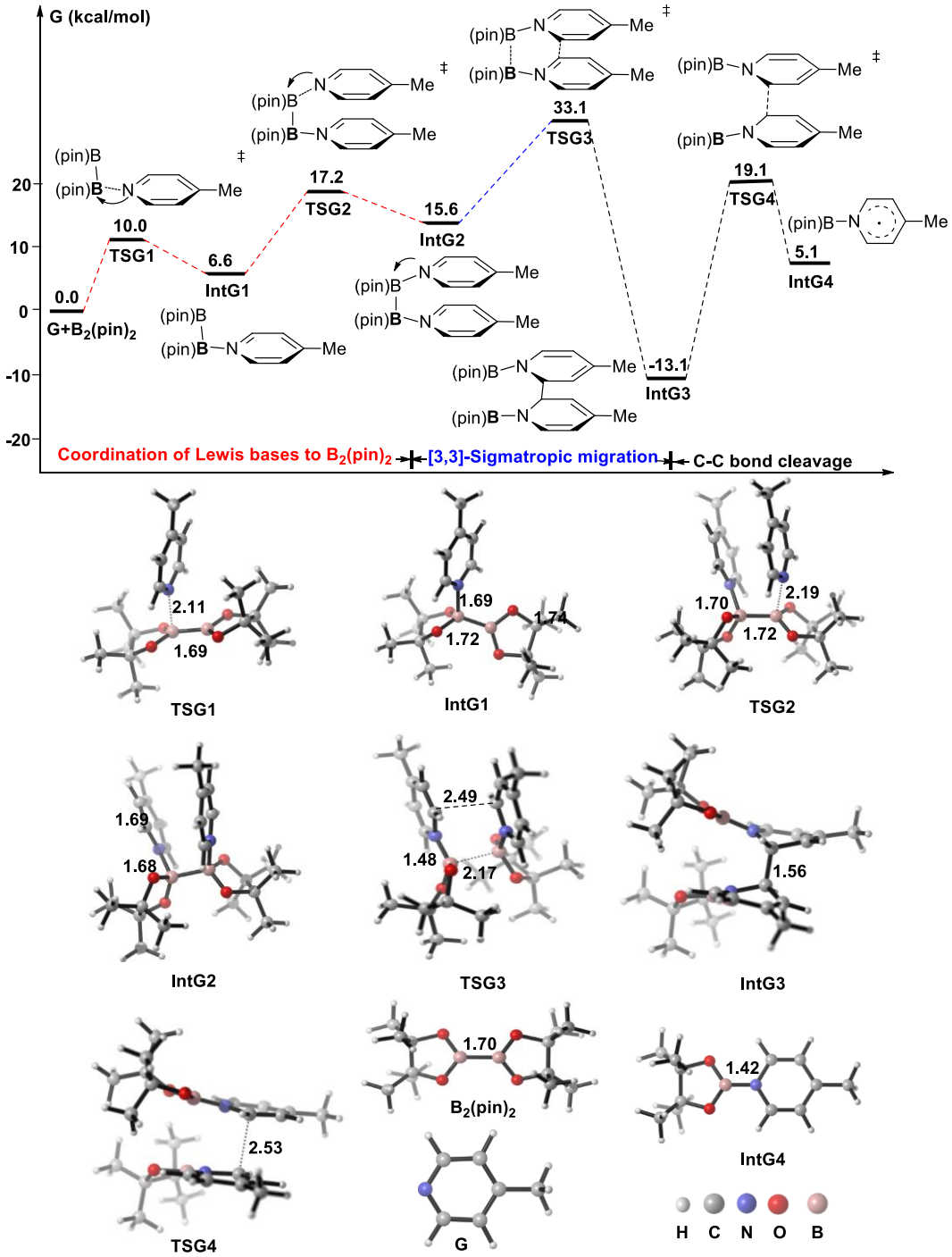


Figure S9. Computed Gibbs energy profile for 4-methylpyridine (**G**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

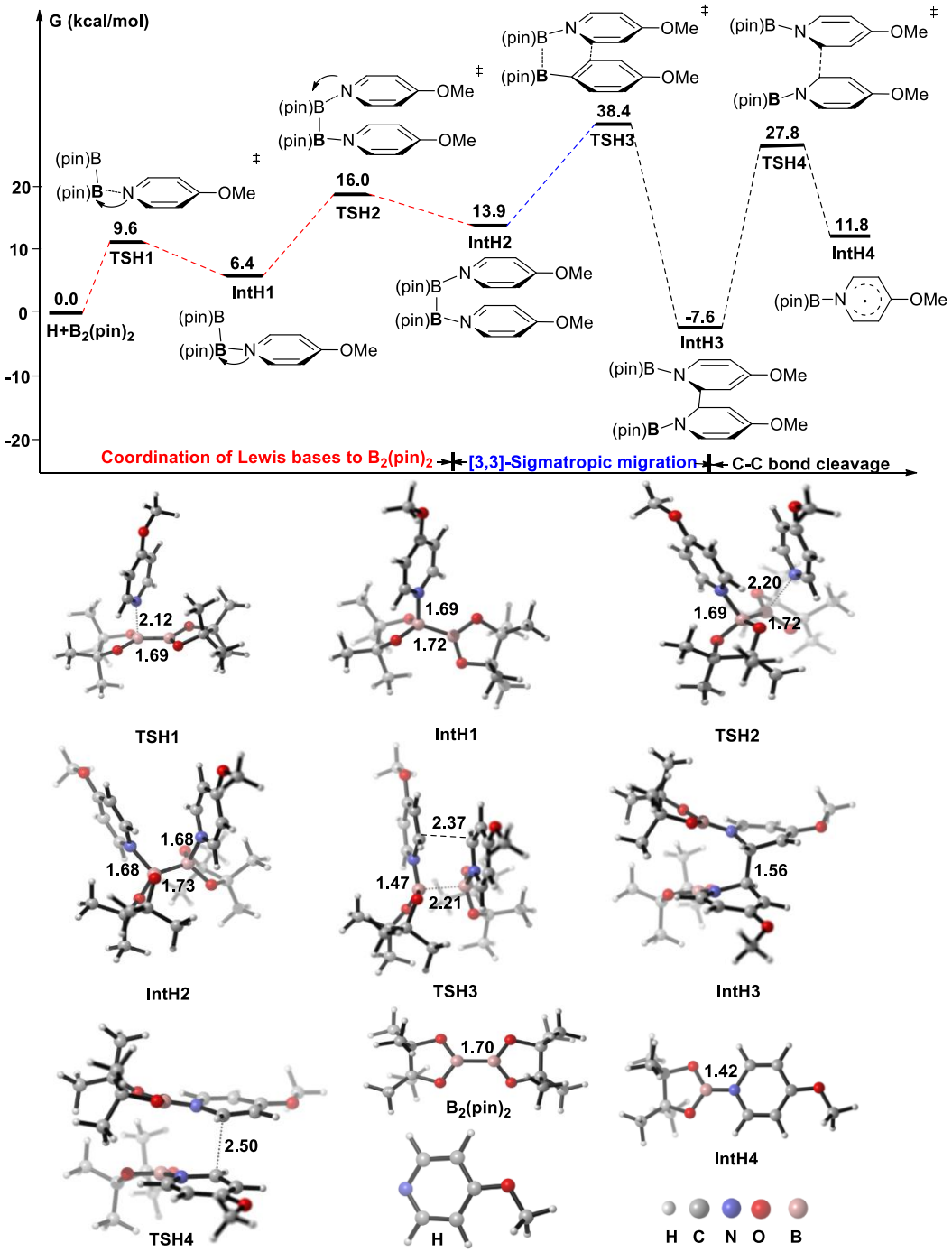


Figure S10. Computed Gibbs energy profile for 4-methoxypyridine (**H**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

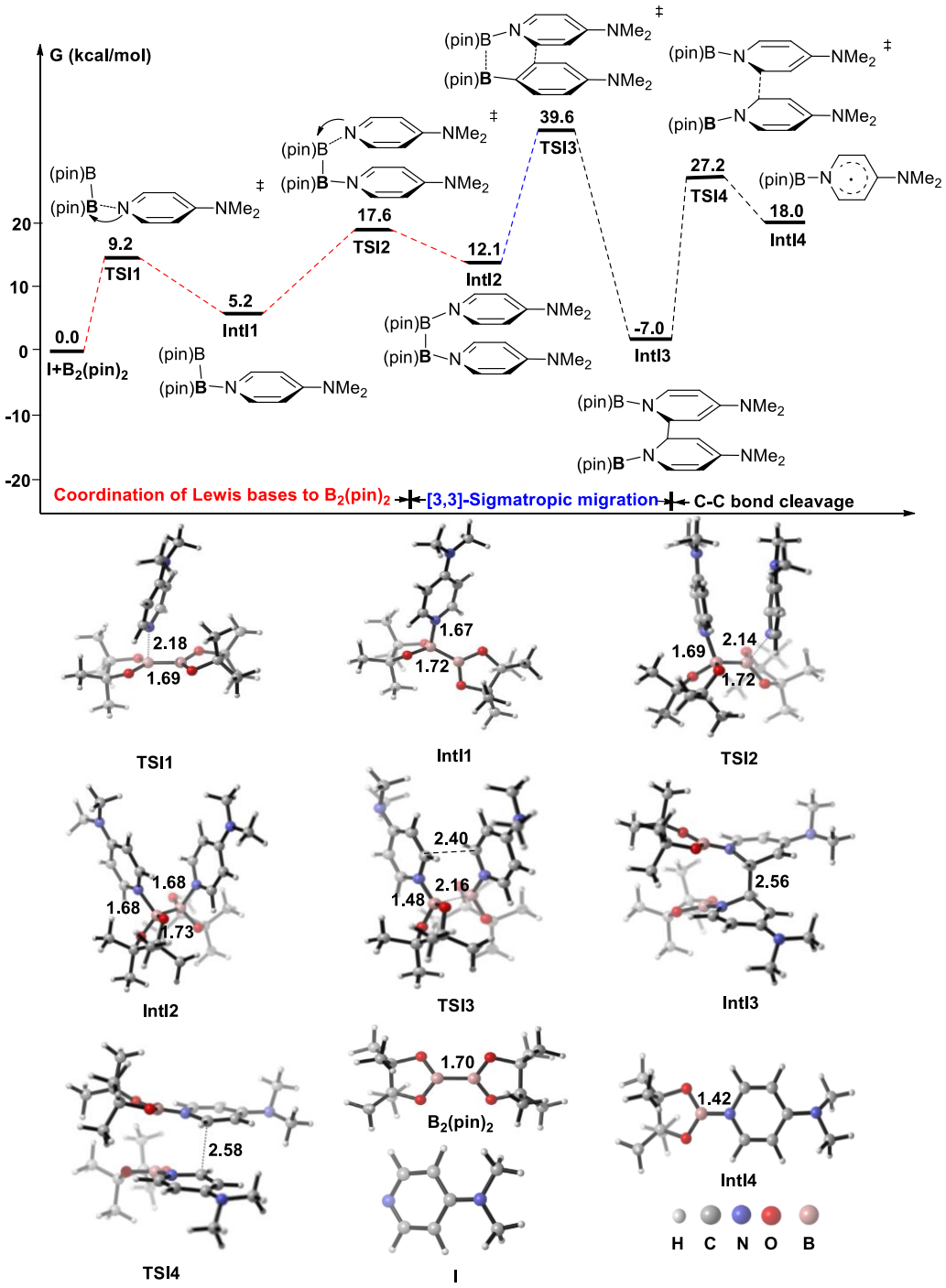


Figure S11. Computed Gibbs energy profile for 4-dimethylaminopyridine (**I**) catalyzed formation of the pyridine-boryl radical using $B_2(pin)_2$ in the benzene. Interatomic distances are in Å.

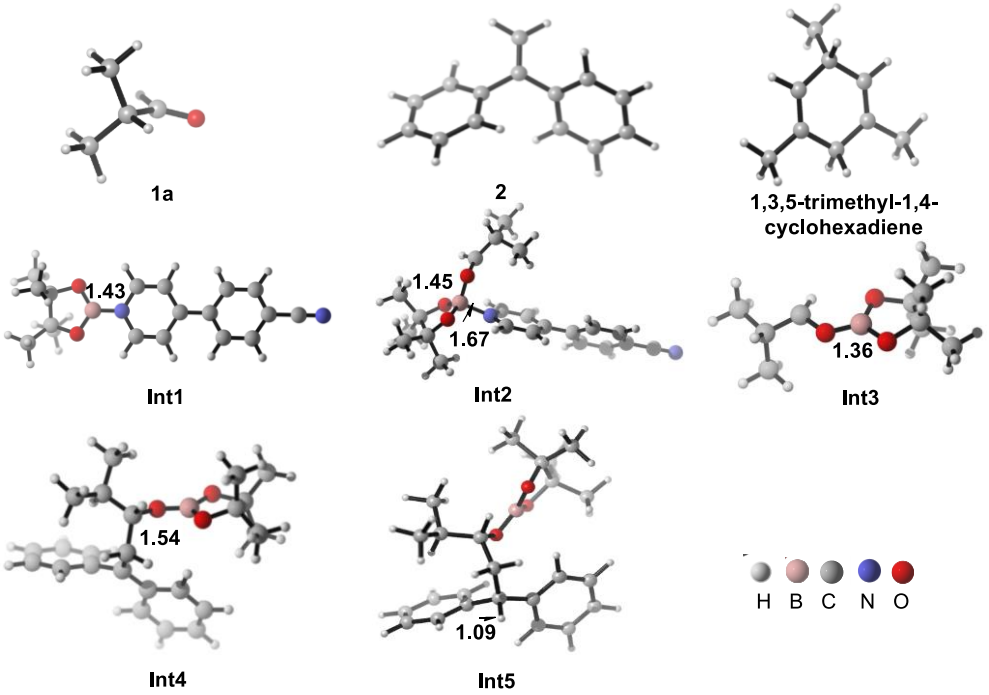


Figure S12. Optimized structures of all minimum species in the reductive coupling reaction between isobutyraldehyde (**1a**) and 1,1-diphenylethylene (**2**) promoted by 4-(4-pyridinyl)benzonitrile-boryl radical (**Int1**). Interatomic distances are in Å.

1.3 The results of single electron transfer (SET) process

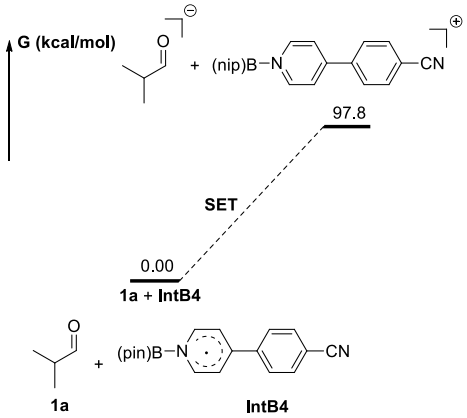


Figure S13. SET process between isobutyraldehyde (1a) and Int4

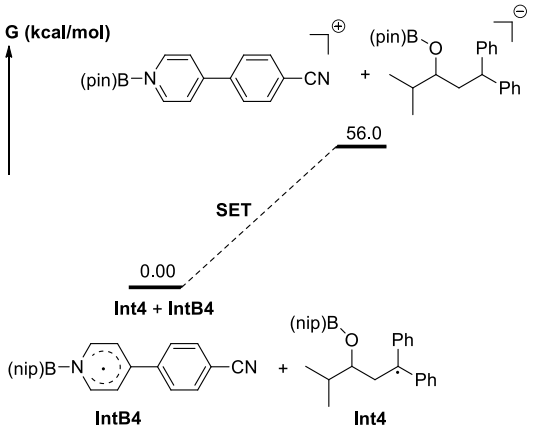


Figure S14. SET process between IntB4 and Int4

Our calculations show that the direct electron transfer process **IntB4** with **Int4** and isobutyraldehyde (**1a**) is not thermodynamically favorable, as shown in Figure S13 and Figure S14.

2. Experimental Studies on Substrate Scope

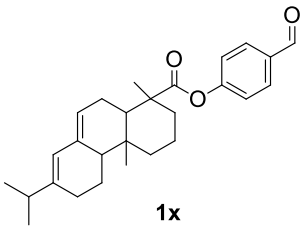
2.1 General information

All reactions were carried out under argon atmosphere. Dry CH_3CN, CH_2Cl_2, methyl tert-butyl ether (MTBE) and THF were purchased from Acros and used as received. All NMR spectra were recorded on a Bruker AVANCE Ⅲ–400 spectrometer at room temperature with $CDCl_3$ as the solvent and TMS as the internal standard. Chemical shifts (δ) were reported in ppm with respect to the residue solvent peak. Coupling constant (*J*) were reported in Hert (Hz), abbreviations for signal couplings are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; br, broad. Infrared spectra were recorded on a ThermoFisher Nicolet iS5 FTIR using neat thin film technique. The electron paramagnetic resonance (EPR) spectra were obtained using a Bruker EMX-10/2 EPR spectrometer at 298.15 K. High-resolution mass spectra (HRMS) were recorded on Thermo Quest Finnigan LCQDECA system equipped with electrospray ionization (ESI), or Atmospheric Pressure Chemical Ionization (APCI). All other commercially available reagents were used without further purification.

2.2 Synthesis of aldehydes

Aldehydes **1u** and **1v**[8]**,** substituted 1,1-diarylalkenes **4a-4n**[9], **4o**[10], **4p**[11] and 4-(4-pyridinyl)benzonitrile (**B**)[12] were synthesized according to the reported procedure.

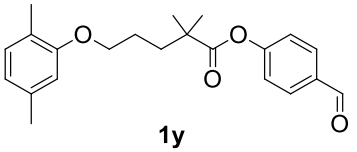
Substrate synthesis **1x**



1x

A sealed reaction bottle charged with a magnetic stir bar, abietic acid (2.0 mmol, 1.0 equiv) DCC (dicyclohexylcarbodiimide) (3.00 mmol, 2.00 equiv), DMAP (4-dimethylaminepyridine) (0.30 mmol, 0.15 equiv) and 4-hydroxybenzaldehyde (2.00 mmol, 1.00 equiv). in CH_2Cl_2 (15 mL). The reaction mixture was stirred at room temperature for 24 h. Then it was filtered, the filtrate was concentrated in *vacuo* and the residue was purified by chromatography on silica gel,[8] eluting with PE/EA = 10:1 (v/v) to afford the product **1x** in 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ; 9.98 (s, 1H), 7.94 – 7.89 (m, 2H), 7.22 – 7.17 (m, 2H), 5.80 (s, 1H), 5.43 – 5.39 (m, 1H), 2.29 – 2.18 (m, 3H), 2.13 – 2.06 (m, 1H), 2.03 – 1.93 (m, 4H), 1.86 – 1.80 (m, 2H), 1.71 – 1.62 (m, 1H), 1.39 (s, 3H), 1.34 – 1.18 (m, 4H), 1.03 – 0.99 (m, 6H), 0.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 176.6, 156.1, 145.7, 135.8, 133.9, 131.2, 122.5, 122.3, 120.2, 51.0, 47.2, 45.2, 38.3, 37.1, 35.0, 34.7, 27.5, 25.9, 22.6, 21.5, 20.9, 18.2, 17.2, 14.1; IR (film): 2931, 2733, 2118, 1747, 1698, 1599, 1508, 1208, 1046, 859, 738; HRMS (ESI-TOF) exact mass calculated for $C_{27}H_{34}O_3$ $[M+Na]^+$ 429.2400, found 429.2396.

Substrate synthesis **1y**



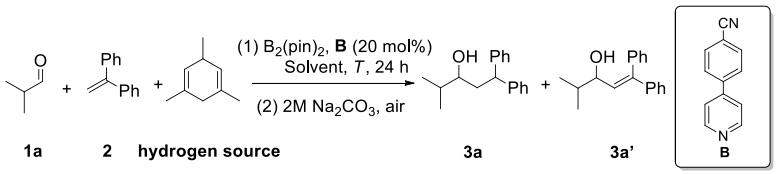
1y

A sealed reaction bottle charged with a magnetic stir bar, abietic acid (2.0 mmol, 1.0 equiv) DCC (dicyclohexylcarbodiimide) (3.00 mmol, 2.00 equiv), DMAP

(4-dimethylaminepyridine) (0.30 mmol, 0.15 equiv) and 4-hydroxybenzaldehyde (2.00 mmol, 1.00 equiv). in CH_2Cl_2 (15 mL). The reaction mixture was stirred at room temperature for 24 h. Then it was filtered, the filtrate was concentrated in *vacuo* and the residue was purified by chromatography on silica gel,[8] eluting with PE/EA = 10:1 (v/v) to afford the product at the colorless oil (40% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.89 – 7.86 (m, 2H), 7.21 – 7.17 (m, 2H), 6.99 (d, *J* = 7.4 Hz, 1H), 6.67 – 6.61 (m, 2H), 4.05 – 3.91 (m, 2H), 2.29 (s, 3H), 2.17 (s, 3H), 1.98 – 1.78 (m, 4H), 1.38 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.9, 175.7， 156.8, 156.8, 136.5, 133.9, 131.2, 130.4, 123.6, 122.4, 120.8, 111.9, 67.6, 42.6, 37.1, 37.0, 25.3, 25.1, 21.4, 15.8; IR (film): 2925, 2733, 1755, 1698, 1599, 1505, 1264, 1104, 803; HRMS (ESI-TOF) exact mass calculated for $C_{22}H_{26}O_4$ $[M+H]^+$ 355.1904, found 355.1901.

2.3 Optimization studies of the reaction conditions

Table S1 Optimization of the reaction conditions[a]



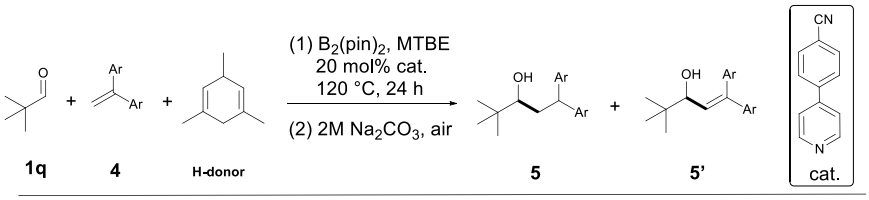
entry	*T*(°C)	Solvent	Ratio (3a/3a′)[b]
1	120	CH_2Cl_2	N R
2	120	CH_3CN	N R
3	120	THF	47%:3%
4	120	MTBE	78%: 6%
5	100	MTBE	55%:8%
6	120	MTBE	30%:2%[c]

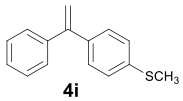
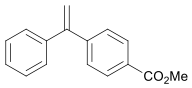
[a]Reaction conditions: isobutyraldehyde (**1a**, 0.2 mmol), $B_2(pin)_2$ (0.2 mmol), 4-(4-pyridinyl)benzonitrile (**B**, 0.04 mmol), 1,1-diphenylethylene (**2**, 0.4 mmol), 1,3,5-trimethyl-1,4-cyclohexadiene (0.2 mmol), solvent (1.0 mL). [b]Yields were determined by ^{1}H-NMR analysis of the crude mixture using CH_2Br_2 as the internal standard. [c]B_2pin_2 (0.5 equiv).

Isobutyraldehyde (**1a**) and 1, 1-diphenylethylene (**2**) were chosen as the model substrates for optimization of the reaction conditions. As shown Table S1, methyl tert-butyl ether (MTBE) was found to be the solvent for this reaction when 4-(4-pyridinyl)benzonitrile (**B**) was adopted as the catalyst (entry 1-4). A reduced

yield was observed at 100 °C (entry 5). With 0.5 equiv $B_2(pin)_2$, the yield of 3a decreased to 30% (entry 6).

Table S2 The effect of adding the hydrogen source on the product distribution

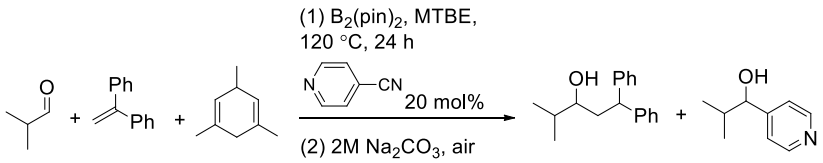


substrates of the1,1-diarylethylenes	combined isolated yield (**5/5'**) with hydrogen	without hydrogen source
 **4i**	68% (1: 0.12)	72% (1: 0.58)
 **4j**	44% (1: 0.08)	55% (1: 0.43)

As shown in Table S2, the addition of the hydrogen source is important for improving the yield of the main product (**5**).

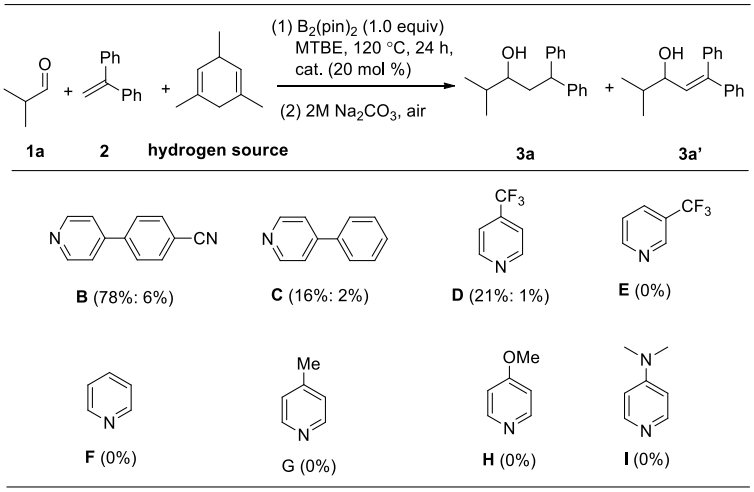
In addition, the catalytic reactivity of different pyridines toward the reductive coupling reaction between isobutyraldehyde (**1a**) and 1, 1-diphenylethylene (**2**) was also tested. As shown in Table S2, 4-(4-pyridinyl)benzonitrile (**B**) was found to be the most effective catalyst. When other pyridines were adopted (For example, **E**-**I**), no desired product was detected, possibly due to the high B-B bond activation barriers of these pyridines (See Figure S1).

With 4-cyanopyridine as the catalyst, the pyridine and aldehydes adduct (**3a"**) was detected and isolated in 7% yield.[13]



	3a	**3a"**
NMR yield	28%	12%
isolated yield	25%	7%

Table S3 Optimization of the pyridines[a]



[a]Reaction conditions: isobutyraldehyde (**1a**, 0.2 mmol), $B_2(pin)_2$ (0.2 mmol), catalyst (0.04 mmol), 1,1-diphenylethylene (**2**, 0.4 mmol), 1,3,5-trimethyl-1,4-cyclohexadiene (0.2 mmol), MTBE (1.0 mL). Yields were determined by ^{1}H-NMR analysis of the crude mixture using CH_2Br_2 as the internal standard.

2.4 General procedures for the organocatalytic reductive coupling between aldehydes (or ketones) and 1,1-diarylalkenes

A sealed reaction tube charged with a magnetic stir bar, aldehydes (or ketones) (0.2 mmol), $B_2(pin)_2$ (0.20 mmol, 1.0 equiv), 1,3,5-trimethyl-1,4-cyclohexadiene (0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (0.04 mmol, 20 mol%), MTBE (1 mL) and the corresponding coupling partner 1,1-diarylalkenes (0.4 mmol, 2.0 equiv) was placed in a heated oil bath (120 °C). After 24 hours, the reaction mixture was cooled and quenched with 2 M Na_2CO_3 aqueous solution (3 mL). Then, the reaction tube was stirred under air for another 15 minutes. The reaction mixture was extracted with EtOAc (3×10 mL). The combined organic layer was dried over Na_2SO_4 and then concentrated in vacuo to afford the crude product. This crude material was purified by preparative TLC on silca gel to afford the desired product.

3. Experimental Studies on the Reaction Mechanism

3.1 Electron Paramagnetic Resonance (EPR) Experiments

The existence of the 4-(4-pyridinyl)benzonitrile-boryl radical from the reaction of 4-(4-pyridinyl)benzonitrile and $B_2(pin)_2$ can be confirmed by its EPR spectrum.

The EPR spectrum (for the Microwave frequency=9.973 GHz, g=2.000) of the pyridine-boryl radical (**Int1**) were obtained (as shown in Figure S15) through the addition of 4-(4-pyridinyl)benzonitrile (1 equiv) to a 0.2 M solution of $B_2(pin)_2$ in MTBE (1 mL) (line 1). This result give supportive evidence for the formation of 4-(4-pyridinyl)benzonitrile-boryl radical, which was consistent with our DFT calculations.

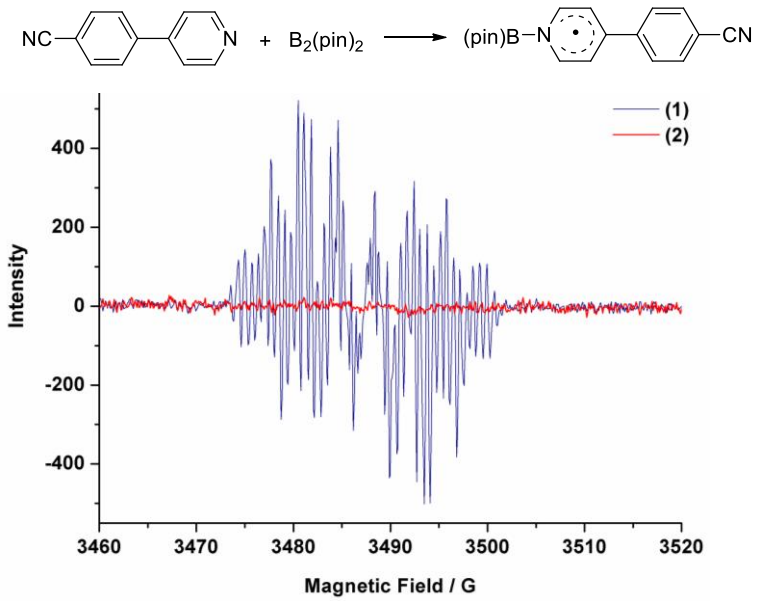
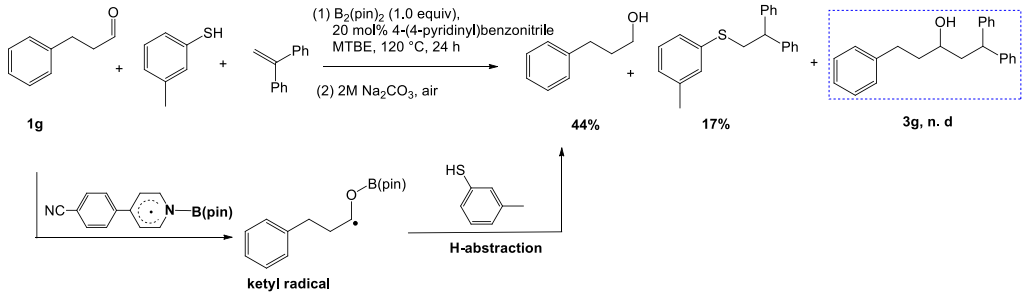


Figure S15. X band and EPR spectrum obtained in MTBE at 298.15 K. (1) Spectrum of 1:1 mixture of 4-(4-pyridinyl)benzonitrile and $B_2(pin)_2$. (2) Spectrum of 0.1 M solution of 4-(4-pyridinyl)benzonitrile.

3.2 The involvement of the ketyl radical

The involvement of the ketyl radical can be confirmed by a competition experiment. As shown below, when the hydrogen source 1,3,5-trimethyl-1,4-cyclohexadiene was replaced by 3-methylbenzenethiol, the ketyl radical quickly abstracted a hydrogen atom from 3-methylbenzenethiol to yield the reductive product, 3-phenyl-1-propanol, so that its addition to 1,1-diphenylethylene (to form the reductive coupling product) was inhibited. This result clearly indicated the involvement of the ketyl radical.



Experimental procedure: A sealed reaction tube charged with a magnetic stir bar, **1g** (0.20 mmol), $B_2(pin)_2$ (0.20 mmol, 1.0 equiv), 3-methylbenzenethiol (0.3 mmol, 1.5 equiv), 4-(4-pyridinyl)benzonitrile (catalyst, 0.04 mmol, 20 mol %), MTBE (1 mL) and 1,1-diphenylethylene (0.4 mmol, 2.0 equiv) were placed in a heated oil bath (120 °C). After 24 hours, the reaction was cooled and quenched with 2M Na_2CO_3 aqueous solution (3 mL). The reaction tube was stirred under air for another 15 minutes. The reaction mixture was extracted with EtOAc (3×10 mL). The combined organic layer was dried over Na_2SO_4 and then concentrated in vacuo to afford the crude product. This crude material was purified by preparative TLC on silca gel (PE/EA=20:1) to afford the 3-phenyl-1-propanol in 44% yield.

3.3 The generation of the radical species Int4 (or its analogues)

The radical species **Int4** (or its analogues), which can be generated via the addition of the ketyl radical to the *β*-position of arylethylene, can be confirmed by an intermolecular trapping experiment. When 2-vinylpyridine and trimethylacetaldehyde was subjected to the standard reaction condition, species **6** and **6'** could be detected by HRMS analysis for the crude reaction mixture. This result suggests that in this reaction, the radical species **Int4-like** was further trapped by another 2-vinylpyridine molecule.

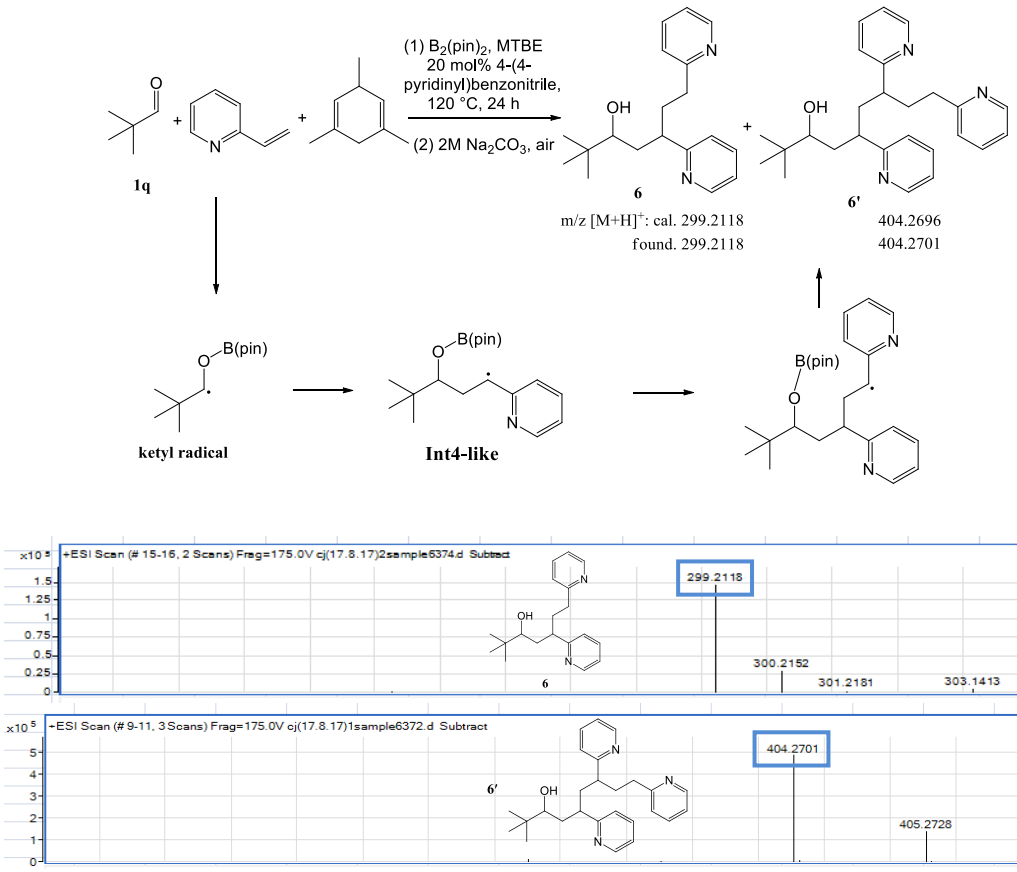


Figure S16. Mass spectrum of the crude reaction mixture of **1q,** 2-vinylpyridine, 1,3,5-trimethyl-1,4-cyclohexadiene, 4-(4-pyridinyl)benzonitrile and $B_2(pin)_2$.

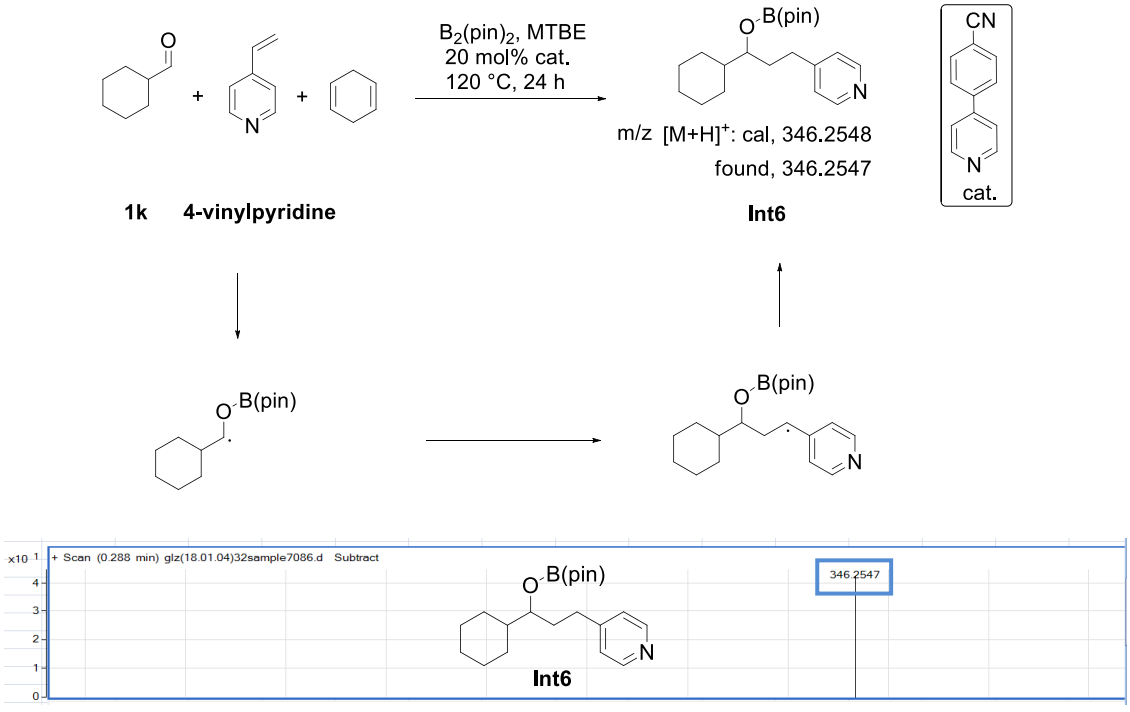


Figure S17. Mass spectrum of the crude reaction mixture of **1k,** 4-vinylpyridine, 1,4-cyclohexadiene, 4-(4-pyridinyl)benzonitrile and $B_2(pin)_2$.

3.3 ^{11}B spectra of $B_2(pin)_2$ and crude reaction mixture

We further conducted ^{11}B NMR analysis to detect the formation of the proposed O-boron intermediate (**Int7**). As shown below, the appearance of a set of signals at 21.2~22.2 ppm in the crude reaction mixture before work-up by Na_2CO_3, characteristic of a neutral boron center bound to three oxygen atoms, provided evidence for the formation of boron intermediate (**Int7**). The ^{11}B NMR shift at ~21 ppm is consistent with the previous report.[14] This result suggests that this reaction proceeded through the transfer of the boryl radical from the pyridine-boryl radical to the oxygen atom of aldehyde.

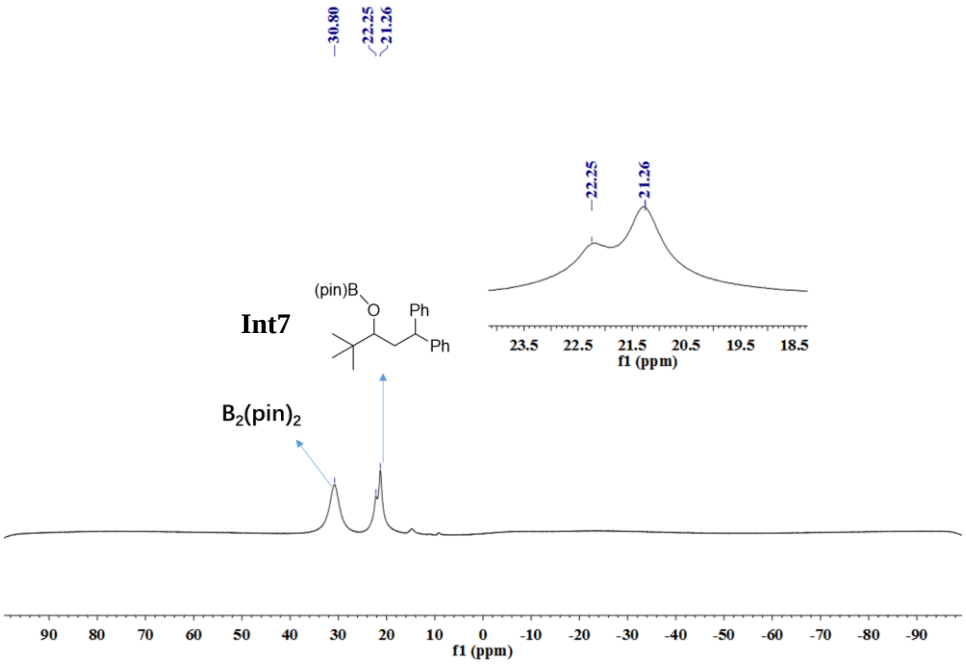
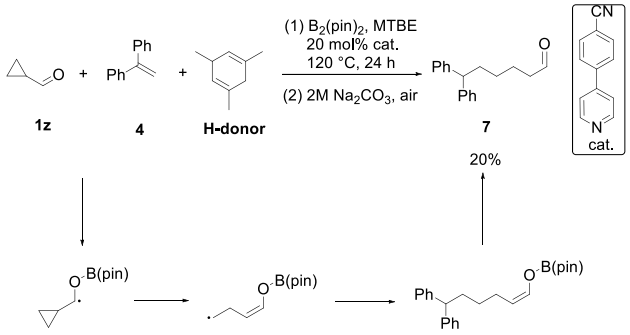


Figure S18. ^{11}B NMR spectrum in THF-d8 of the crude reaction mixture of 1q, 1,1-diphenylethylene, 1,3,5-trimethyl-1,4-cyclohexadiene, 4-(4-pyridinyl)benzonitrile and $B_2(pin)_2$.

Experimental procedure: A sealed reaction tube charged with a magnetic stir bar, 1q (0.20 mmol), $B_2(pin)_2$ (0.20 mmol, 1.0 equiv), 1,3,5-trimethyl-1,4-cyclohexadiene (0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (catalyst, 0.04 mmol, 20 mol %), THF-d8 (1 mL) and 1,1-diphenylethylene (0.4 mmol, 2.0 equiv) were placed in a heated oil bath (120 °C). After 24 hours, the reaction mixture was used to detection of ^{11}B NMR.

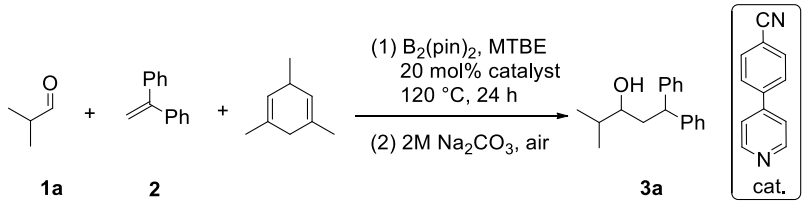
3.4 radical clock experiment



Experimental procedure: A sealed reaction tube charged with a magnetic stir bar, **1z** (0.20 mmol), $B_2(pin)_2$ (0.20 mmol, 1.0 equiv), 1,3,5-trimethyl-1,4-cyclohexadiene (0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (catalyst, 0.04 mmol, 20 mol %), MTBE (1 mL) and 1,1-diphenylethylene (0.4 mmol, 2.0 equiv) were placed in a heated oil bath (120 °C). After 24 hours, the reaction was cooled and quenched with 2M Na_2CO_3 aqueous solution (3 mL). The reaction tube was stirred under air for another 15 minutes. The reaction mixture was extracted with EtOAc (3×10 mL). The combined organic layer was dried over Na_2SO_4 and then concentrated in vacuo to afford the crude product. This crude material was purified by preparative TLC on silca gel (PE/EA=20:1) to afford the product **7** in 20% yield.

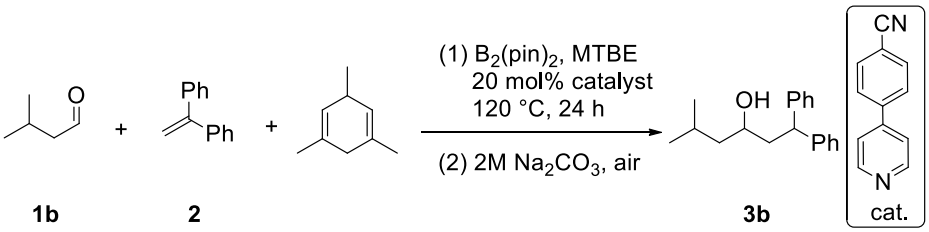
7: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.34 – 7.21 (m, 8H), 7.20 – 7.17 (m, 2H), 3.64 – 3.59 (m, 1H), 2.55 – 2.48 (m, 1H), 2.39 – 2.34 (m, 1H), 2.12 – 2.03 (m, 3H), 1.96 – 1.90 (m, 1H), 1.68 – 1.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 147.5, 144.6, 128.4, 128.3, 128.2, 126.6, 126.5, 126.1, 58.6, 58.1, 38.5, 25.0, 22.1; IR (film): 3056, 2957, 2957, 2873, 2735, 1717, 1492, 1492, 700; HRMS (ESI-TOF) exact mass calculated for $C_{17}H_{19}O$ $[M+H]^+$ 253.1587, found 253.1596.

4. Spectroscopic Characterization of the Coupling Products



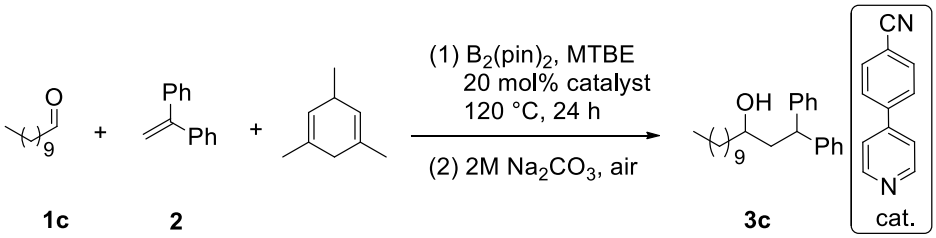
3a: Prepared following *general procedure* using **1a** (18.3 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg, 1.0 equiv), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 20:1) to afford the product **3a** (36 mg, 70% yield). NMR spectrums of the compounds **3a** are consistent with previous reported results.[15]

3a: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 8H), 7.24 – 7.15 (m, 2H), 4.28 (dd, *J* = 10.8, 4.6 Hz, 1H), 3.30-3.24 (m, 1H), 2.33-2.25 (m, 1H), 2.08-2.01 (m, 1H), 1.64-1.72 (m, 2H, with -OH), 0.91 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 144.0, 128.6, 128.6, 128.3, 127.8, 126.4, 126.2, 74.2, 47.7, 40.0, 34.1, 18.7, 17.2; IR (film): 3398, 3084, 3026, 2957, 1727, 1599, 1450, 1385; HRMS (ESI-TOF) exact mass calculated for $C_{18}H_{22}NaO$ $[M+Na]^+$ 277.1563, found 277.1560.



3b: Prepared following *general procedure* using **1b** (21.5 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 20:1) to afford the product **3b** (37 mg, 70% yield). NMR spectrums of the compounds **3b** are consistent with previous reported results.[15]

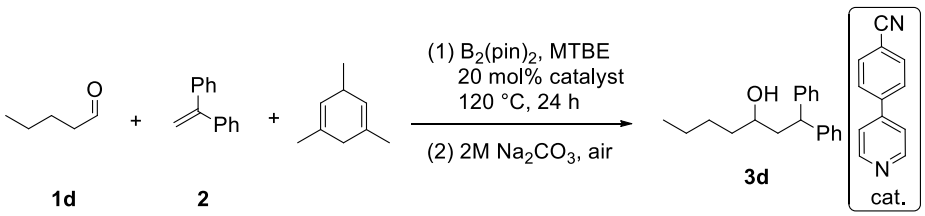
3b: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.26 (m, 8H), 7.22 – 7.16 (m, 2H), 4.25 (dd, *J* = 9.9, 5.9 Hz, 1H), 3.53 – 3.39 (m, 1H), 2.28 – 2.21 (m, 1H), 2.13 – 2.06 (m, 1H), 1.70 – 7.77 (m, 1H), 1.45 – 1.29 (m, 3H, with -OH), 0.87 (d, *J* = 6.6 Hz, 3H), 0.83 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 144.2, 128.6, 128.6, 128.1, 127.1, 126.4, 126.2, 68.0, 47.7, 47.4, 43.8, 24.7, 23.4, 22.3.; IR (film): 3602, 2956, 2869, 1598, 1493, 1450, 1364, 1007; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{24}NaO$ $[M+Na]^+$ 291.1719, found 291.1713.



1c 2 3c

3c: Prepared following *general procedure* using **1c** (41.3 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 20:1) to afford the product **3c** (50 mg, 71% yield).

3c: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 8H), 7.25 – 7.15 (m, 2H), 4.27 (dd, *J* = 10.2, 5.7 Hz, 1H), 3.52 – 3.44 (m, 1H), 2.31 – 2.22 (m, 1H), 2.15 – 2.06 (m, 1H), 1.5 – 1.45 (m, 2H), 1.35 – 1.21 (m, 17H, with -OH), 0.94 – 0.88 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.2, 128.6, 128.6, 128.2, 127.8, 126.4, 126.2, 69.9, 47.6, 43.3, 38.1, 32.0, 29.8, 29.7, 29.7, 29.7, 29.4, 25.6, 22.8, 14.2; IR (film): 3355, 3026, 2925, 2853, 1599, 1494, 1451, 1377; HRMS (ESI-TOF) exact mass calculated for $C_{25}H_{36}NaO$ $[M+Na]^+$ 375.2658, found 375.2655.

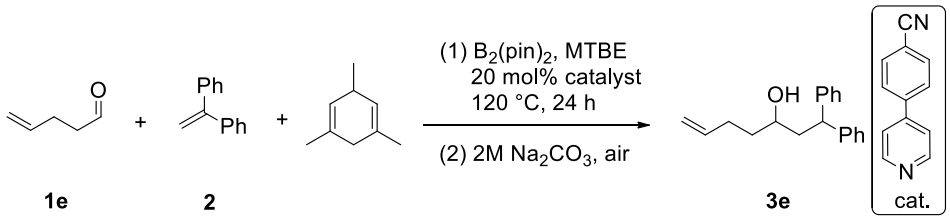


1d 2 3d

3d: Prepared following *general procedure* using **1d** (21.3 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg),

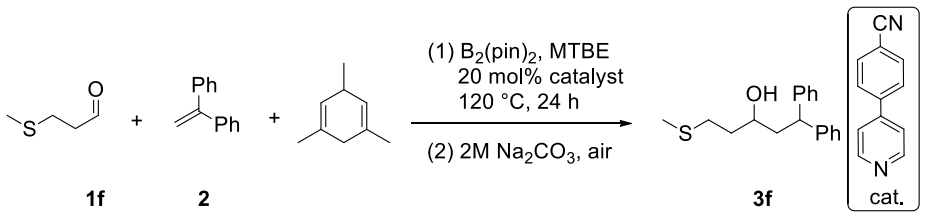
1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3d** (38 mg, 72% yield). NMR spectrums of the compounds **3d** are consistent with previous reported results.[15]

3d: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 8H), 7.24 – 7.16 (m, 2H), 4.26 (dd, *J* = 9.5, 5.8 Hz, 1H), 3.52 – 3.44 (m, 1H), 2.30 – 2.22 (m, 1H), 2.15 – 2.07 (m, 1H), 1.51 – 1.26 (m, 7H, with -OH), 0.92 – 0.88 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 144.2, 128.6, 128.5, 128.1, 127.7, 126.3, 126.1, 69.7, 47.6, 43.2, 37.8, 27.7, 22.7, 14.1; IR (film):3365, 3060, 2930, 2857, 1494, 1450, 1378, 1031; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{28}NaON$ $[M+NH_4]^+$ 286.2165, found 286.2162.



3e: Prepared following *general procedure* using **1e** (19.8 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3e** (33 mg, 61% yield).

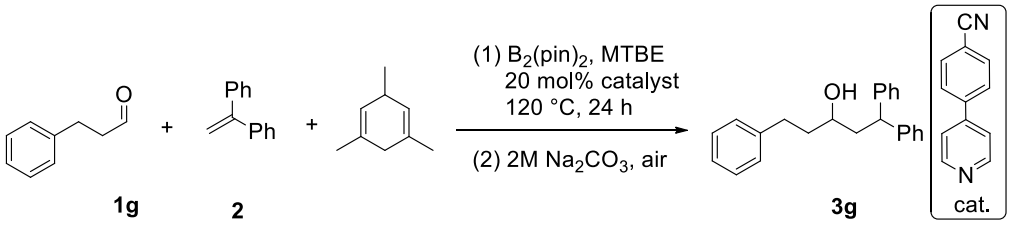
3e: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 8H), 7.24 – 7.16 (m, 2H), 5.87 – 5.76 (m, 1H), 5.05 – 4.94 (m, 2H), 4.30 – 4.22 (m, 1H), 3.56 – 3.48 (m, 1H), 2.29 – 2.08 (m, 3H, with -OH), 1.68 – 1.51 (m, 4H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 144.1, 138.5, 128.6, 128.6, 128.2, 127.8, 126.4, 126.3, 114.9, 69.5, 47.6, 43.2, 37.1, 30.0; IR (film): 3564, 3373, 3061, 3026, 2934, 1639, 1494, 911; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{26}ON$ $[M+NH_4]^+$ 284.2009, found 284.1999.



1f 2 3f

3f: Prepared following *general procedure* using **1f** (20.4 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3f** (38 mg, 67% yield).

3f: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 8H), 7.23 – 7.15 (m, 2H), 4.7 – 4.21 (dd, *J* = 9.7, 6.2 Hz, 1H), 3.66 – 3.58 (m, 1H), 2.61 – 2.54 (m, 2H), 2.27 – 2.14 (m, 2H), 2.07 (brs, 4H, with -OH), 1.81 – 1.71 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 144.0, 128.7, 128.6, 128.1, 127.8, 126.4, 126.3, 69.3, 47.5, 43.3, 36.5, 30.8, 15.5; IR (film): 3419, 3025, 2916, 1493, 1450, 1060, 1000, 901; HRMS (ESI-TOF) exact mass calculated for $C_{18}H_{22}OSNa$ $[M+Na]^+$ 309.1284, found 309.1280.

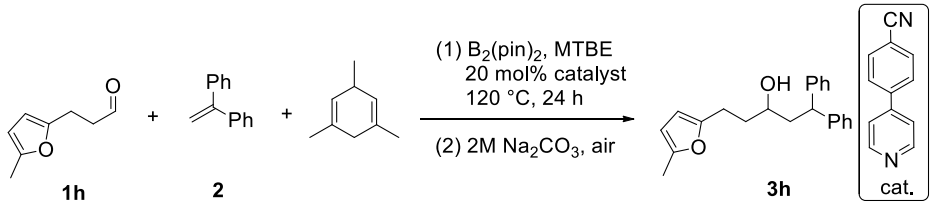


1g 2 3g

3g: Prepared following *general procedure* using **1g** (26.33 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.2 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3g** (35 mg, 55% yield). NMR spectrums of the compounds **3g** are consistent with previous reported results.[15]

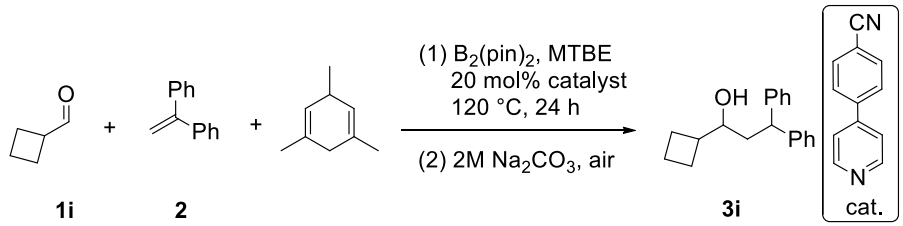
3g: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 10H), 7.23 – 7.11 (m, 5H), 4.24 (dd, *J* = 9.8, 6.0 Hz, 1H), 3.59 – 3.52 (m, 1H), 2.80 – 2.70 (m, 1H),

2.66 – 2.57 (m, 1H), 2.33 – 2.25 (m, 1H), 2.89 – 2.74(m, 1H), 1.90 – 1.70 (m, 3H, with -OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 144.1, 142.1, 128.7, 128.6, 128.5, 128.4, 128.1, 127.8, 126.4, 126.3, 125.9, 69.6, 47.7, 43.3, 39.8, 32.1. IR (film): 3366, 3060, 2928, 1600, 1494, 1451, 763; HRMS (ESI-TOF) exact mass calculated for $C_{23}H_{28}NO$ $[M+NH_4]^+$ 334.2165, found 334.2165.



3h: Prepared following *general procedure* using **1h** (27.6 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3h** (29 mg, 46% yield).

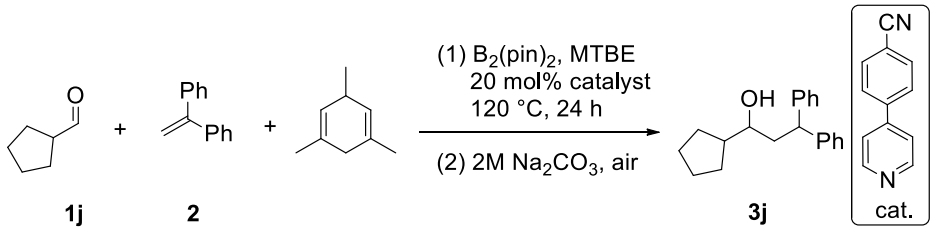
3h: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.25 (m, 8H), 7.21 – 7.16 (m, 2H), 5.81 (m, 2H), 4.25 (dd, *J* = 9.9, 5.9 Hz, 1H), 3.59 – 3.51 (m, 1H), 2.74 – 2.60 (m, 2H), 2.31 – 2.25 (m, 1H), 2.23 (s, 3H), 2.20 – 2.14 (m, 1H), 1.87 – 1.75 (m, 2H), 1.61 (brs, 1H, with -OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 150.4, 145.2, 144.1, 128.6, 128.6, 128.1, 127.8, 126.4, 126.3, 105.9, 105.6, 69.3, 47.6, 43.3, 36.4, 24.4, 13.6. IR (film): 3565, 3060, 2921, 1966, 1599, 1450, 1218, 1062; HRMS (ESI-TOF) exact mass calculated for $C_{22}H_{24}NaO_2$ $[M+Na]^+$ 343.1669, found 343.1663.



3i: Prepared following *general procedure* using **1i** (16.8 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24

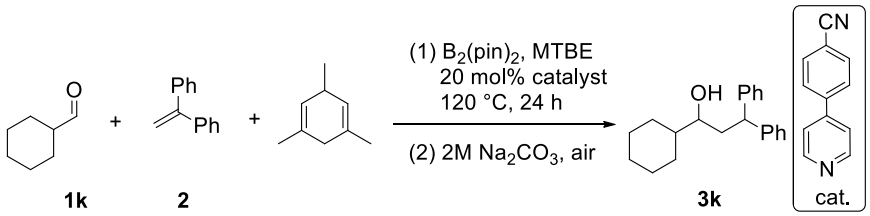
h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3i** (34 mg, 63% yield).

3i: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 8H), 7.24 – 7.14 (m, 2H), 4.27 (dd, *J* = 10.9, 5.0 Hz, 1H), 3.39 – 3.32 (m, 1H), 2.40 – 2.32 (m, 1H), 2.23 – 2.14 (m, 1H), 2.00 – 1.65 (m, 8H, with -OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 144.1, 128.6, 128.5, 128.2, 127.7, 126.4, 126.2, 73.4, 47.4, 41.8, 40.3, 24.3, 24.1, 17.9; IR (film): 3383, 3060, 2933, 2857, 1493, 1449, 1074, 749; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{26}NO$ $[M+NH_4]^+$ 284.2009, found 284.1998.



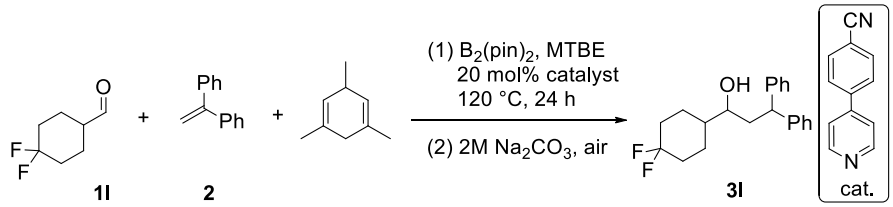
3j: Prepared following *general procedure* using **1j** (21.6 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3j** (41 mg, 74% yield). NMR spectrums of the compounds **3j** are consistent with previous reported results.[15]

3j: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 8H), 7.23 – 7.15 (m, 2H), 4.31 (dd, *J* = 11.1, 4.7 Hz, 1H), 3.31 – 3.25 (m, 1H), 2.37 – 2.29 (m, 1H), 2.08 – 1.99 (m, 1H), 1.95 – 1.86 (m, 1H), 1.80 – 1.68 (m, 2H), 1.61 – 1.50 (m, 4H, with -OH), 1.36 – 1.23 (m, 2H), 1.19 – 1.12 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 144.1, 128.6, 128.5, 128.3, 127.7, 126.3, 126.2, 73.6, 47.6, 47.0, 42.2, 29.2, 28.5, 25.8, 25.7. IR (film): 3385, 3060, 3025, 2049, 2866, 1599, 1493, 750; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{28}NO$ $[M+NH_4]^+$ 298.2165, found 298.2169.



3k: Prepared following *general procedure* using **1k** (24.2 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3k** (45 mg, 76% yield). NMR spectrums of the compounds **3k** are consistent with previous reported results.[15]

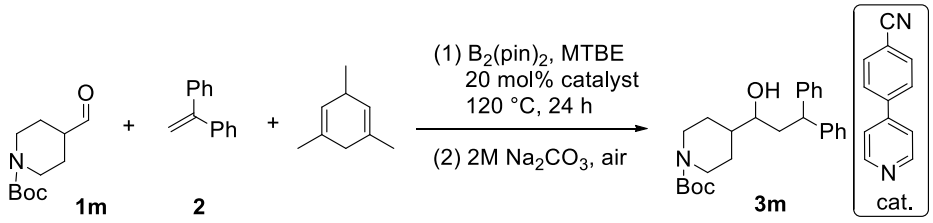
3k: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 8H), 7.23 – 7.14 (m, 2H), 4.28 (dd, *J* = 11.0, 4.8 Hz, 1H), 3.28 – 3.23 (m, 1H), 2.36 – 2.27 (m, 1H), 2.08 – 1.99 (m, 1H), 1.82 – 1.63 (m, 5H, with -OH), 1.37 – 0.97 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 144.0, 128.6, 128.5, 128.3, 127.8, 126.3, 126.2, 73.8, 47.7, 44.3, 40.1, 29.2, 27.8, 26.6, 26.4, 26.3. IR (film): 3390, 3060, 2924, 2815, 1738, 1494, 1031, 739; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{26}NaO$ $[M+Na]^+$ 317.1876 , found 317.1887.



3l: Prepared following *general procedure* using **1l** (27.0 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3l** (34 mg, 51% yield).

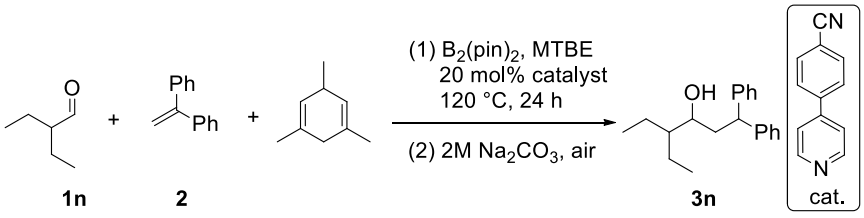
3l: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 8H), 7.23 – 7.15 (m, 2H), 4.25 (dd, *J* = 10.8, 5.0 Hz, 1H), 3.37 – 3.31 (m, 1H), 2.26 – 2.34 (m, 1H),

2.16 – 2.02 (m, 3H), 1.88 – 1.81 (m, 1H), 1.76 – 1.58 (m, 4H), 1.44 – 1.36 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 143.7, 128.8 and 128.7 ($d_{C\text{-}F}$, J = 11.3 Hz), 128.2, 127.7, 126.6, 126.4, 72.7, 47.8, 42.5, 40.4, 33.8 (d, $J_{C\text{-}F}$ = 10.0 Hz), 33.56 (dd, $J_{C\text{-}F}$ = 9.9, 3.0 Hz), 33.32 (d, $J_{C\text{-}F}$ = 9.7 Hz), 25.2 (d, $J_{C\text{-}F}$ = 9.9 Hz). 24.1 (d, $J_{C\text{-}F}$ = 9.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -91.3 (d, J = 234.9 Hz), -102.4 (d, J = 234.8 Hz). IR (film): 3586, 3060, 2938, 1732, 1599, 1494, 1114, 1002, 702; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{24}F_2NaO$ $[M+Na]^+$ 353.1687, found 353.1677.



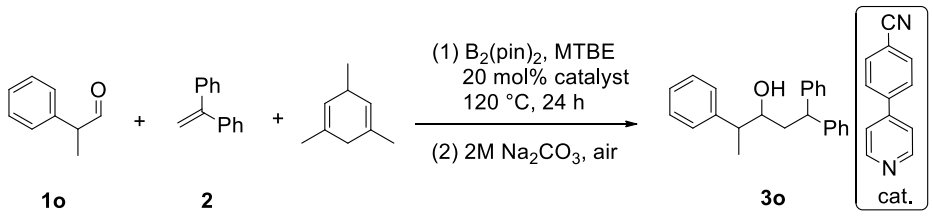
3m: Prepared following *general procedure* using **1m** (42.6 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **3m** (56 mg, 71% yield).

3m: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.18 (m, 8H), 7.16 – 7.08 (m, 2H), 4.21 (dd, J = 11.0, 4.7 Hz, 1H), 4.07 (br, 2H), 3.24 – 3.18 (m, 1H), 2.57 (br, 2H), 2.29 – 2.22 (m, 1H), 2.02 – 1.94 (m, 1H), 1.80 (brs, 1H, with-OH), 1.69 – 1.63 (m, 1H), 1.56 – 1.49 (m, 1H), 1.39 (s, 9H), 1.22 – 1.08 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 254.8, 145.4, 143.7, 128.7, 128.6, 128.2, 127.7, 126.5, 126.2, 79.4, 72.8, 47.6, 43.7, 42.7, 40.1, 28.5, 28.2; IR (film):3445, 2975, 2855, 1668, 1449, 1365, 1168, 739; HRMS (ESI-TOF) exact mass calculated for $C_{25}H_{33}NaNO_3$ $[M+Na]^+$ 418.2353, found 418.2357.



3n: Prepared following *general procedure* using **1n** (24.6 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3n** (33 mg, 59% yield).

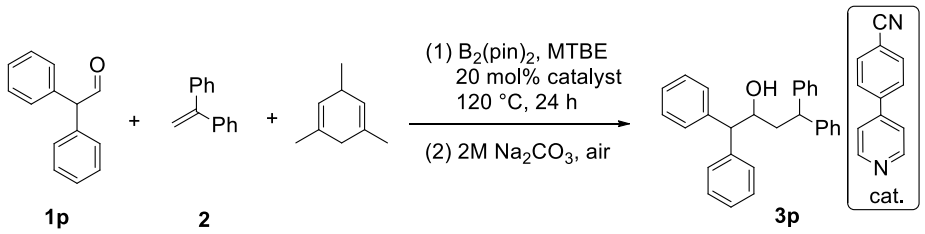
3n: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 8H), 7.24 – 7.15 (m, 2H), 4.26 (dd, *J* = 10.7, 5.1 Hz, 1H), 3.56 – 3.49 (m, 1H), 2.30 – 2.22 (m, 1H), 2.12 – 2.03 (m, 1H), 1.46 – 1.21 (m, 6H, with -OH), 0.84 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 144.1, 128.6, 128.6, 128.2, 127.8, 126.4, 126.2, 70.9, 47.9, 47.6, 39.7, 22.1, 21.6, 12.1, 11.9; IR (film): 3396, 3026, 2960, 2873, 1493, 1450, 1031, 700; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{26}NaO$ $[M+Na]^+$ 305.1876, found 305.1877.



3o: Prepared following *general procedure* using **1o** (26.8 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3o** (36 mg, 59% yield, d.r. =1:1). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

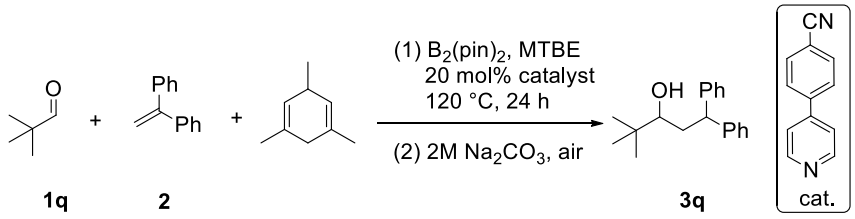
3o: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.16 (m, 15H), 4.34 (dd, *J* = 11.3, 4.5 Hz, 1H), 3.57 – 3.51 (m, 1H), 2.85 – 2.77 (m, 1H), 2.48 – 2.44 (m, 1H), 2.02 – 1.94 (m, 1H), 1.31 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 143.8, 143.2, 128.7, 128.6, 128.5, 128.3, 128.3, 127.8, 126.8, 126.3, 126.1, 73.8, 47.4,

46.6, 40.6, 17.6; IR (film): 3566, 3059, 3025, 1597, 1493, 1450, 1060, 700; HRMS (ESI-TOF) exact mass calculated for $C_{23}H_{24}NaO$ $[M+Na]^+$ 339.1719, found 339.1717.



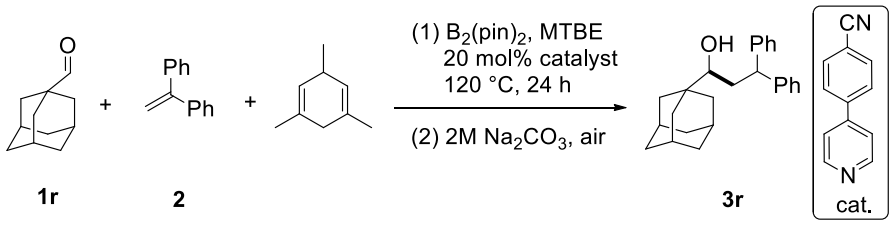
3p: Prepared following *general procedure* using **1p** (35.5 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3p** (42 mg, 56% yield).

3p: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.06 (m, 20H), 4.34 – 4.27 (m, 1H), 4.17 – 4.08 (m, 1H), 3.88 (dd, *J* = 9.1, 5.5 Hz, 1H), 2.34 – 2.23 (m, 1H), 2.06 – 1.96 (m, 1H). 1.61 (brs, 1H, with -OH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 143.6, 142.1, 141.5, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 127.7, 126.9, 126.7, 126.4, 126.1, 71.5, 59.5, 47.4, 41.1; IR (film):3566, 3059, 3025, 1597, 1493, 1450, 1060, 700; HRMS (ESI-TOF) exact mass calculated for $C_{28}H_{26}NaO$ $[M+Na]^+$ 401.1876, found 401.1875.



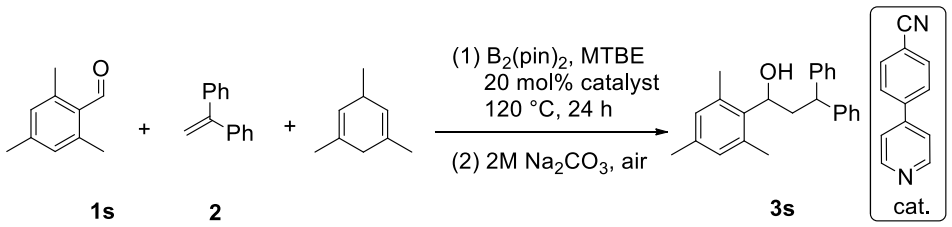
3q: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3q** (38 mg, 71% yield). NMR spectrums of the compounds **3q** are consistent with previous reported results.[15]

3q: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.28 (m, 8H), 7.28-7.16 (m, 2H), 4.34 (dd, *J* = 11.6, 2.4 Hz, 1H), 3.14 (d, *J* = 10.7 Hz, 1H), 2.45-2.35 (m, 1H), 2.01-1.92 (m, 1H), 1.56 (brs, 1H, with -OH), 0.92 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 143.8, 128.6, 128.5, 128.4, 127.7, 126.4, 126.1, 77.3, 48.0, 37.6, 35.0, 25.7. IR (film): 3464, 3060, 3026, 2956, 1598, 1493, 1477, 1030, 700; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{24}NaO$ $[M+Na]^+$ 291.1719, found 291.1713.



3r: Prepared following *general procedure* using **1r** (32.9 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **3r** (41 mg, 60% yield).

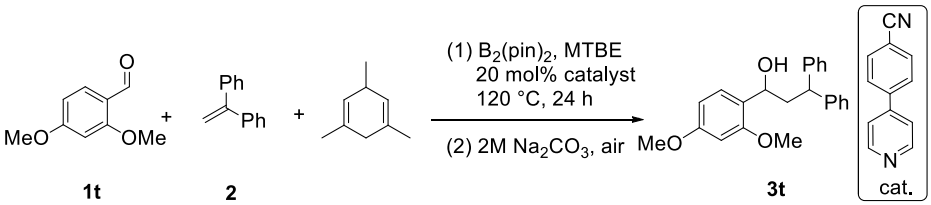
3r: White solid, 134.6-136.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.25 (m, 8H), 7.24 – 7.15 (m, 2H), 4.31 (dd, *J* = 11.7, 4.0 Hz, 1H), 2.97 – 2.92 (m, 1H), 2.43 – 2.34 (m, 1H), 2.00 (brs, 2H, with -OH), 1.75 – 1.61 (m, 7H), 1.60 – 1.47 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 143.8, 128.6, 128.5, 128.4, 127.8, 126.3, 126.1, 77.4, 47.9, 38.0, 37.3, 36.8, 36.2, 28.4; IR (film): 3446, 3025, 2903, 2847, 1493, 1449, 1050, 700; HRMS (ESI-TOF) exact mass calculated for $C_{25}H_{30}NaO$ $[M+Na]^+$ 369.2189, found 369.2180.



3s: Prepared following *general procedure* using **1s** (29.6 μL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv),

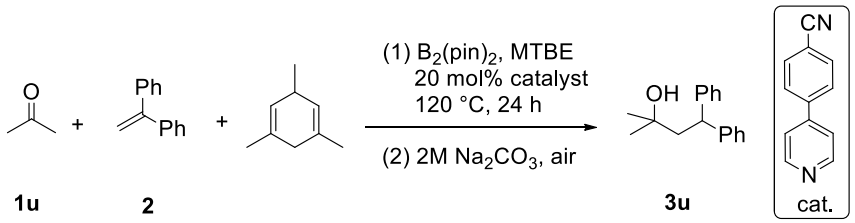
4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3s** (30 mg, 46% yield).

3s: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 8H), 7.25 – 7.16 (m, 2H), 6.80 (s, 2H), 4.93 (dd, *J* = 10.3, 3.4 Hz, 1H), 4.33 (dd, *J* = 11.0, 4.8 Hz, 1H), 2.80 – 2.72 (m, 1H), 2.35 – 2.14 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 144.4, 136.9, 136.7, 136.2, 130.2, 128.7, 128.6, 128.3, 127.8, 126.5, 126.3, 69.0, 47.9, 41.2, 20.8, 20.4; IR (film): 3558, 3025, 2921, 1609, 1493, 1450, 1053, 701; HRMS (ESI-TOF) exact mass calculated for $C_{24}H_{26}NaO$ $[M+Na]^+$ 353.1876, found 353.1879.



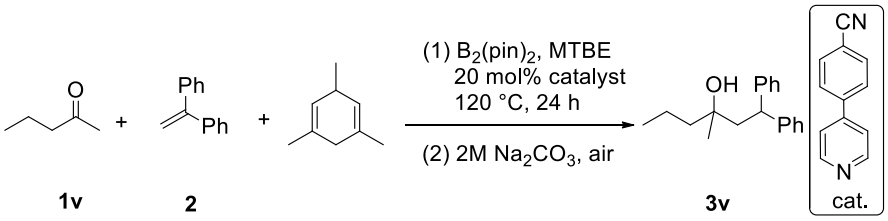
3t: Prepared following *general procedure* using **1t** (33.2 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3t** (33 mg, 46% yield).

3t: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.25 (m, 8H), 7.23 – 7.10 (m, 3H), 6.48 – 6.43 (m, 2H), 4.66 – 4.61 (m, 1H), 4.24 – 4.18 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 2.61 – 2.46 (m, 3H, with -OH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 157.7, 145.3, 144.3, 128.6, 128.5, 128.2, 127.9, 127.7, 126.2, 126.1, 124.9, 104.0, 98.8, 69.1, 55.4, 55.2, 47.8, 43.1; IR (film): 3445, 3025, 2934, 2835, 1613, 1504, 1207, 749; HRMS (ESI-TOF) exact mass calculated for $C_{23}H_{24}NaO_3$ $[M+Na]^+$ 371.1618, found 371.1615.



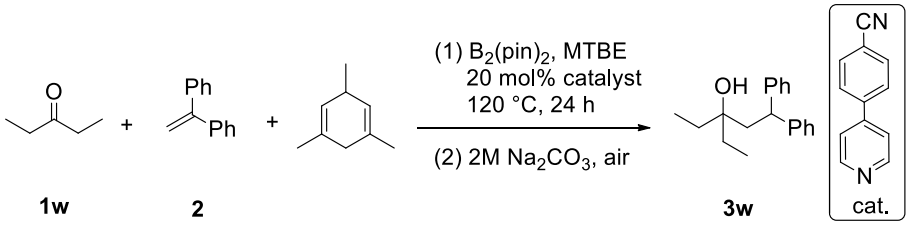
3u: Prepared following *general procedure* using **1u** (14.7 uL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3u** (20 mg, 42% yield).

3u: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.26 (m, 8H), 7.20 – 7.14 (m, 2H), 4.23 (t, *J* = 7.0 Hz, 1H), 2.41 – 2.37 (d, *J* = 7.0 Hz, 2H), 1.74 (brs, 1H, -OH), 1.19 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 128.7, 127.8, 126.3, 71.5, 48.8, 47.6, 30.1; IR (film): 3566, 3419, 3060, 2969, 1493, 1373, 1133, 743; HRMS (ESI-TOF) exact mass calculated for $C_{17}H_{20}NaO$ $[M+Na]^+$ 263.1406, found 263.1400.



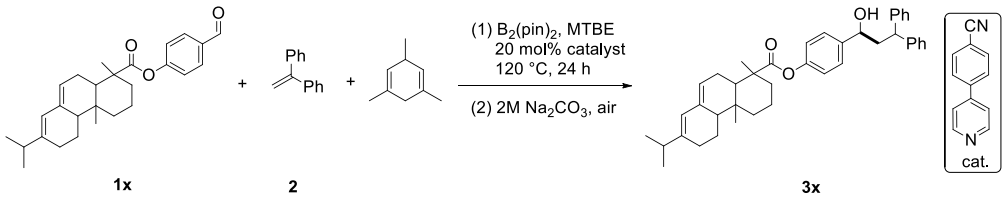
3v: Prepared following *general procedure* using **1v** (21.3 uL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3v** (17 mg, 27% yield).

3v: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 8H), 7.19 – 7.14 (m, 2H), 4.21 (t, *J* = 7.0 Hz, 1H), 2.35 (dd, *J* = 7.0, 1.5 Hz, 2H), 1.64 (brs, 1H, -OH), 1.46 – 1.41 (m, 2H), 1.33 – 1.27 (m, 2H), 1.11 (s, 3H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 128.7, 127.8, 126.3, 73.4, 47.2, 47.0, 45.3, 27.5, 17.3, 14.7; IR (film): 3566, 3446, 3025, 2958, 2931, 1493, 1451, 1030, 702; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{24}NaO$ $[M+Na]^+$ 291.1719, found 291.1715.



3w: Prepared following *general procedure* using **1w** (21.0 uL, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **3w** (17 mg, 27% yield).

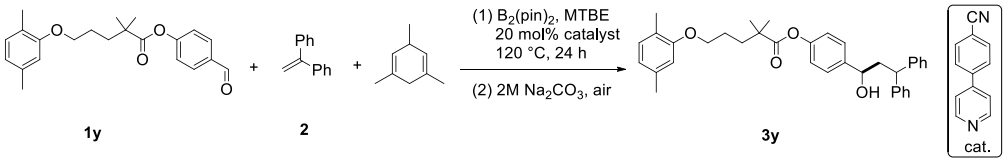
3w: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.25 (m, 8H), 7.19 – 7.14 (m, 2H), 4.19 (t, *J* = 6.9 Hz, 1H), 2.32 (d, *J* = 6.9 Hz, 2H), 1.62 (brs, 1H, -OH), 1.47 (t, *J* = 7.5 Hz, 4H), 0.80 (d, *J* = 7.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 128.7, 127.9, 126.3, 75.4, 46.8, 44.1, 31.3, 8.0; IR (film): 3586, 2966, 2937, 1598, 1493, 1451, 973, 745; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{24}NaO$ $[M+Na]^+$ 291.1719, found 291.1719.



3x: Prepared following *general procedure* using **1x** (61.2 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **3x** (47 mg, 40% yield).

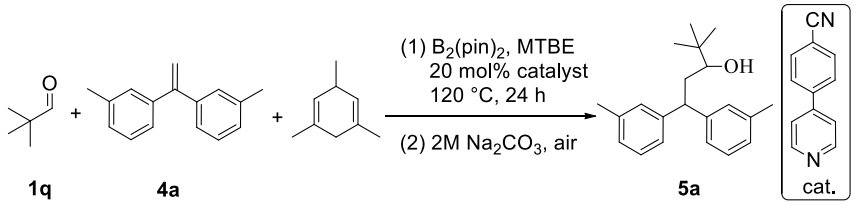
3x: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 10H), 7.22 – 7.13 (m, 2H), 6.97 (m, 2H), 5.81 (s, 1H), 5.42 (s, 1H), 4.47 (dd, *J* = 8.4, 5.1 Hz, 1H), 4.11 (m, 1H), 2.56 – 2.46 (m, 1H), 2.44 – 2.35 (m, 1H), 2.28 – 2.20 (m, 2H), 2.12 – 2.07 (m, 2H), 2.03 – 1.90 (m, 5H, with -OH), 1.88 – 1.78 (m, 2H), 1.69 – 1.61 (m,

2H), 1.38 (s, 3H), 1.30 – 1.18 (m, 3H), 1.05 – 0.99 (m, 6H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.2, 150.6, 145.6, 144.6, 144.2, 142.0, 135.7, 128.70, 128.6, 128.0, 127.9, 127.1, 126.4, 126.3, 122.4, 121.7, 120.5, 71.9, 51.0, 47.6, 47.0, 45.2, 44.8, 38.3, 37.1, 35.0, 34.7, 27.5, 25.9, 22.6, 21.5, 20.9, 18.2, 17.2, 14.1; IR (film): 3467, 2929, 1744, 1504, 1227, 1199, 1057, 908, 734; HRMS (ESI-TOF) exact mass calculated for $C_{41}H_{48}KO_3$ $[M+K]^+$ 627.3235, found 627.3234.



3y: Prepared following *general procedure* using **1y** (61.2 mg, 0.2 mmol, 1.0 equiv), 1,1-diphenylethylene (70.6 μL, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **3y** (34 mg, 32% yield).

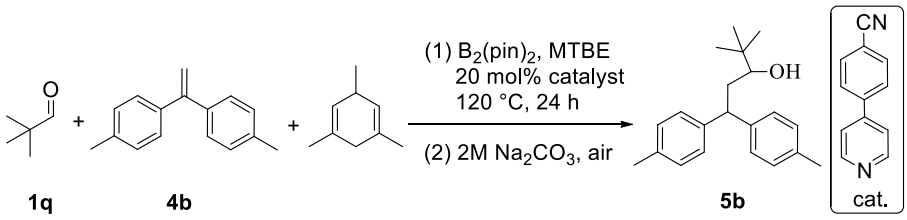
3y: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.24 (m, 10H), 7.23 – 7.13 (m, 2H), 7.04 – 6.96 (m, 3H), 6.69 – 6.60 (m, 2H), 4.49 (dd, *J* = 8.5, 5.1 Hz, 1H), 4.12 (dd, *J* = 9.1, 6.8 Hz, 1H), 3.98 (m, 2H), 2.51 (m, 1H), 2.40 (m, 1H), 2.30 (s, 3H), 2.18 (s, 3H), 1.88 (d, *J* = 2.6 Hz, 5H, with-OH), 1.37 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.5, 156.9, 150.5, 144.6, 142.2, 142.1, 136.6, 130.4, 128.7, 128.6, 128.1, 127.9, 127.1, 126.4, 126.4, 123.7, 121.7, 120.8, 112.0, 71.9, 67.9, 47.6, 44.8, 42.5, 37.2, 25.4, 25.2, 25.2, 21.5, 15.9; IR (film): 3428, 2924, 1749, 1507, 1264, 1198, 1115, 1046, 701; HRMS (ESI-TOF) exact mass calculated for $C_{36}H_{40}NaO_4$ $[M+Na]^+$ 559.2819, found 559.2812.



5a: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4a** (83.3 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv),

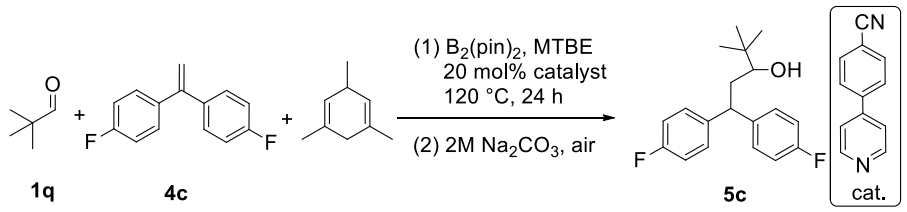
4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5a** (41 mg, 70% yield).

5a: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.04 (m, 6H), 7.02 – 6.94 (m, 2H), 4.19 (d, *J* = 11.4 Hz, 1H), 3.10 (d, *J* = 10.6 Hz, 1H), 2.36 – 2.28 (m, 7H), 1.92 – 1.82 (m, 1H), 1.40 (brs, 1H, -OH), 0.88 (d, *J* = 1.7 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 143.6, 138.0, 129.3, 128.5, 128.4, 127.0, 126.8, 125.0, 124.6, 77.35, 48.0, 37.6, 35.0, 25.6, 21.5; IR (film): 3461, 2955, 2868, 1604, 1478, 1363, 1067, 773; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{32}NO$ $[M+NH_4]^+$ 314.2478, found 314.2477.



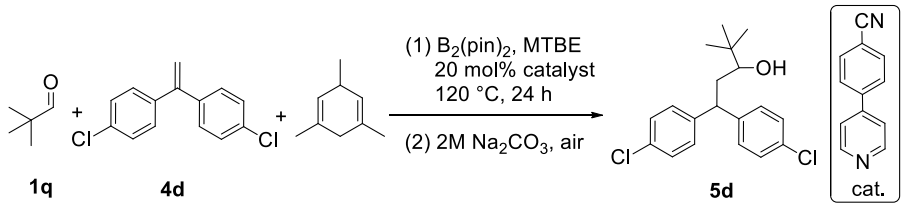
5b: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4b** (83.3 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5b** (38 mg, 64% yield).

5b: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.08 (m, 8H), 4.22 (dd, *J* = 11.5, 4.3 Hz, 1H), 3.14 (d, *J* = 10.4 Hz, 1H), 2.35 – 2.30 (m, 7H), 1.96 – 1.86 (m, 1H), 1.44 (brs, 1H, with -OH), 0.90 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 140.9, 135.7, 135.6, 129.3, 129.3, 128.1, 127.5, 77.4, 47.3, 37.7, 35.0, 25.7, 21.1, 21.0; IR (film): 3447, 2954, 2868, 1051, 1447, 1275, 1065, 764; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{28}NaO$ $[M+Na]^+$ 319.2032, found 319.2030.



5c: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4c** (86.49 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5c** (27 mg, 41% yield).

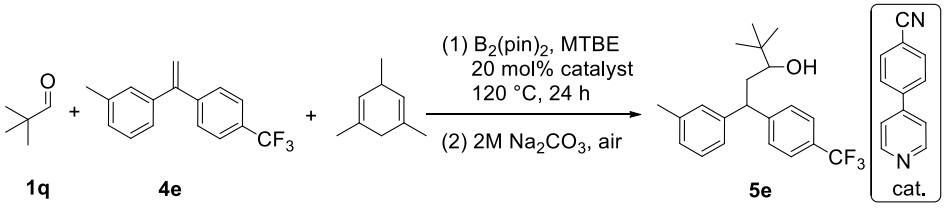
5c: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 4H), 7.03 – 6.91 (m, 4H), 4.27 (dd, *J* = 11.8, 3.9 Hz, 1H), 3.03 (dd, *J* = 10.8, 1.7 Hz, 1H), 2.28 – 2.18 (m, 1H), 1.92 – 1.83 (m, 1H), 1.59 (brs, 1H, -OH), 0.87 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, $J_{C\text{-}F}$ = 18.4 Hz), 160.3 (d, $J_{C\text{-}F}$ = 18.3 Hz), 141.6 (d, $J_{C\text{-}F}$ = 3.2 Hz), 139.5 (d, $J_{C\text{-}F}$ = 3.3 Hz), 129.7 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.0 (d, $J_{C\text{-}F}$ = 7.8 Hz). 115.5 (d, $J_{C\text{-}F}$ = 21.4 Hz), 115.3 (d, $J_{C\text{-}F}$ = 21.3 Hz), 77.1, 46.4, 37.8, 35.0, 25.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.69, -117.17; IR (film): 3612, 3480, 2957, 2870, 1603, 1505, 1224, 1033, 747; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{22}F_2NaO$ $[M+Na]^+$ 327.1531, found 327.1532.



5d: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4d** (99.66 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5d** (41 mg, 61% yield).

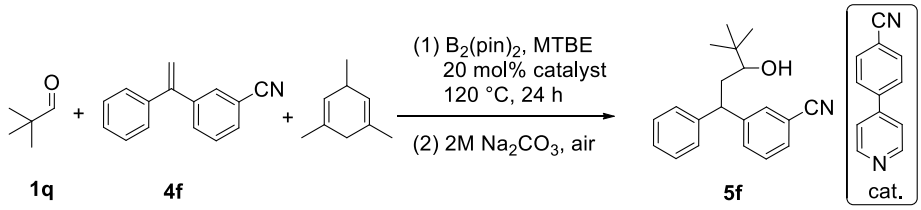
5d: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.19 (m, 4H), 7.18 – 7.12 (m, 4H), 4.25 (dd, *J* = 11.9, 3.8 Hz, 1H), 3.01 (dd, *J* = 10.7, 1.7 Hz, 1H), 2.27 – 2.17 (m, 1H), 1.90 – 1.81 (m, 1H), 1.44 (brs, 1H, OH), 0.86 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 141.9, 132.3, 132.0, 129.6, 129.0, 128.9, 128.7, 77.0, 46.6, 37.2 ,

35.0, 25.7; IR (film): 3480, 2958, 2869, 1490, 1405, 1364, 1091, 1013, 814; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{20}Cl_2O$ [M-H]$^-$ 335.0975, found 335.0937.



5e: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4e** (104.9 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5e** (50 mg, 72% yield, d. r. = 1:1.5). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

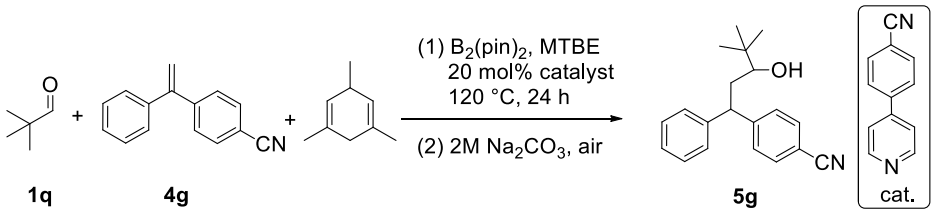
5e: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.36 (m, 4H), 7.27 – 7.00 (m, 4H), 4.38 – 4.32 (m, 1H), 3.15 – 3.02 (m, 1H), 2.41 – 2.32 (m, 4H), 2.00 – 1.85 (m, 1H), 1.62 (brs, 1H, -OH), 0.90 (d, J = 1.1 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 148.2, 144.9, 142.6, 138.44 (d, $J_{C\text{-}F}$ = 7.5 Hz), 129.4, 128.7, 128.5, 128.0, 127.5, 127.3, 125.56 (dd, $J_{C\text{-}F}$ = 15.4, 3.9 Hz), 125.2, 124.6, 77.2, 77.0, 47.8, 37.3, 37.2, 35.1, 25.7, 21.6, 21.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.28 (d, J = 4.8 Hz). IR (film): 3473, 2959, 2870, 1618, 1417, 1395, 1325, 1164, 1017, 721; HRMS (APCI-TOF) exact mass calculated for $C_{21}H_{24}O$ [M-H]$^-$ 349.1785, found 349.1785.



5f: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4f** (82.1 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg),

1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **5f** (27 mg, 46% yield, d. r. = 1:1.5). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

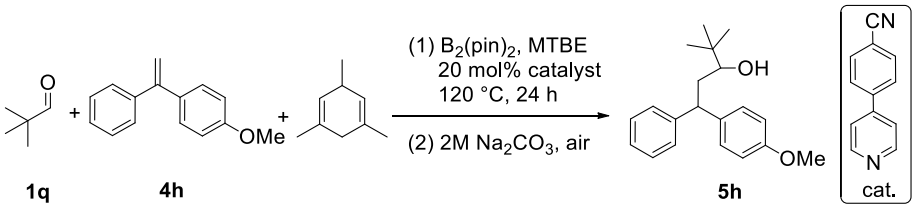
5f: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.43 (m, 3H), 7.37 – 7.31 (m, 3H), 7.27 – 7.22 (m, 3H), 4.34 (dd, *J* = 11.9, 3.7 Hz, 1H), 3.06 (dd, *J* = 10.8, 1.6 Hz, 1H), 2.35 – 2.26 (m, 1H), 1.91 – 1.83 (m, 1H), 1.60 (brs, 1H, -OH), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 142.4, 132.5, 131.3, 129.9, 129.3, 129.0, 128.4, 127.0, 119.1, 112.5, 76.9, 47.5, 37.1, 35.0, 25.7; IR (film): 3523, 2956, 2869, 2229, 1494, 1480, 1009, 719; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{23}NaNO$ $[M+Na]^+$ 316.1672, found 316.1671.



5g: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4g** (82.1 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 10:1) to afford the product **5g** (28 mg, 48% yield, d. r. = 1:1.1). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

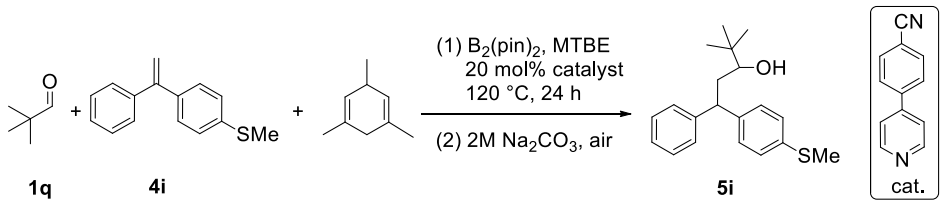
5g: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.52 (m, 2H), 7.41 – 7.20 (m, 7H), 4.41 – 4.33 (m, 1H), 3.07 and 2.98 (dd, *J* = 10.7, 1.6 Hz, 0.46 H, dd, *J* = 10.8, 1.7 Hz, 0.54 H), 2.36 – 2.27 (m, 1H), 2.00 – 2.83 (m, 1H), 1.64 (brs, 1H, -OH), 0.88

(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 149.8, 144.4, 142.3, 132.5, 132.3, 129.2, 128.9, 128.8, 128.6, 128.4, 127.7, 127.0, 126.7, 119.1, 119.0, 110.3, 109.9, 76.9, 48.0, 37.1, 37.0, 35.1, 35.0, 25.7, 25.6; IR (film): 3501, 2957, 2869, 2228, 1606, 1479, 1275, 1031, 764; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{23}NaNO$ $[M+Na]^+$ 316.1672, found 316.1672.



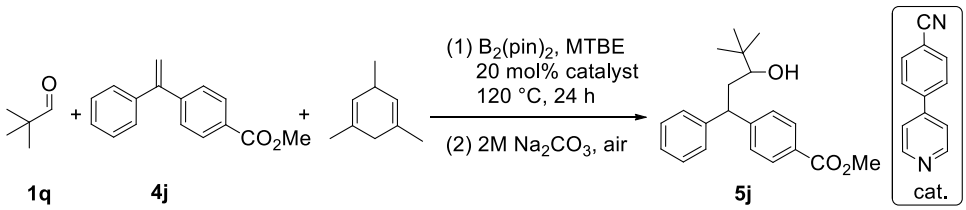
5h: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4h** (84.1 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5h** (31 mg, 52% yield, d. r. = 1:1). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

5h: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.16 (m, 7H), 6.89 – 6.81 (m, 2H), 4.29 – 4.22 (m, 1H), 3.79 and 3.77 (s, 1.55H, s, 1.45H), 3.14 – 3.07 (m, 1H), 2.38 – 2.27 (m, 1H), 1.96 – 1.87 (m, 1H), 1.62 (brs, 1H), 0.89 (d, J = 1.4 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 157.9, 146.4, 144.2, 138.2, 135.8, 129.2, 128.6, 128.5, 128.2, 127.6, 126.3, 126.0, 114.0, 113.9, 77.3, 77.2, 55.2, 47.2, 47.1, 37.7, 35.0, 25.7; IR (film): 3479, 2954, 2869, 1609, 1494, 1247, 1177, 1034, 829; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{26}NaO_2$ $[M+Na]^+$ 321.1825, found 321.1827.



5i: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4i** (90.5 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5i** (36 mg, 58% yield, d. r. = 1:1.2). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

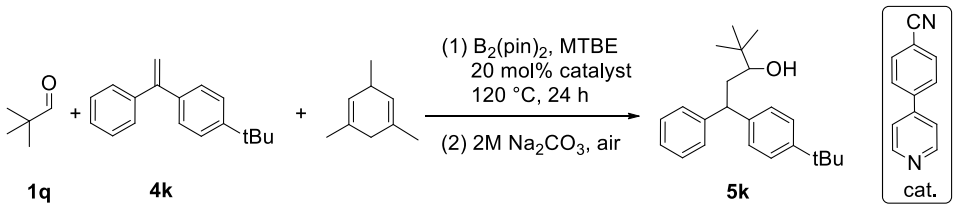
5i: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 4H), 7.22 – 7.14 (m, 5H), 4.28 – 4.22 (m, 1H), 3.11 – 3.06 (m, 1H), 2.45 and 2.42 (s, 1.66H, s, 1.34H), 2.36 – 2.27 (m, 1H), 1.95 – 1.85 (m, 1H), 1.59 (brs, 1H, -OH), 0.88 (br. s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 143.7, 143.2, 140.8, 136.0, 135.7, 128.9, 128.6, 128.5, 128.3, 128.2, 127.7, 127.2, 127.1, 126.4, 126.2, 77.2, 77.2, 47.5, 47.5, 37.5, 35.0, 25.7, 16.2, 16.0; IR (film): 3462, 3025, 2955, 2868, 1600, 1492, 1478, 1008, 762; HRMS (APCI-TOF) exact mass calculated for $C_{20}H_{25}O$ $[M-H]^-$ 313.1632, found 313.1634.



5j: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4j** (95.3 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24

h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5j** (26 mg, 40% yield, d. r. = 1:1.1). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

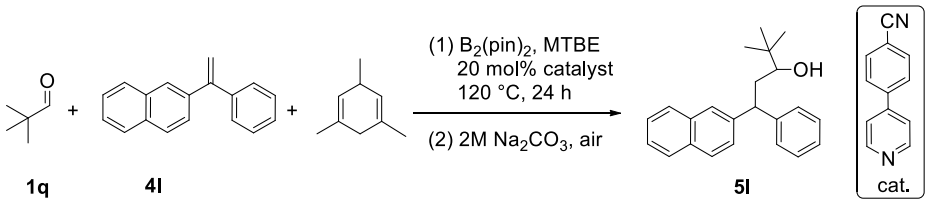
5j: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.90 (m, 2H), 7.37 – 7.17 (m, 7H), 4.38 – 4.33 (m, 1H), 3.89 and 3.88 (s, 2.16H, s, 0.85H), 3.10 – 2.99 (m, 1H), 2.39 – 2.29 (m, 1H), 1.99 – 1.86 (m, 1H), 1.61 (brs, 1H, -OH), 0.87 (d, *J* = 3.5 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 151.5, 149.4, 145.1, 143.0, 130.0, 129.9, 128.8, 128.7, 128.5, 128.4, 128.4, 127.8, 127.7, 126.7, 126.5, 77.2, 52.1, 52.1, 48.0, 37.3, 37.2, 35.1, 25.7, 25.7; IR (film): 3565, 2953, 1722, 1609, 1435, 1278, 1111, 1019, 756; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{26}NaO_3$ $[M+Na]^+$ 349.1774, found 349.1775.



5k: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4k** (94.5 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5k** (26 mg, 40% yield, d. r. = 1:0.8). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

5k: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.19 (m, 9H), 4.35 – 4.28 (m, 1H), 3.21 and 3.16 (dd, *J* = 10.5, 1.6 Hz, 0.55H, dd, *J* = 10.6, 1.6 Hz, 0.44H), 2.47 – 2.37 (m, 1H), 2.04 – 1.92 (m, 1H), 1.67 (brs, 1H), 1.36 (d, *J* = 6.4 Hz, 9H), 0.94 (d, *J* = 4.4 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 148.8, 146.4, 144.0, 142.9,

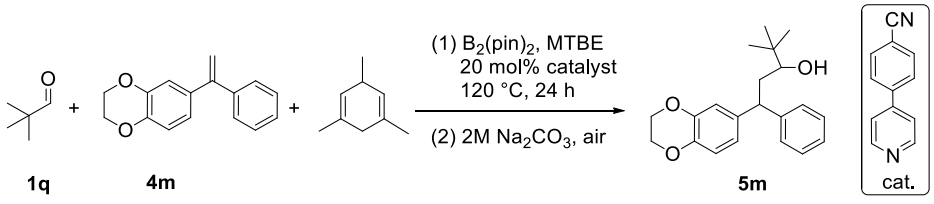
140.6, 128.6, 128.5, 128.4, 127.8, 127.8, 127.8, 126.3, 126.0, 125.5, 125.4, 77.4, 77.3, 47.8, 47.7, 37.8, 34.1, 35.1, 35.0, 34.4, 34.4, 31.5, 31.5, 25.8, 25.7; IR (film): 3447, 2960, 2904, 1477, 1363, 1286, 1030, 700; HRMS (ESI-TOF) exact mass calculated for $C_{23}H_{36}NO$ $[M+NH_4]^+$ 342.2791, found 342.2786.



1q 4l 5l

5l: Prepared following *general procedure* using **1q** (21.7μL, 0.2 mmol, 1.0 equiv), **4l** (92.1 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5l** (48 mg, 76% yield, d. r. = 1:1.1). The diastereoselectivities (d. r.) was determined by GC-MS analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

5l: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.71 (m, 4H), 7.47 – 7.15 (m, 8H), 4.53 – 4.43 (m, 1H), 3.20 – 3.10 (m, 1H), 2.54 – 2.41 (m, 1H), 2.09 – 2.96 (dm, 1H), 1.58 (brs, 1H), 0.90 (dd, *J* = 8.8, 3.3 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 143.7, 143.5, 141.3, 133.6, 132.3, 132.1, 128.7, 128.6, 128.5, 128.4, 128.1, 127.8, 127.8, 127.7, 127.6, 126.9, 126.8, 126.8, 126.4, 126.2, 126.1, 126.0, 125.5, 125.4, 125.4, 77.3, 77.2, 48.1, 48.0, 37.3, 37.3 , 35.1, 25.7; HRMS (ESI-TOF) exact mass calculated for $C_{23}H_{26}NaO$ $[M+Na]^+$ 341.1876, found 341.1876.

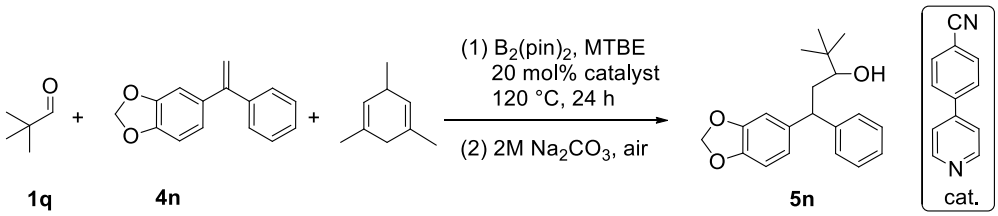


1q 4m 5m

5m: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4m** (92.1 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv),

4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5m** (44 mg, 68% yield, d. r. = 1:1.2). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

5m: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 4H), 7.21 – 7.12 (m, 1H), 6.80 – 6.72 (m, 3H), 4.26 – 4.13 (m, 5H), 3.14 and 3.06 (dd, *J* = 10.6, 1.6 Hz, 0.55H, dd, *J* = 10.6, 1.6 Hz, 0.45H), 2.32 – 2.22 (m, 1H), 1.91 – 1.81 (m, 1H), 1.39 (brs, 1H, with -OH), 0.88 (d, *J* = 7.1 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 143.9, 143.4, 143.2, 139.4, 137.1, 128.5, 128.4, 128.1, 127.5, 126.2, 126.0, 121.1, 120.6, 117.2, 117.1, 116.8, 116.2, 121.1, 120.6, 77.2, 64.4, 64.3, 64.2, 47.3, 37.5, 37.5, 34.9, 34.9, 25.6, 25.6; IR (film): 3501, 2955, 2871, 1732, 1589, 1505, 1284, 1036, 763; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{25}O$ $[M-H]^-$ 325.1809, found 325.1806.

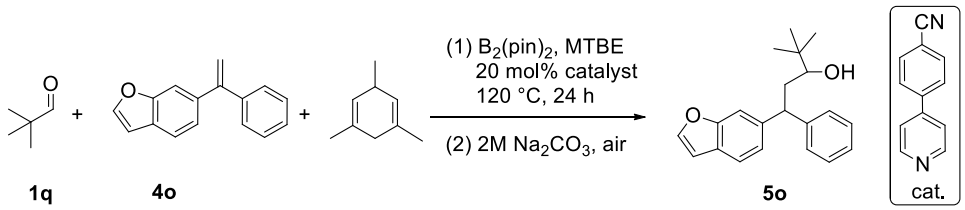


1q 4n 5n

5n: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4n** (89.7 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5n** (42 mg, 68% yield, d. r. =1: 1.1). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

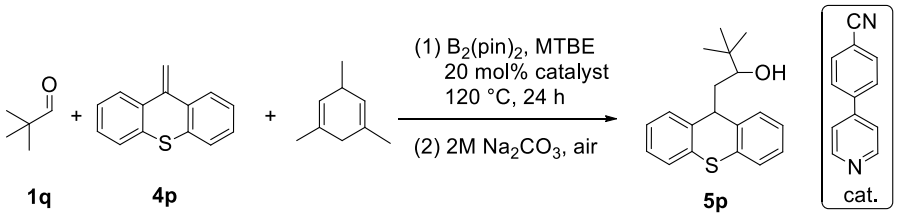
5n: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.15 (m, 5H), 6.76 – 6.67 (m, 3H), 5.91 and 5.90 (d, *J* = 1.5 Hz, 0.51H, d, *J* = 1.4 Hz, 0.49H), 5.88 (s, 1H), 4.23

– 4.16 (m, 1H), 3.13 – 3.04 (m, 1H), 2.33 – 2.21 (m, 1H), 1.91 – 1.83 (m, 1H), 1.44 (brs, 1H, with -OH), 0.87 (d, *J* = 4.6 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 147.6, 146.0, 145.7, 143.8, 140.0, 137.7, 128.6, 128.5, 128.1, 127.5, 126.3, 126.1, 121.2, 120.3, 108.4, 108.2, 108.1, 100.8, 77.2, 77.1, 47.7, 47.5, 37.5, 37.4, 34.9, 25.6, 25.6; HRMS (ESI-TOF) exact mass calculated for $C_{20}H_{24}NaO_3$ $[M+Na]^+$ 335.1618, found 335.1625.



5o: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4o** (89.7 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5o** (21 mg, 34% yield, d. r. = 1:1.2). The diastereoselectivities (d. r.) was determined by ^{1}H NMR analysis of the crude mixture. The two diastereomers were not separated by preparative TLC. Reported as a mixture of diastereomers.

5o: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.49 (m, 2H), 7.46 – 7.39 (m, 1H), 7.35 – 7.19 (m, 6H), 6.73 and 6.71 (dd, *J* = 2.2, 0.9 Hz, 0.45H, dd, *J* = 2.2, 1.0 Hz, 0.55H), 4.44 – 4.37 (m, 1H), 3.18 – 3.08 (m, 1H), 2.46 – 2.35 (m, 1H), 2.03 – 1.94 (m, 1H), 1.56 (brs, 1H, with -OH), 0.90 (d, *J* = 5.5 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 153.7, 146.4, 145.3, 145.3, 144.3, 140.8, 138.5, 128.7, 128.5, 128.3, 127.7, 127.6, 126.3, 126.1, 124.8, 124.5, 120.7, 119.7, 111.4, 111.3, 106.7, 106.7, 77.3, 48.0, 47.9, 38.1, 37.9, 35.1, 35.0, 25.8; IR (film): 3565, 3461, 2956, 2867, 1503, 1439, 1245, 1040, 700; IR (film): 3561, 3481, 2955, 2868, 1466, 1261, 1125, 1031, 738; HRMS (ESI-TOF) exact mass calculated for $C_{21}H_{24}NaO_2$ $[M+Na]^+$ 331.1669, found 331.1671.

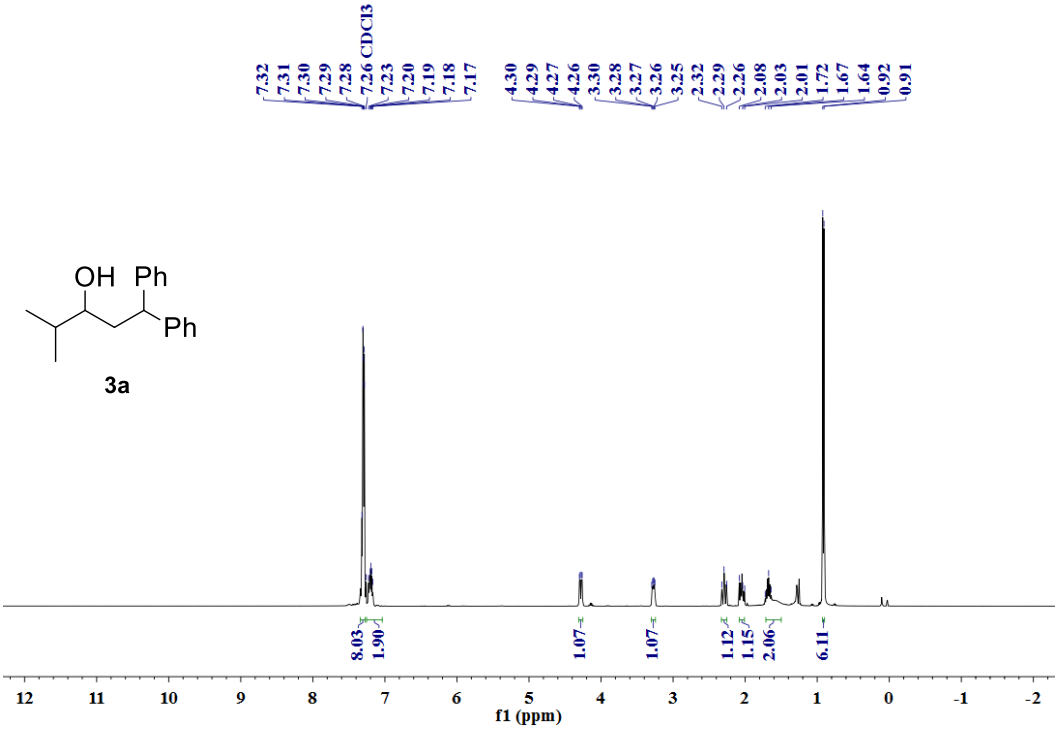


5p: Prepared following *general procedure* using **1q** (21.7 μL, 0.2 mmol, 1.0 equiv), **4p** (84 mg, 0.4 mmol, 2.0 equiv), $B_2(pin)_2$ (50.8 mg), 1,3,5-trimethyl-1,4-cyclohexadiene (24.5 mg, 0.2 mmol, 1.0 equiv), 4-(4-pyridinyl)benzonitrile (7.2 mg, 20 mol%) and MTBE (1 mL) at 120 °C. After 24 h, following the described step, the reaction mixture was isolated with prepared TLC on silica (PE/EA = 50:1) to afford the product **5p** (15 mg, 25% yield).

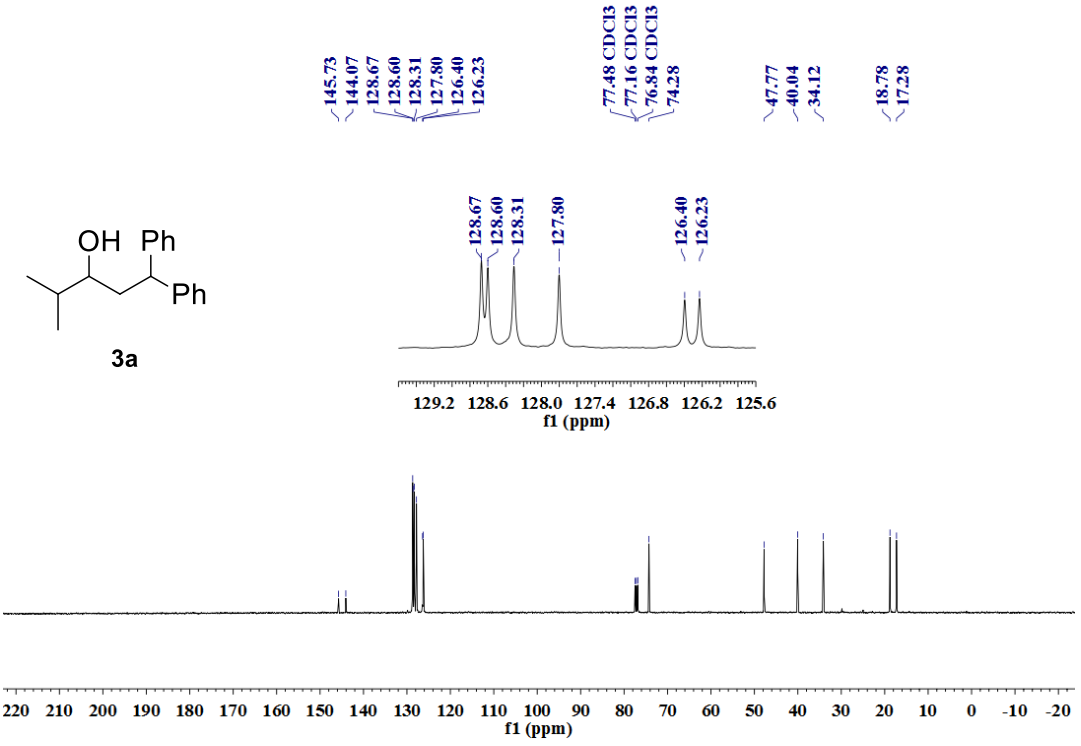
5p: Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 4H), 7.26 – 7.16 (m, 4H), 4.36 (dd, *J* = 11.4, 4.4 Hz, 1H), 2.92 (dd, *J* = 10.8, 1.7 Hz, 1H), 2.30 – 2.20 (m, 1H), 1.62 (brs, 1H, with -OH), 1.39 – 1.33 (m, 1H), 0.74 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.1, 132.7, 132.4, 129.8, 128.4, 127.2, 127.1, 126.9, 126.6, 126.5, 126.3, 77.03, 46.2, 34.9, 33.5, 25.6; IR (film):3566, 3481, 2956, 1464, 1441, 1276, 1063, 1007, 752; HRMS (ESI-TOF) exact mass calculated for $C_{19}H_{22}NaOS$ $[M+Na]^+$ 321.1284, found 321.1283.

5. NMR Spectra

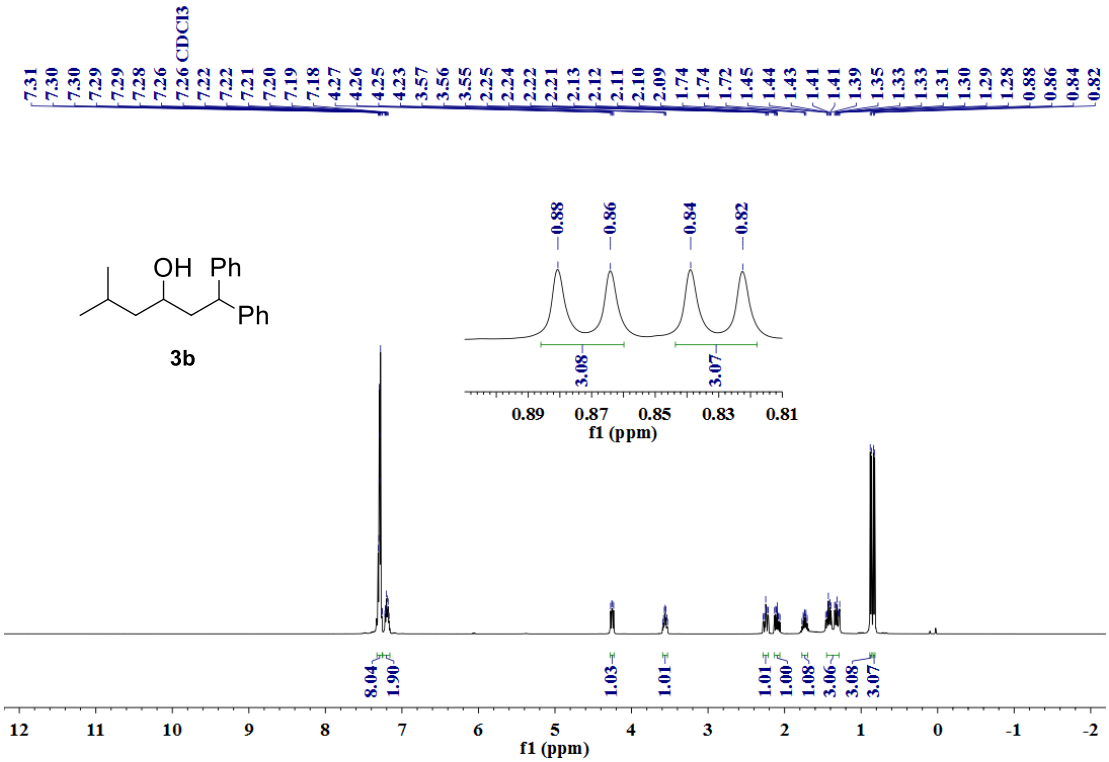
^{1}H NMR (400 MHz, $CDCl_3$):



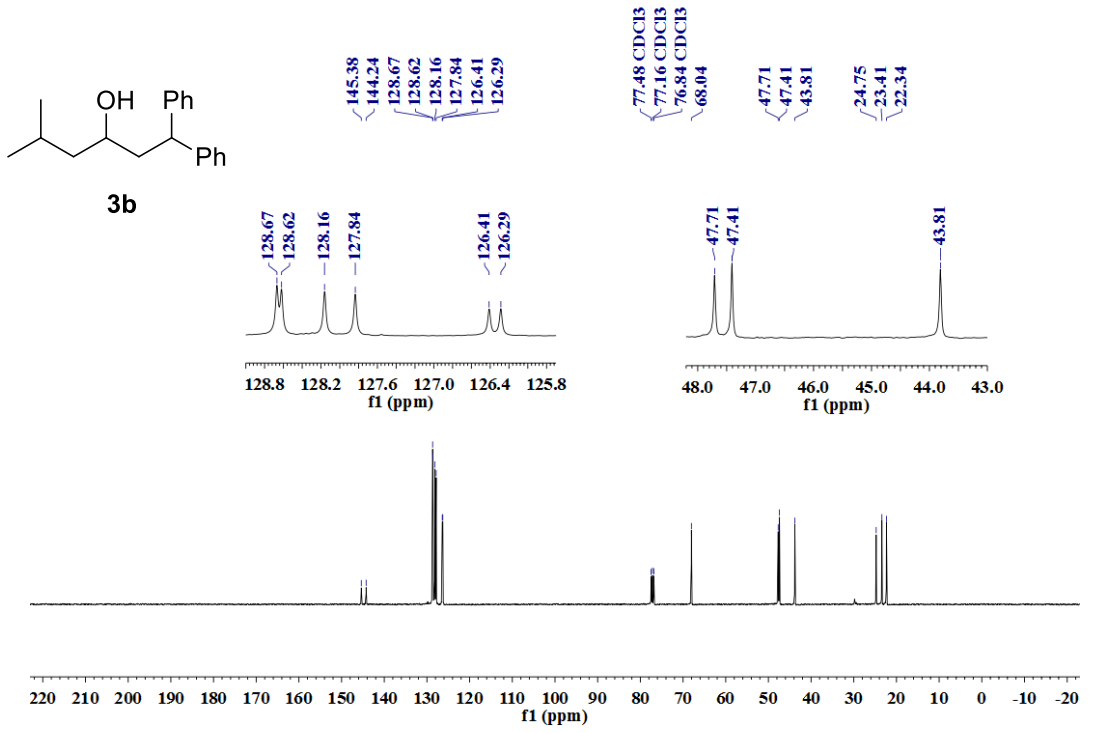
^{13}C NMR (100 MHz, $CDCl_3$):



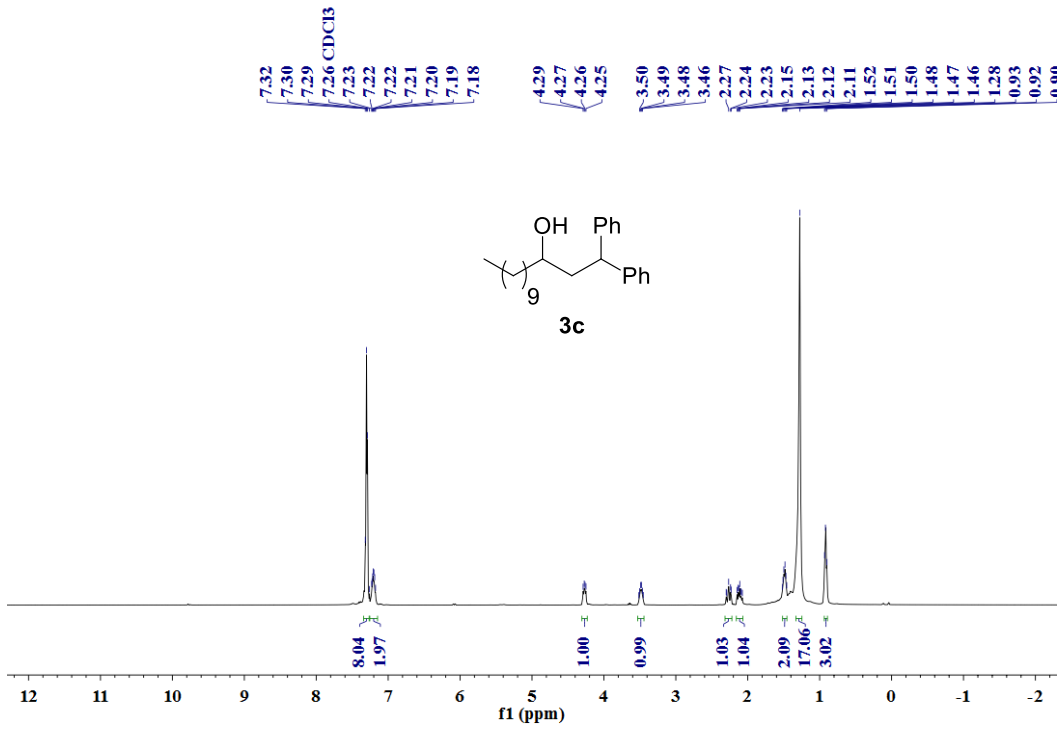
^{1}H NMR (400 MHz, $CDCl_3$):



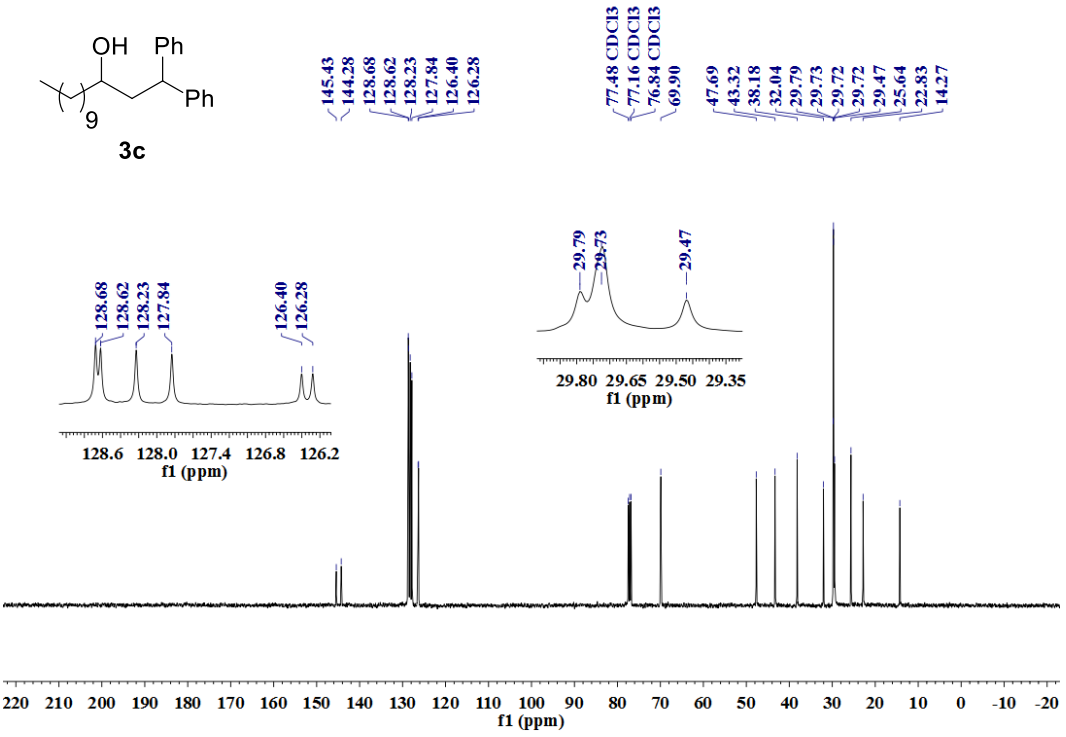
^{13}C NMR (100 MHz, $CDCl_3$):



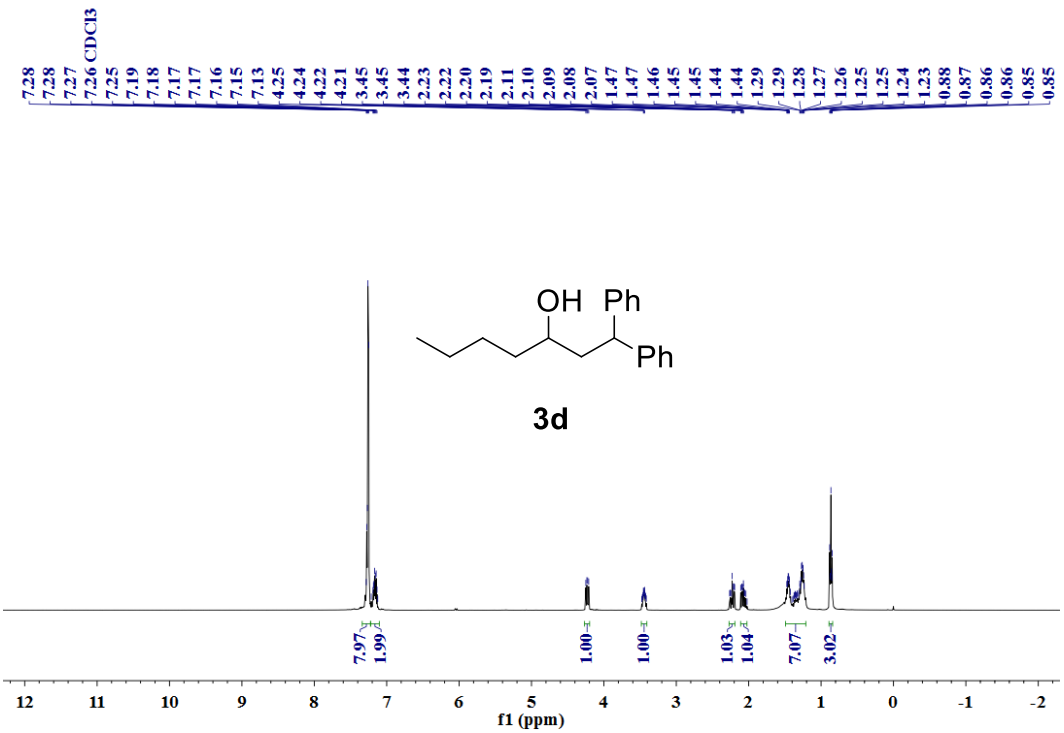
^{1}H NMR (400 MHz, $CDCl_3$):



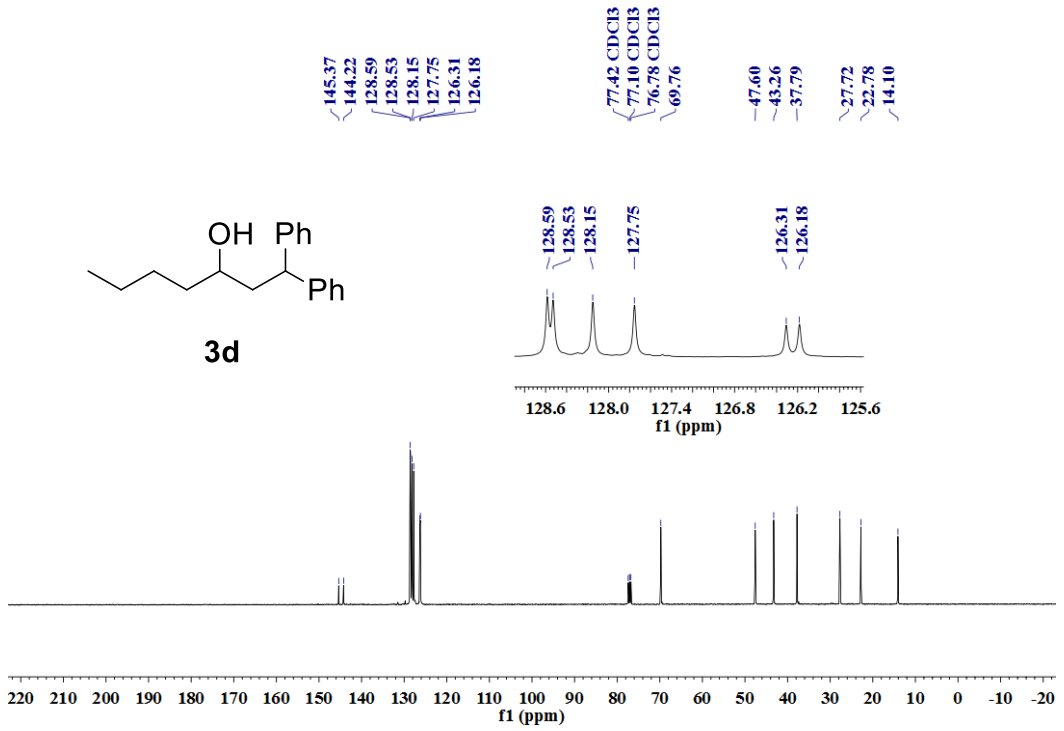
^{13}C NMR (100 MHz, $CDCl_3$):



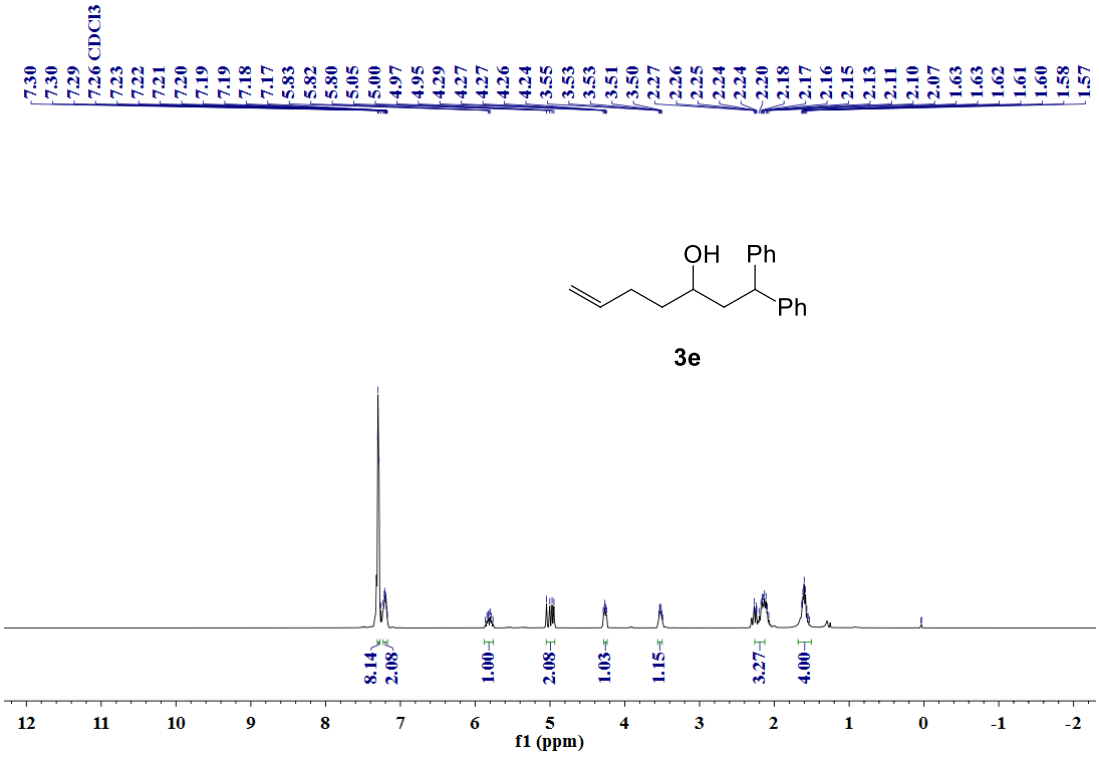
^{1}H NMR (400 MHz, $CDCl_3$):



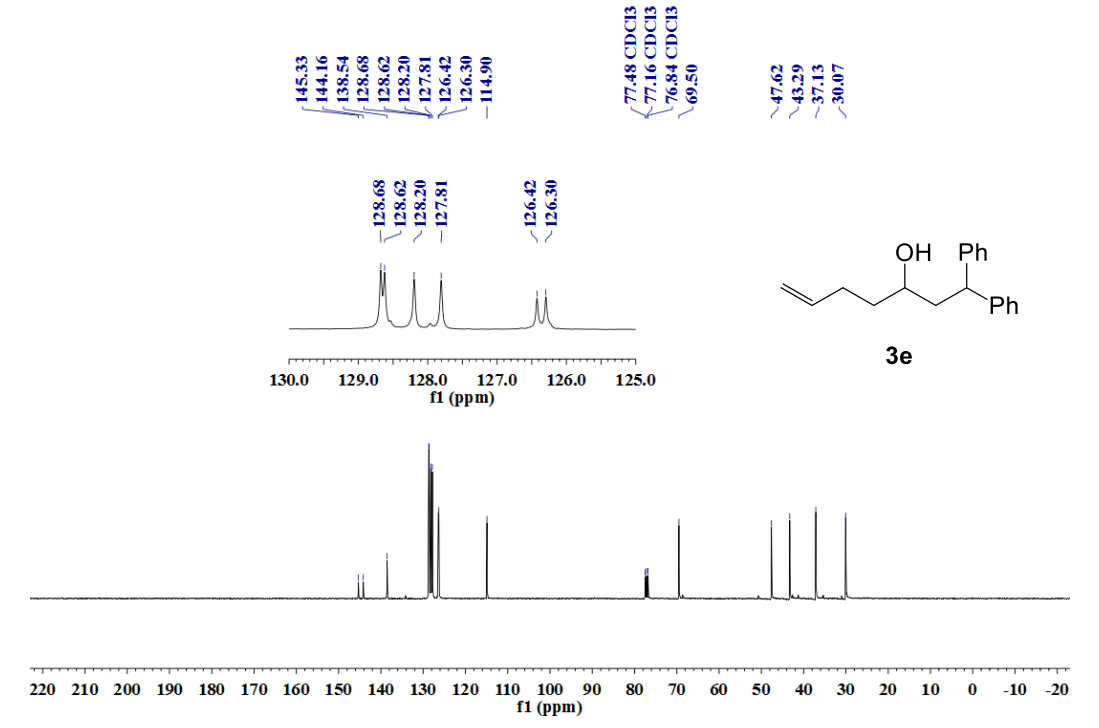
^{13}C NMR (100 MHz, $CDCl_3$):



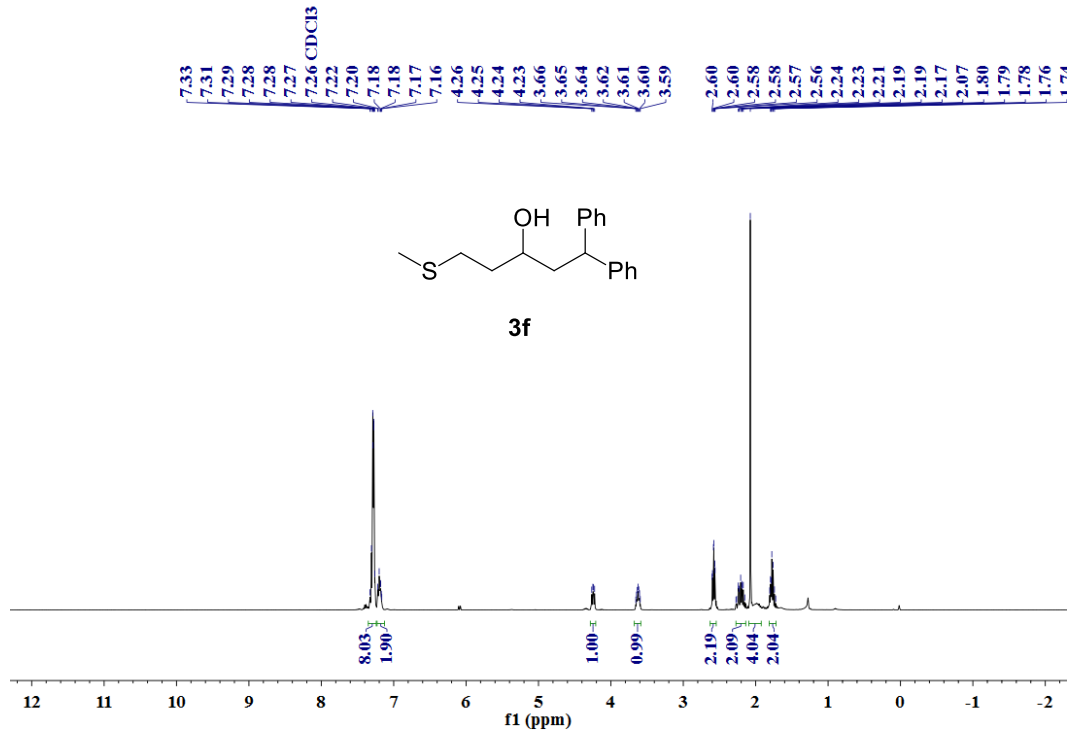
^{1}H NMR (400 MHz, $CDCl_3$):



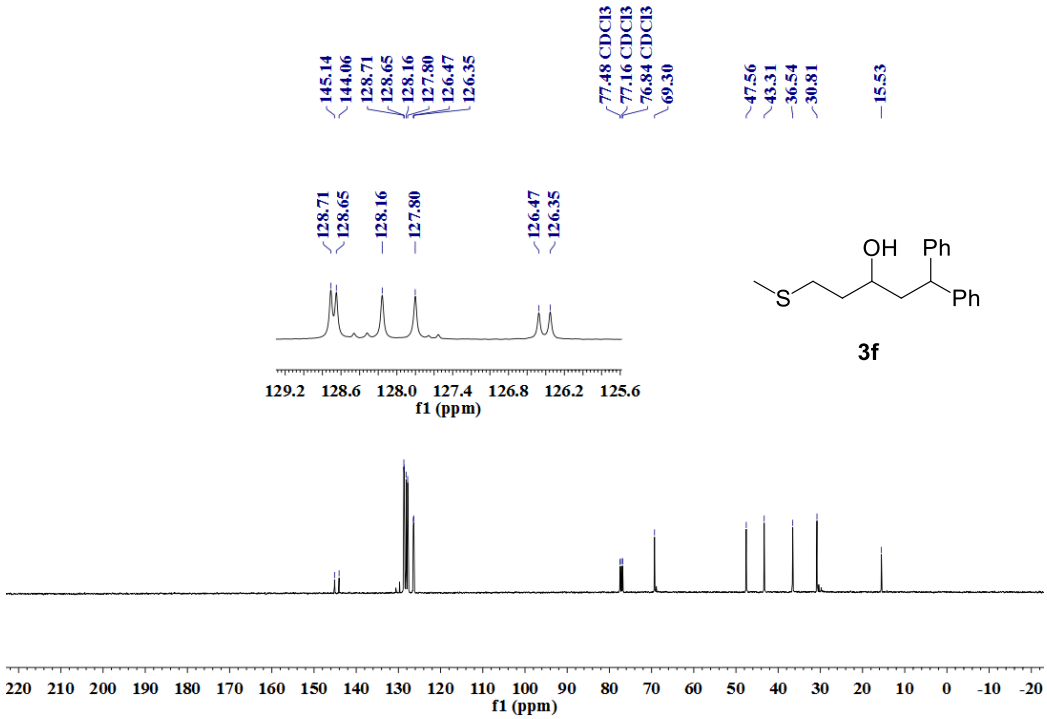
^{13}C NMR (100 MHz, $CDCl_3$):



^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (100 MHz, $CDCl_3$):



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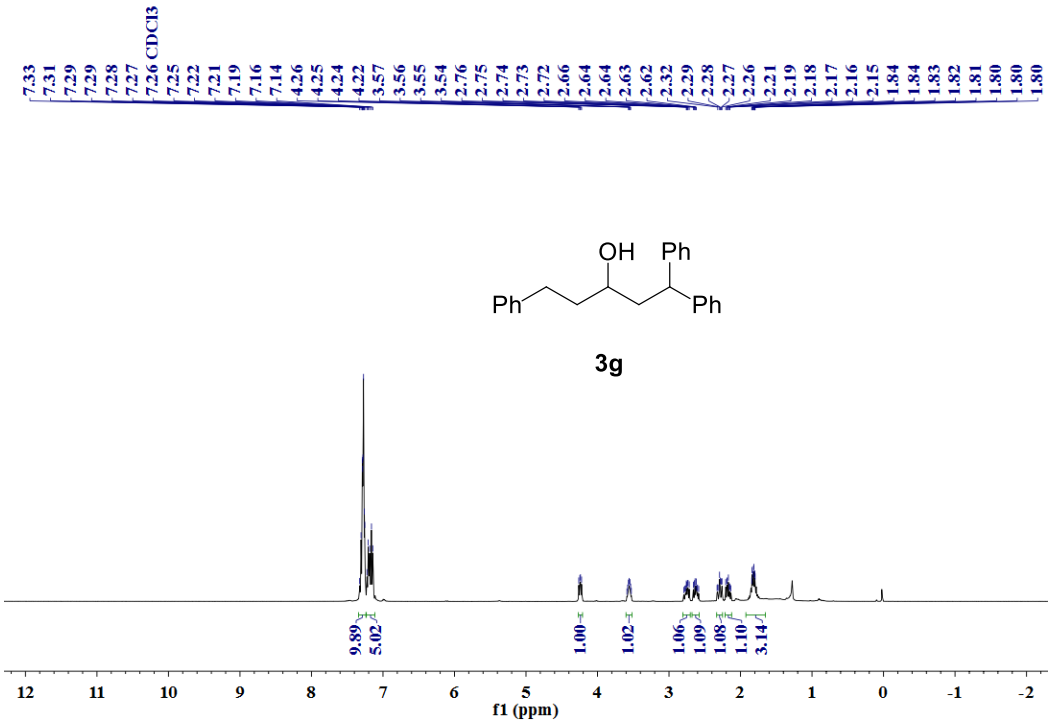

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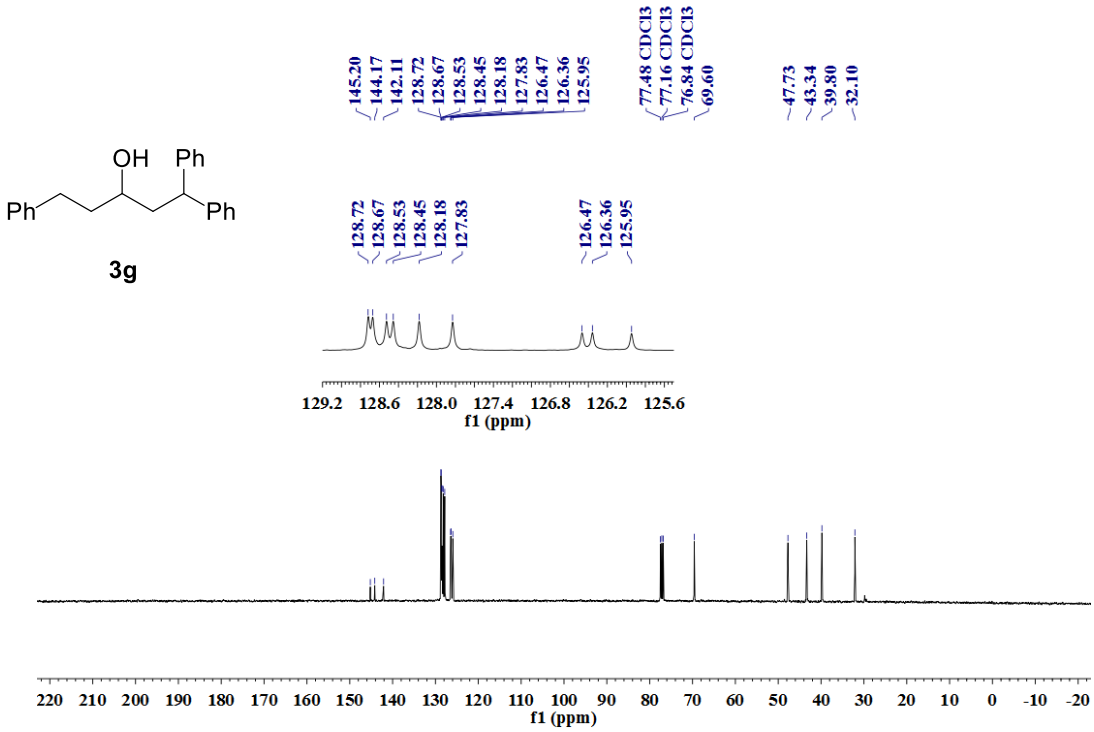

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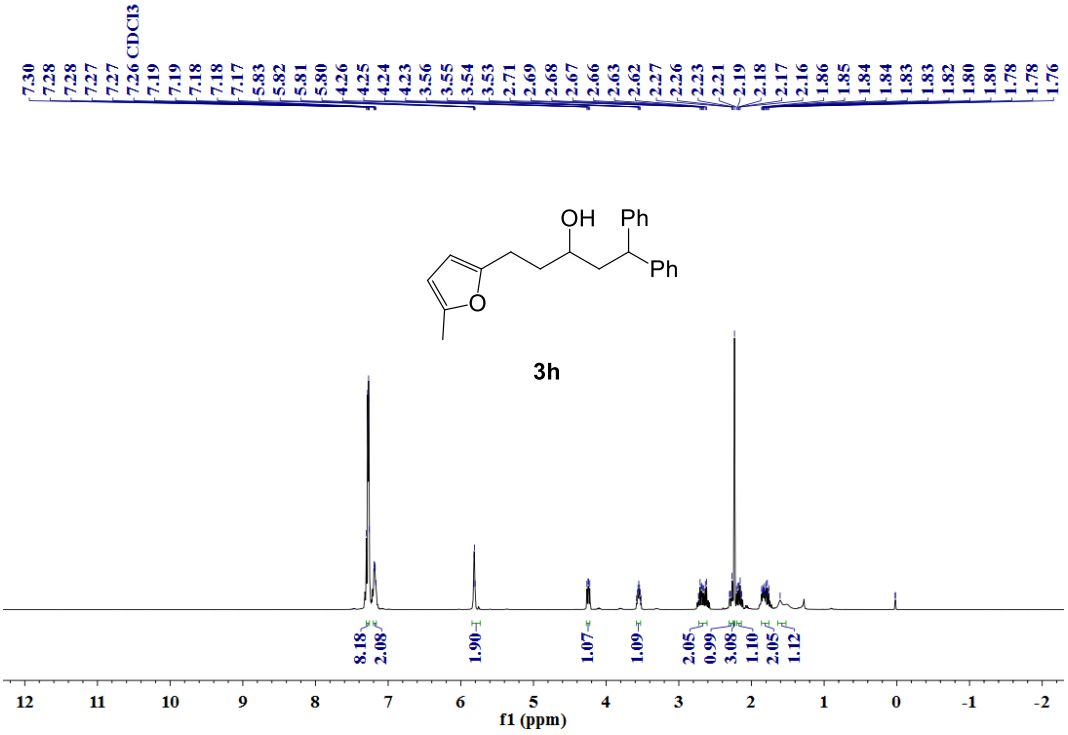
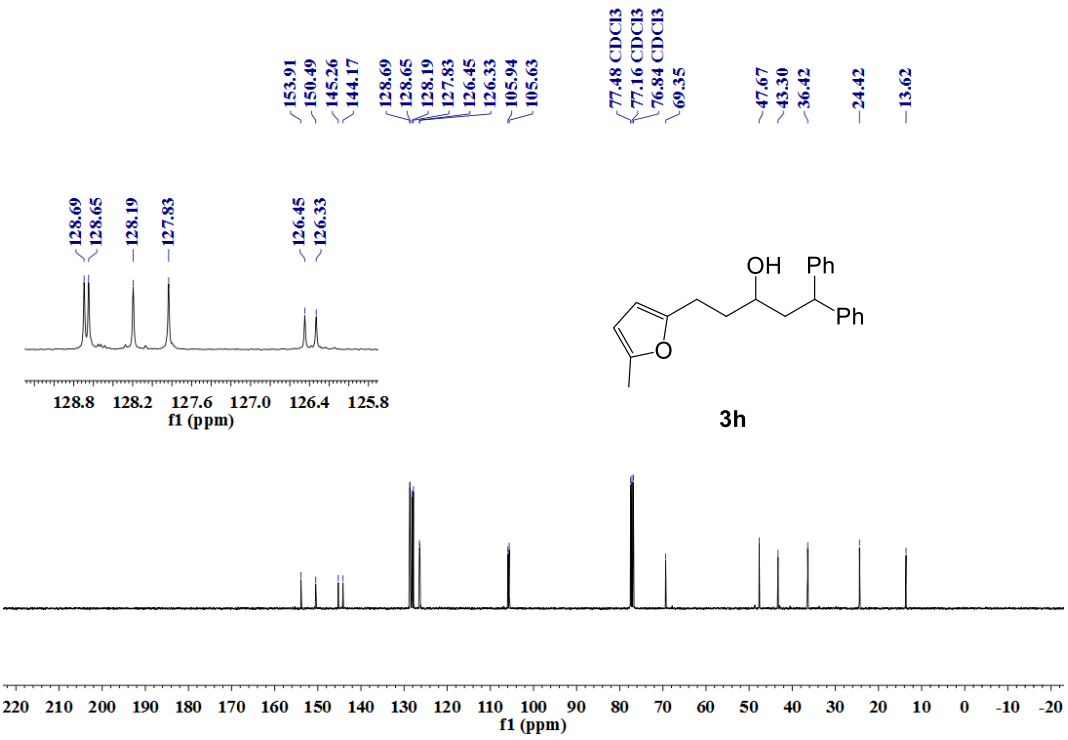


^{13}C NMR (100 MHz, $CDCl_3$):



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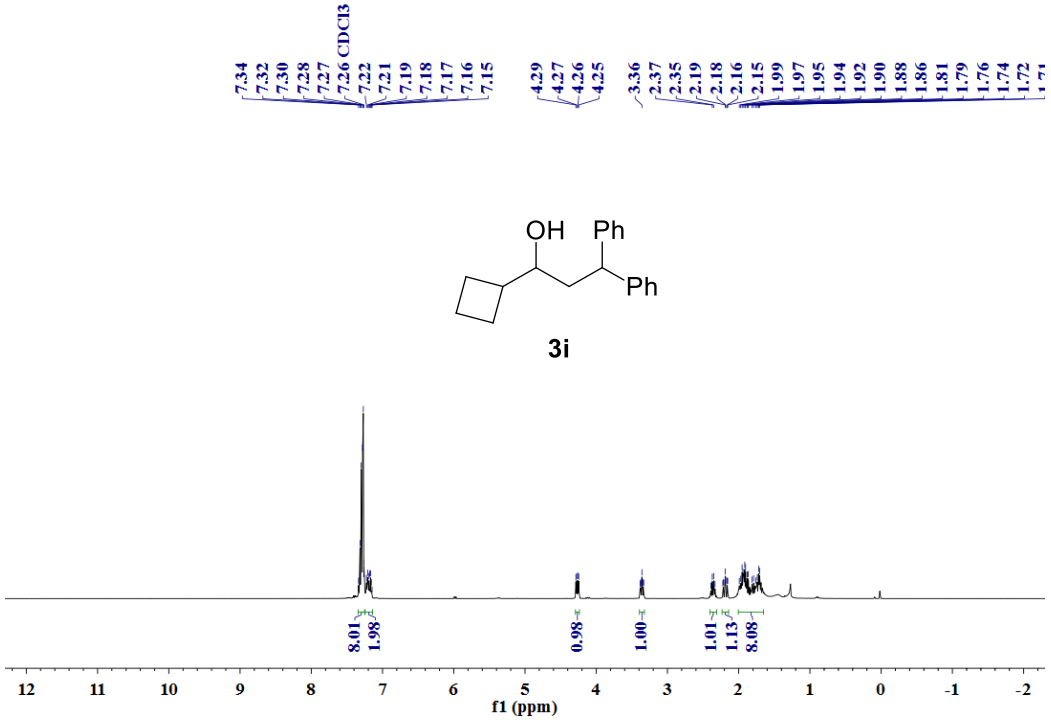

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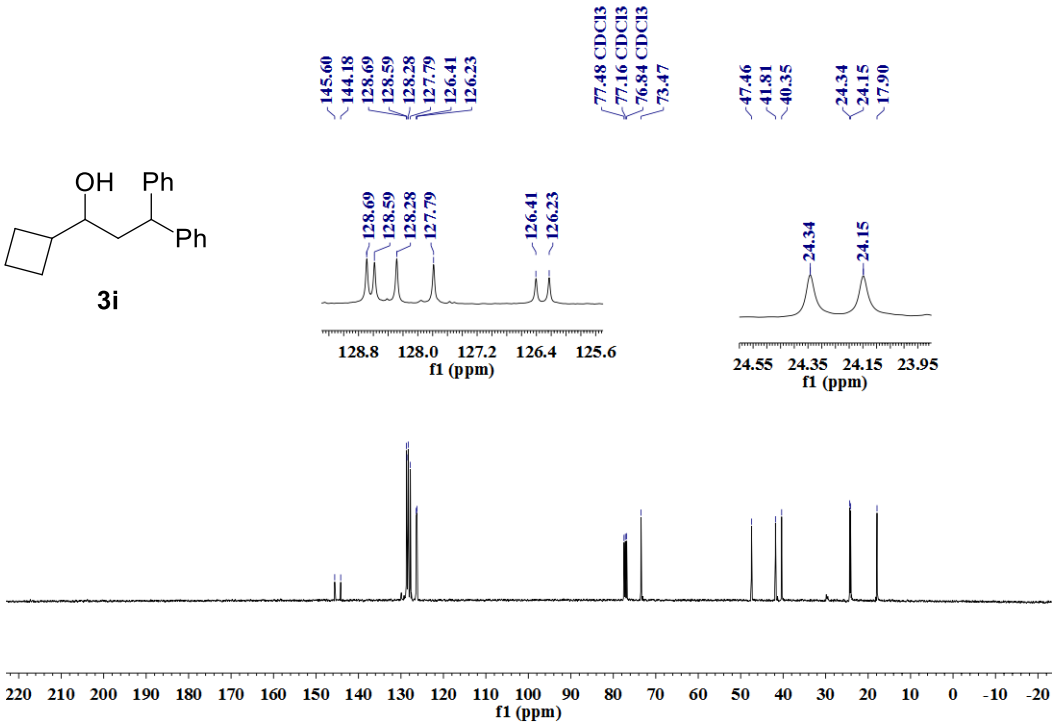

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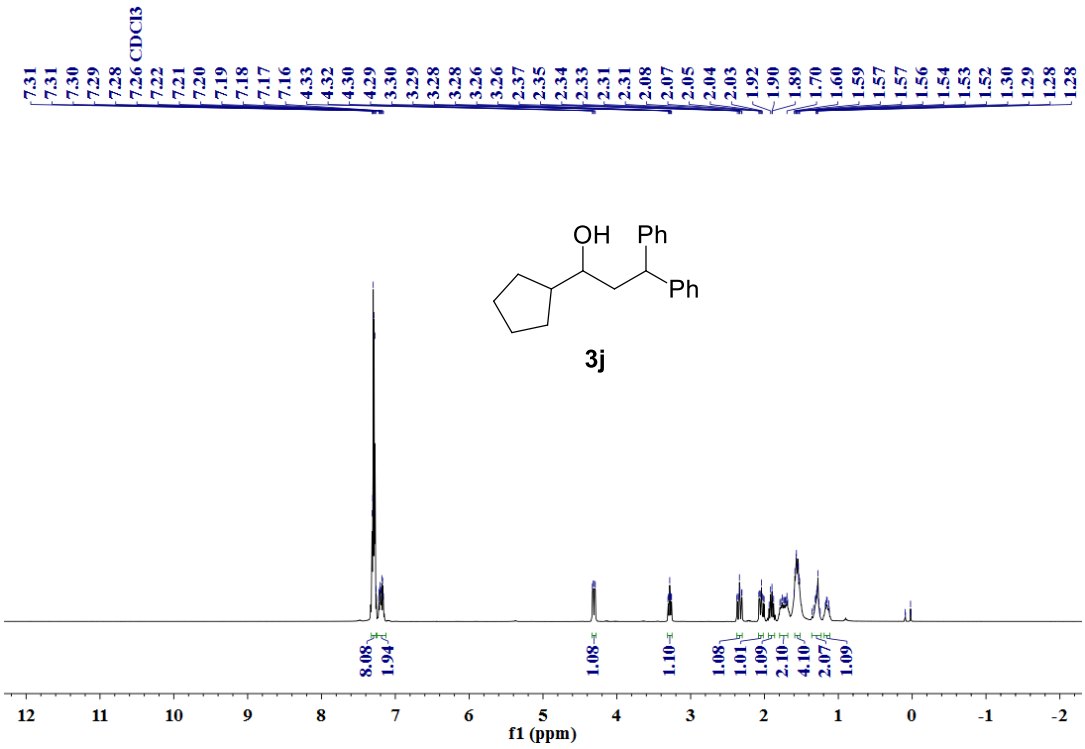

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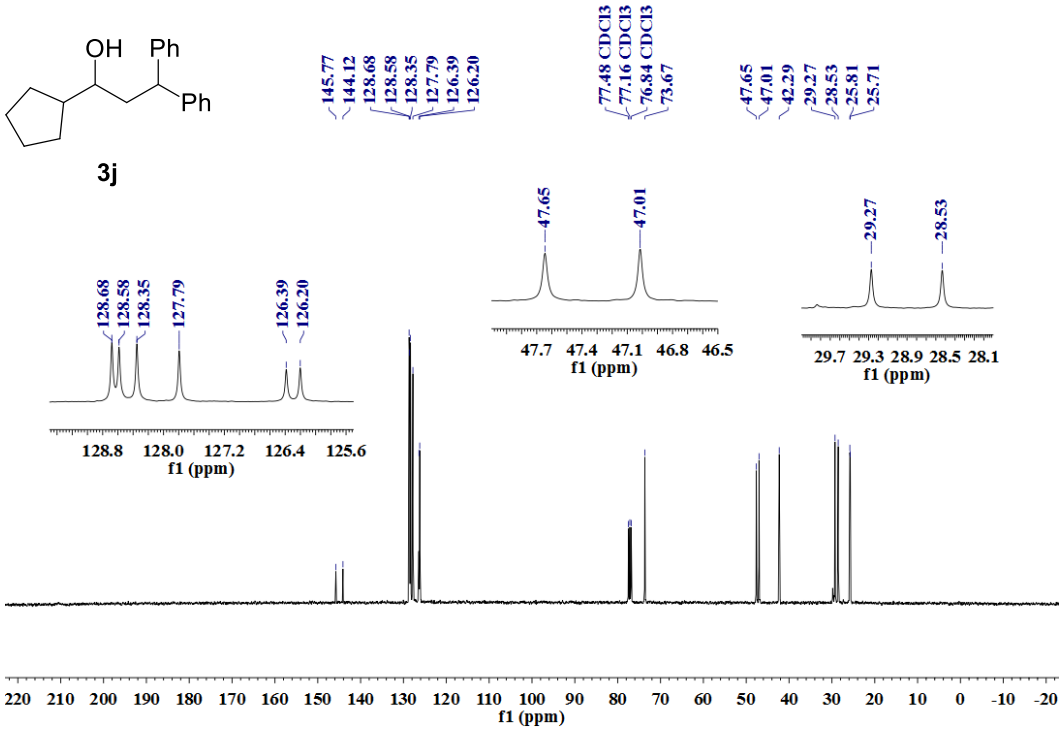

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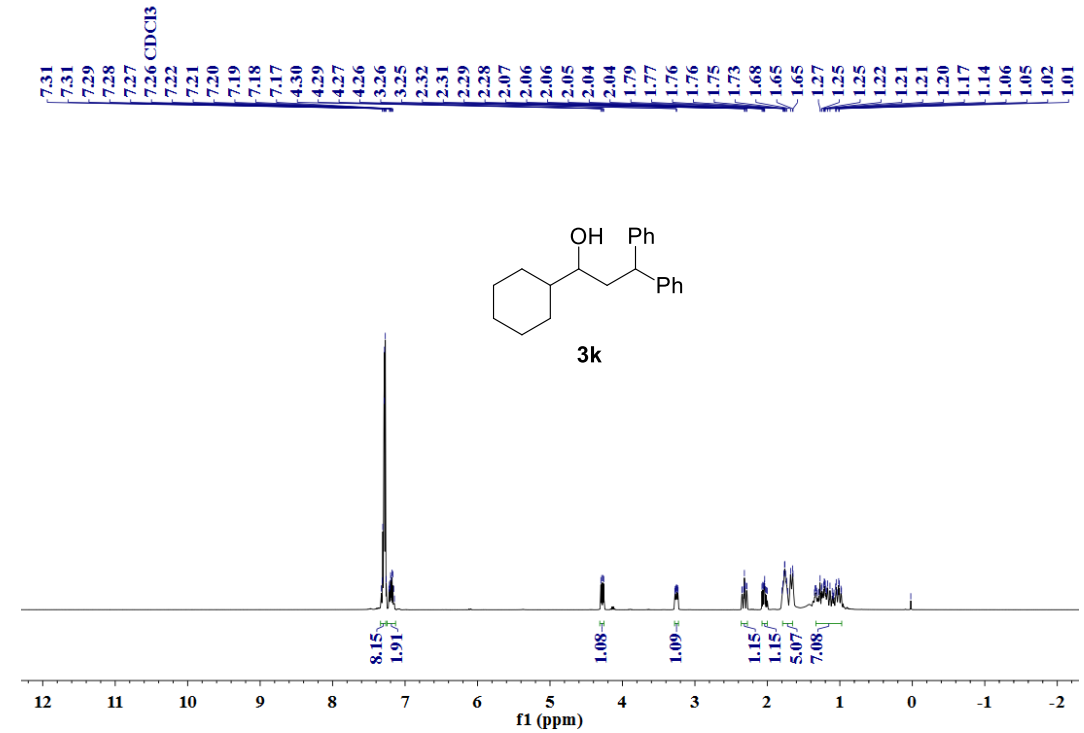

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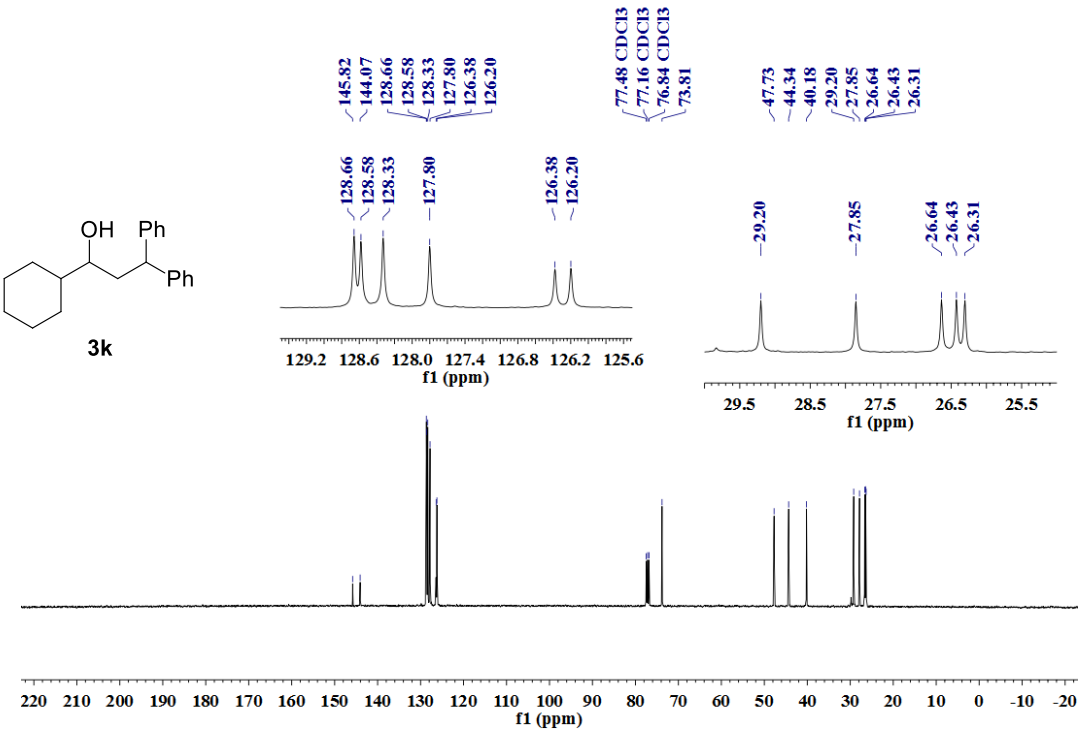

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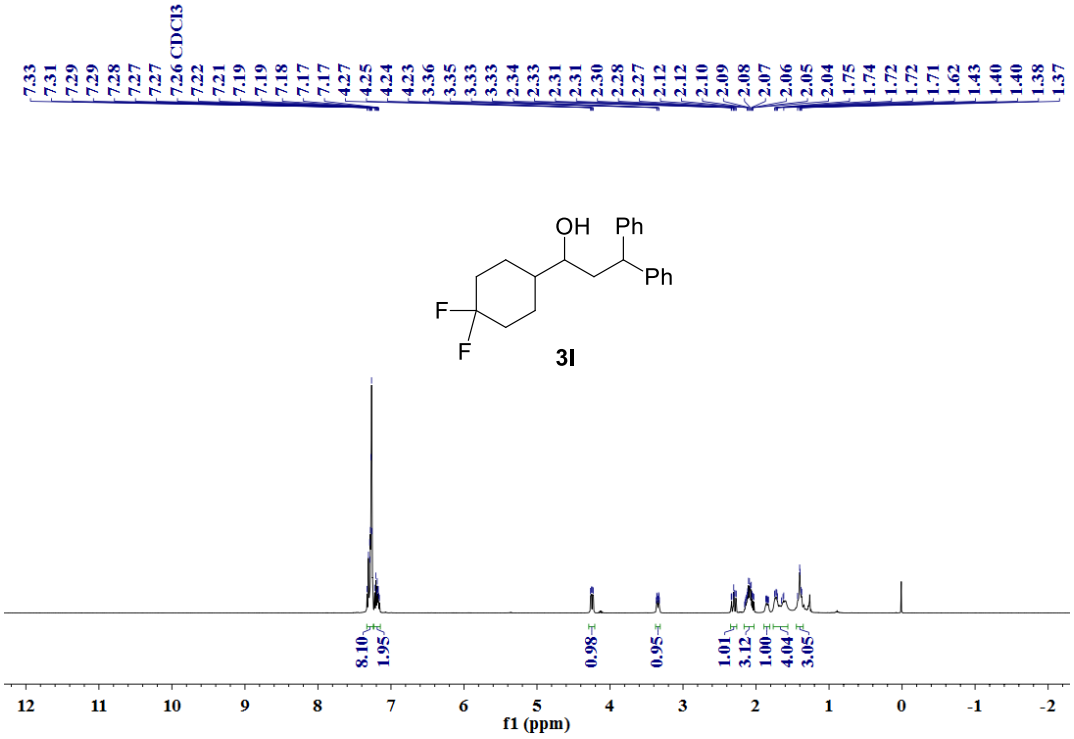

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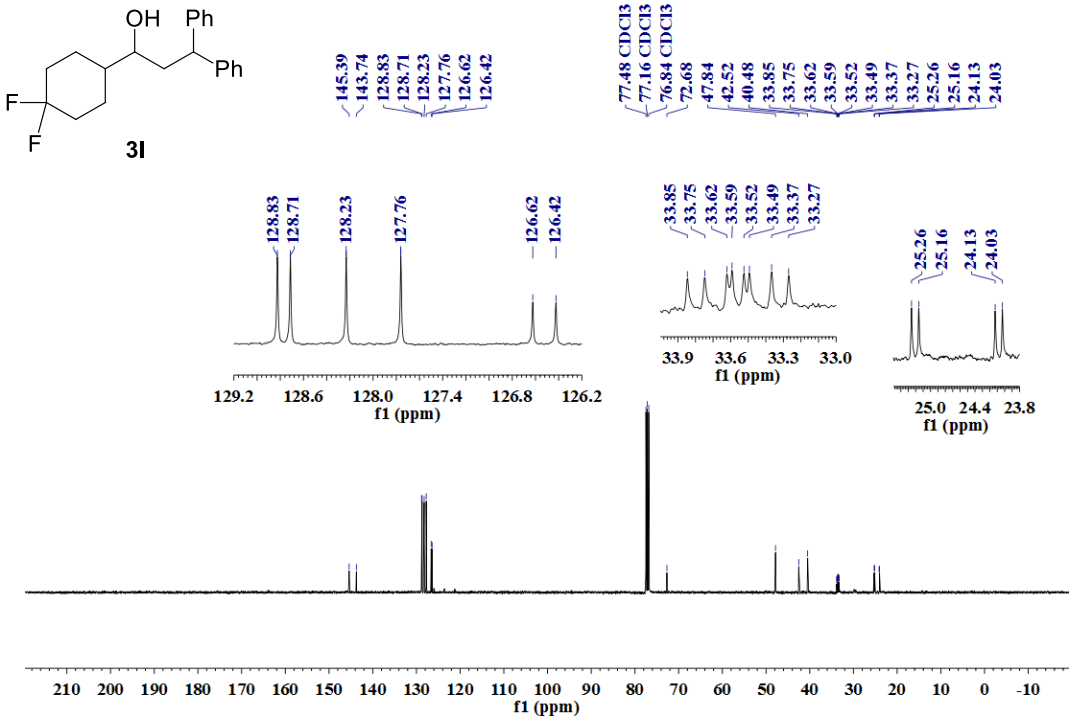
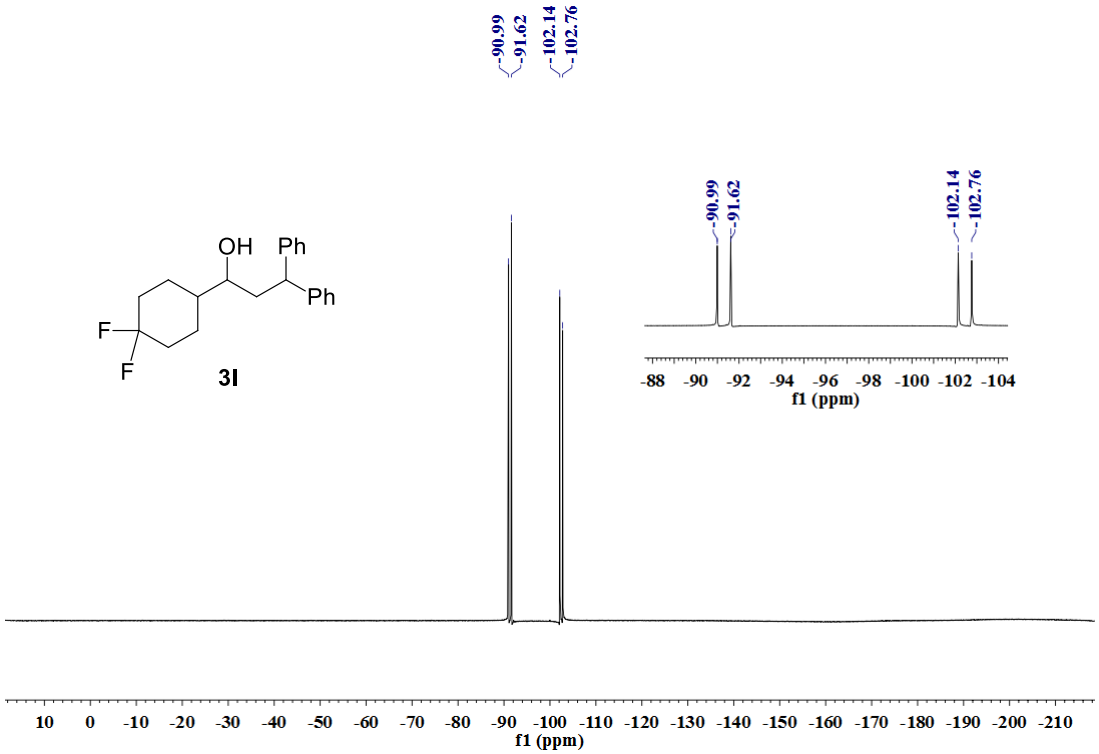


^{19}F NMR (376 MHz, $CDCl_3$):



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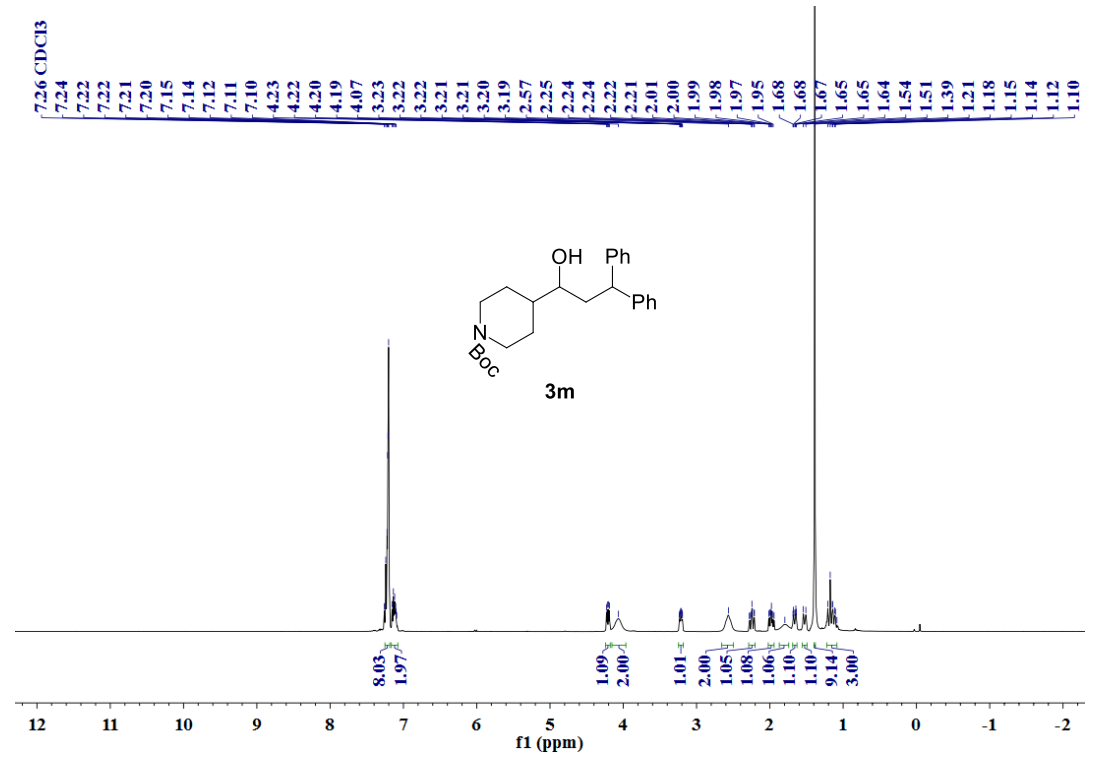

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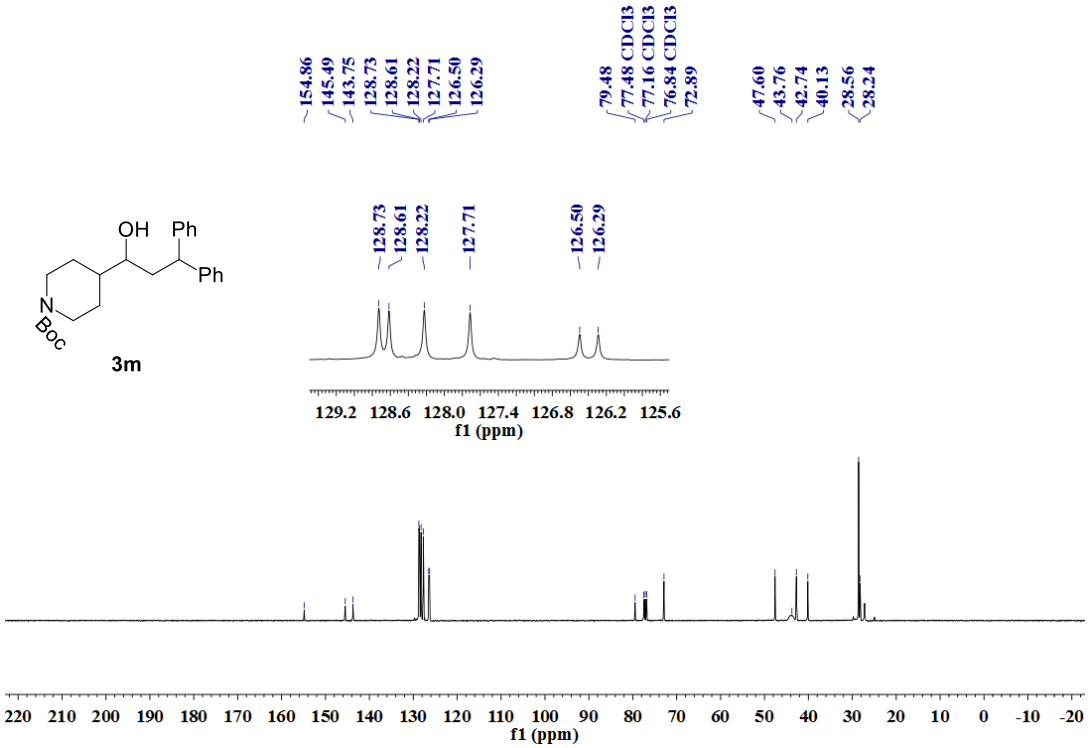

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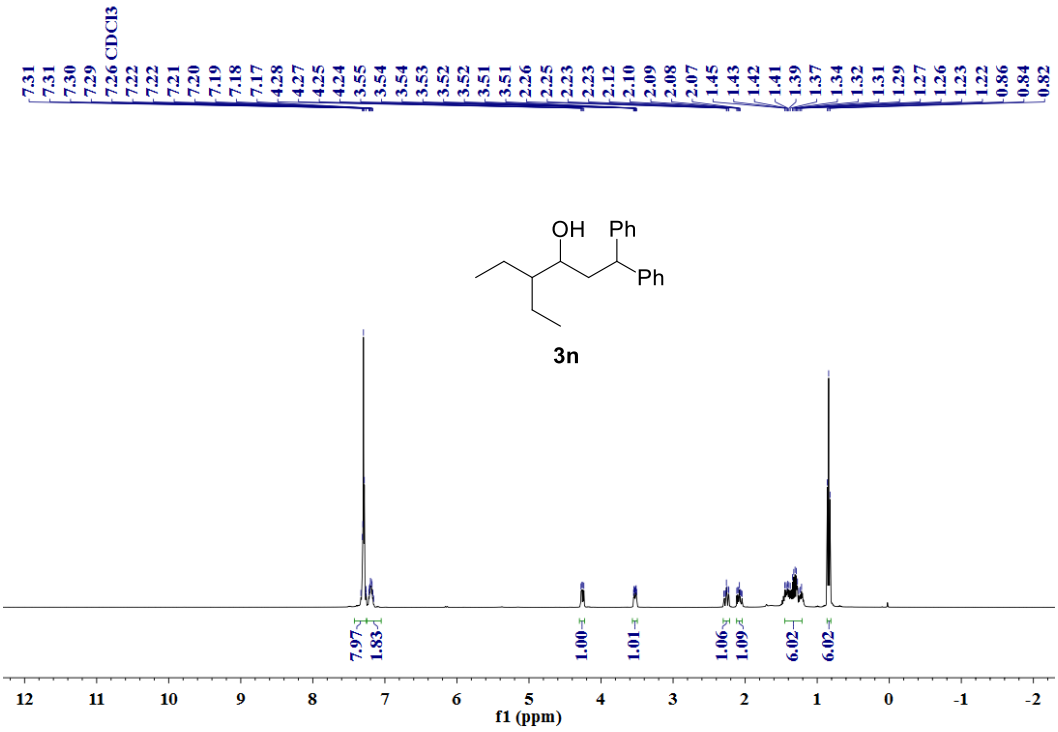

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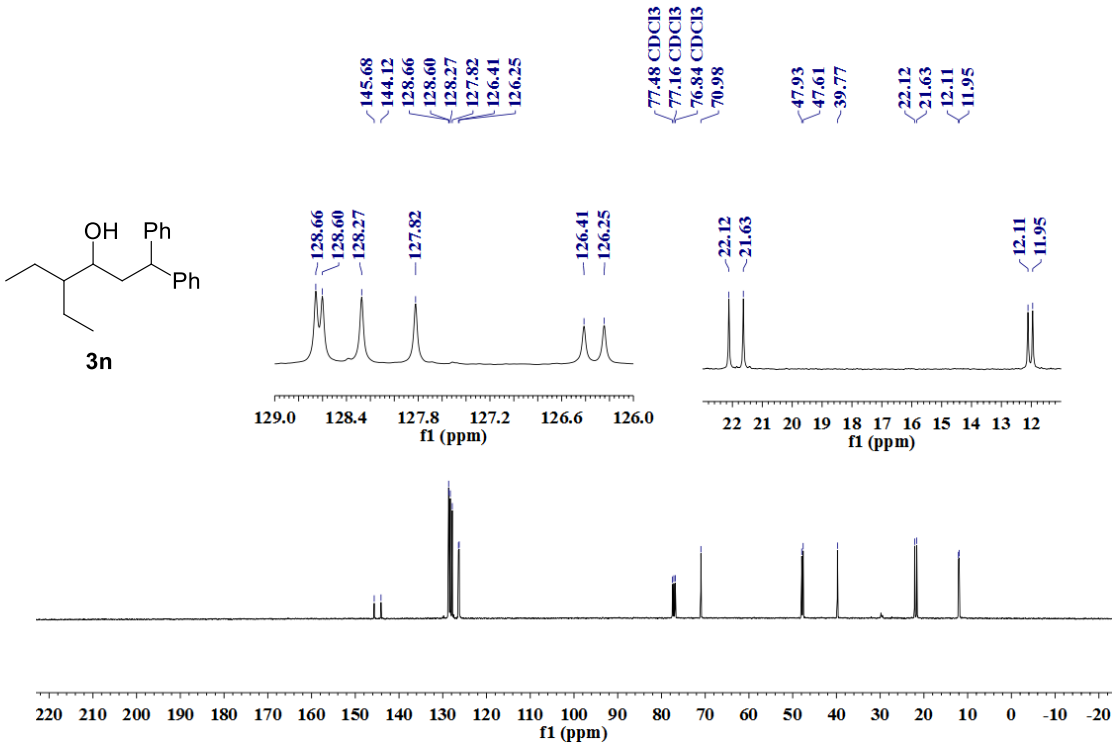

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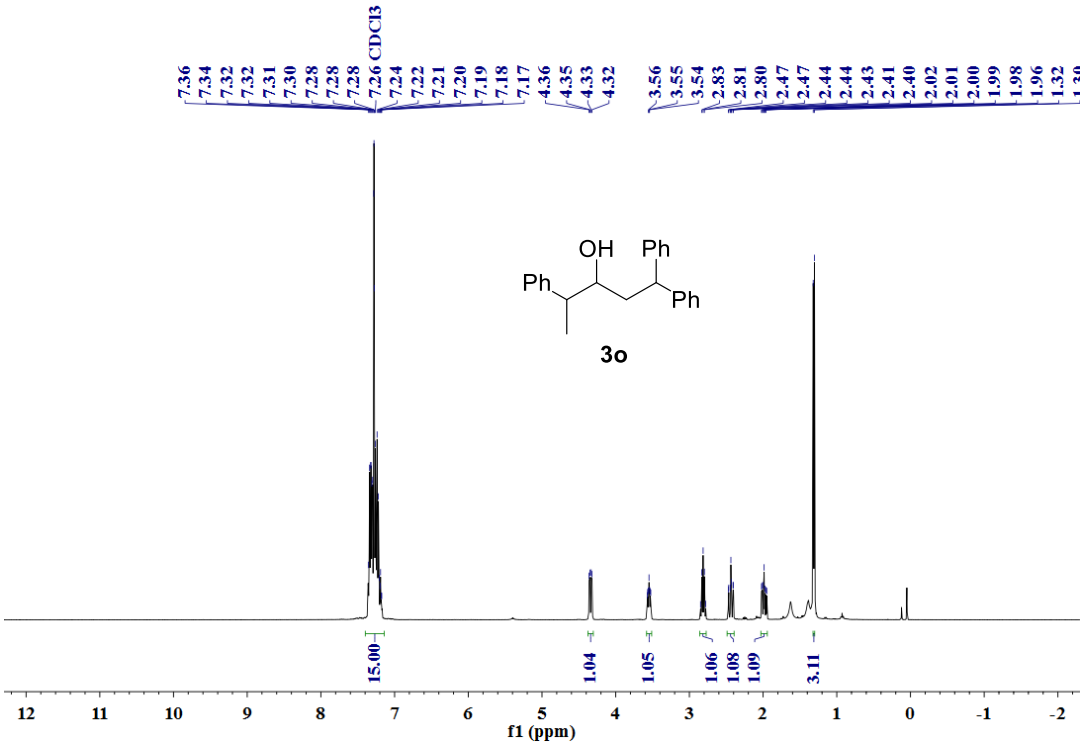

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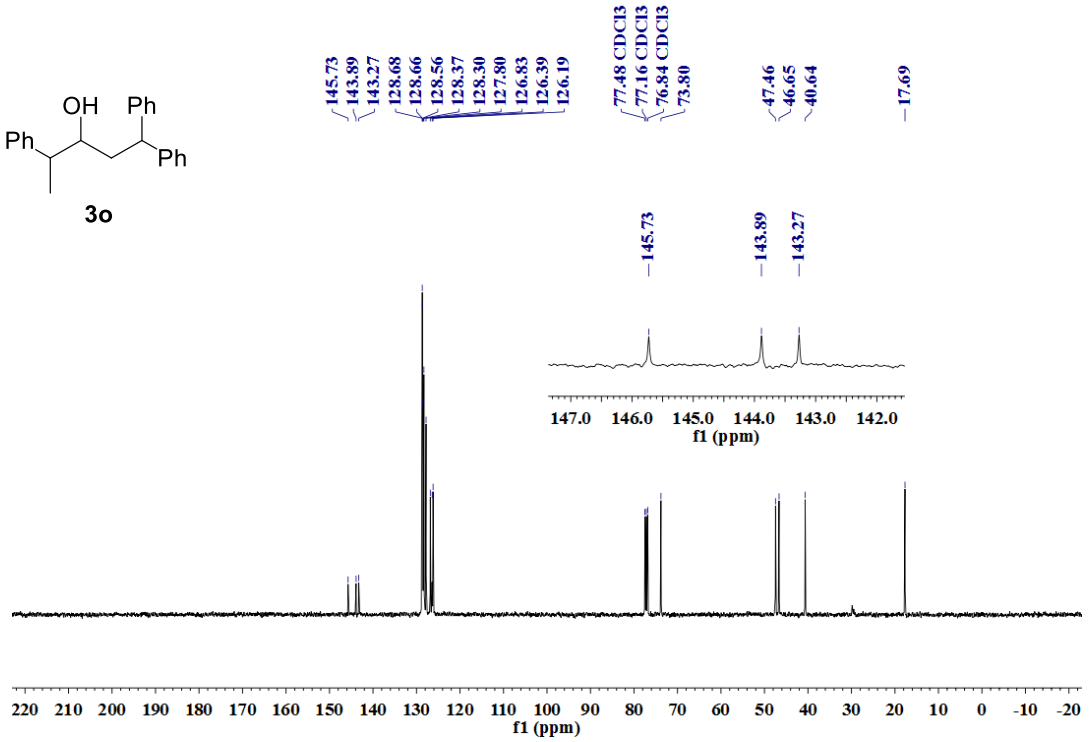

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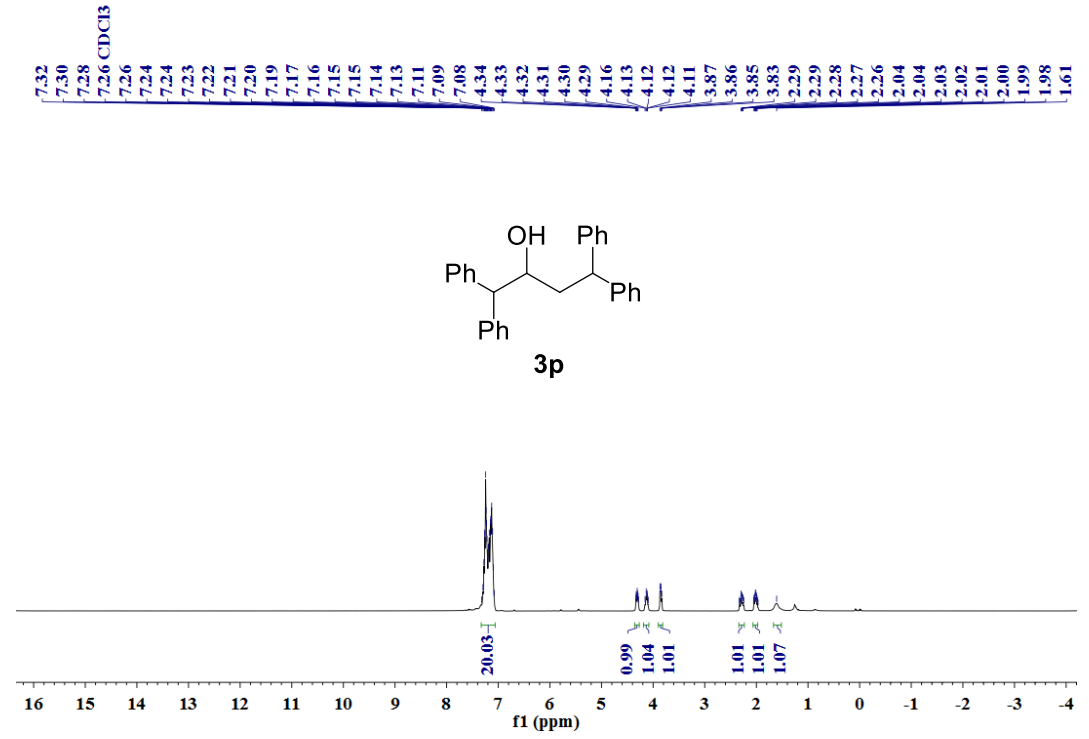

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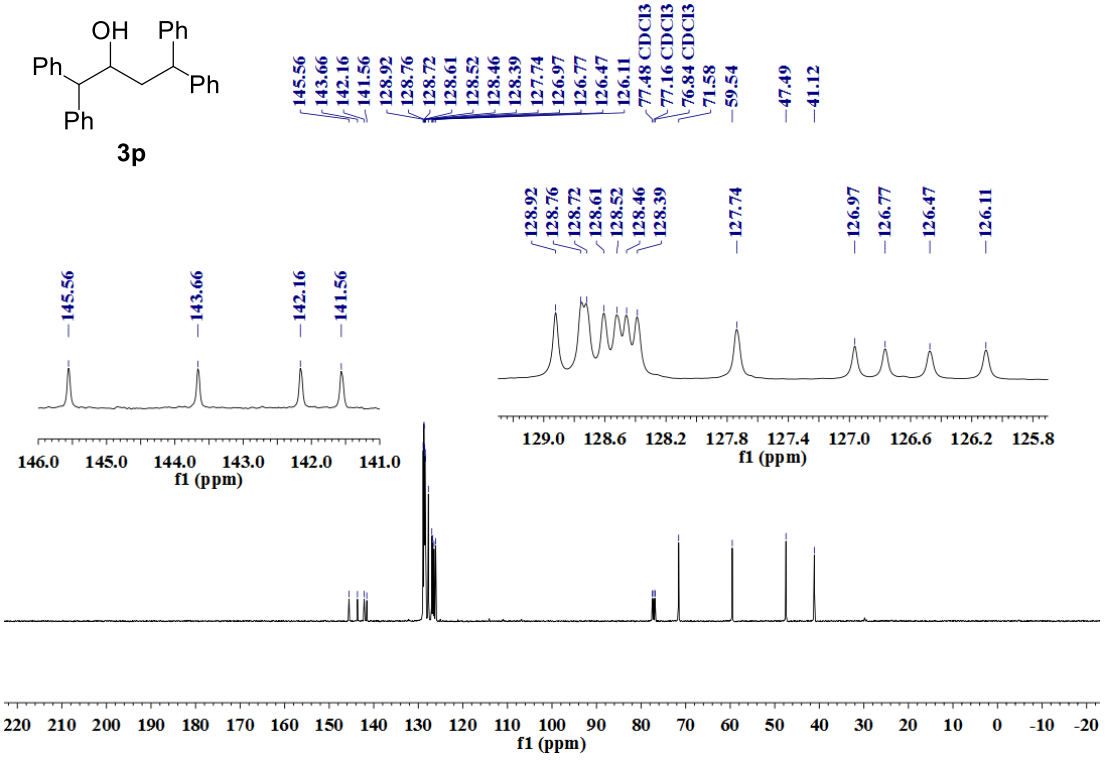

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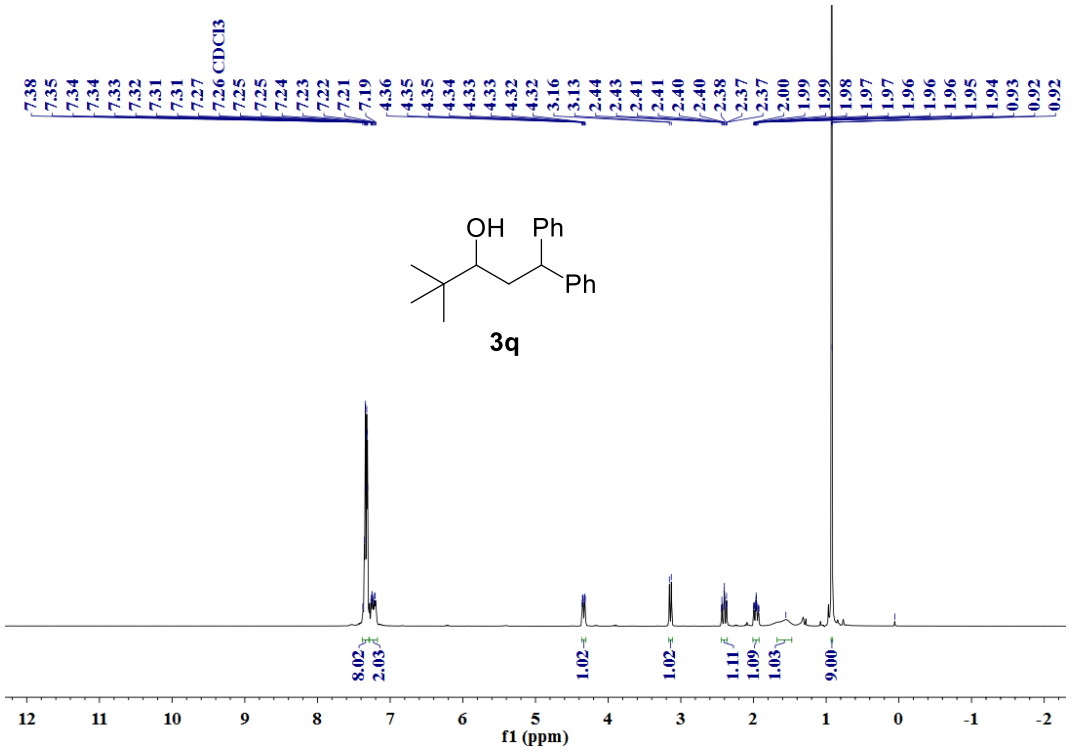

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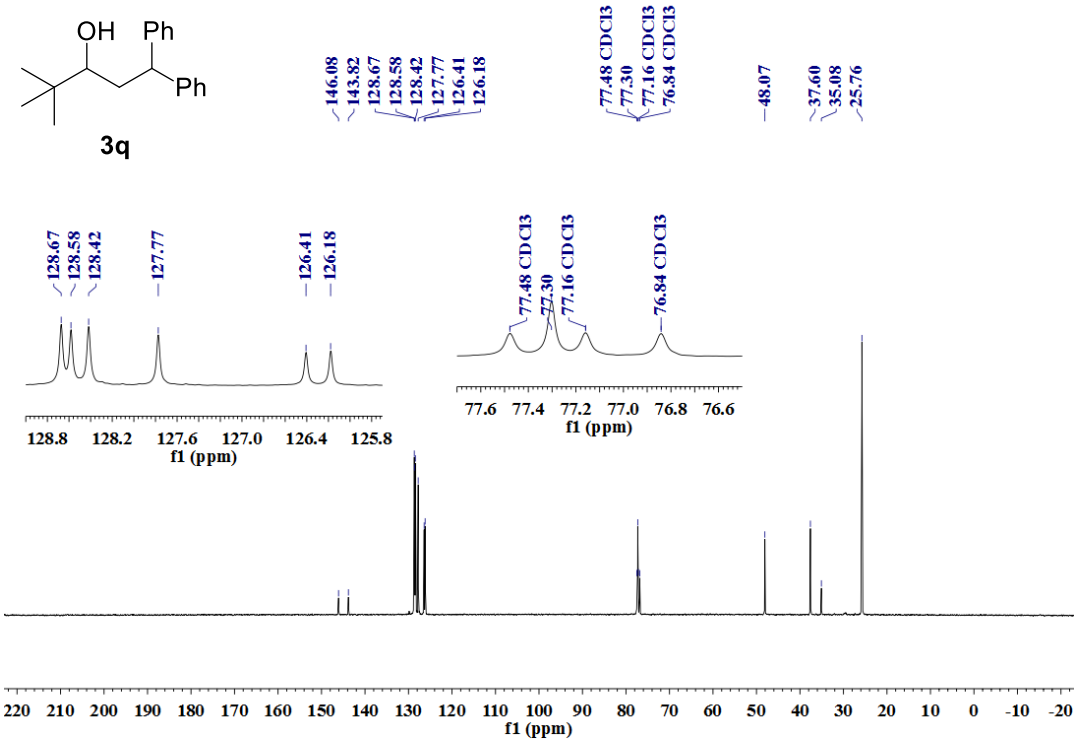

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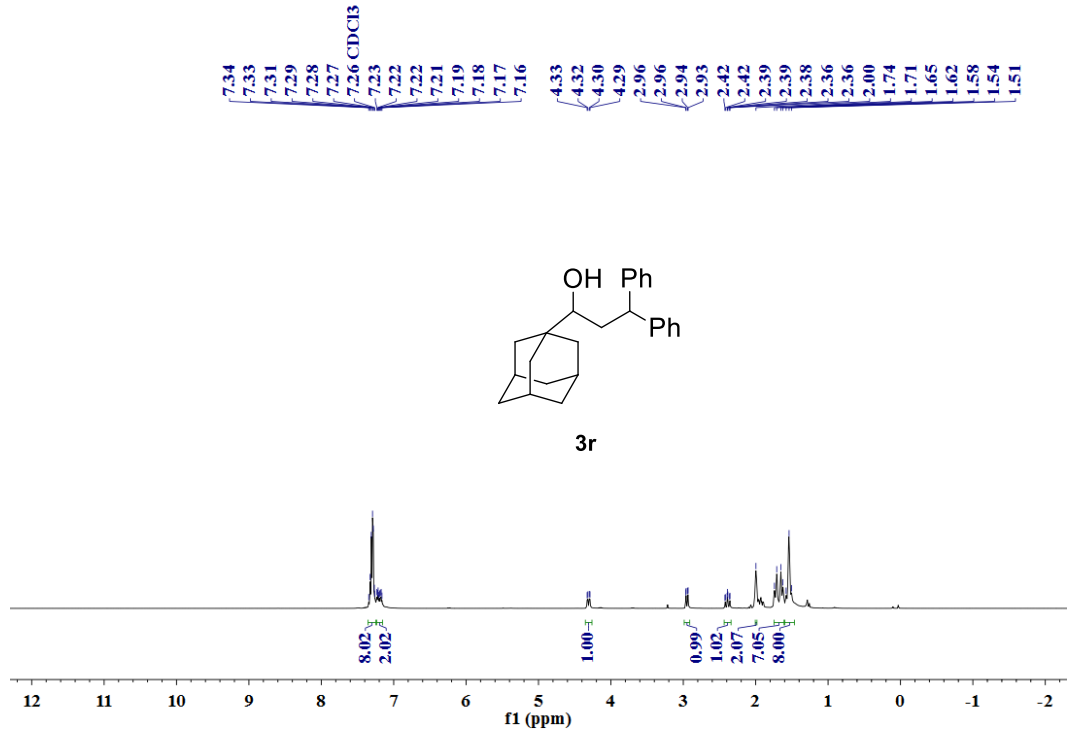

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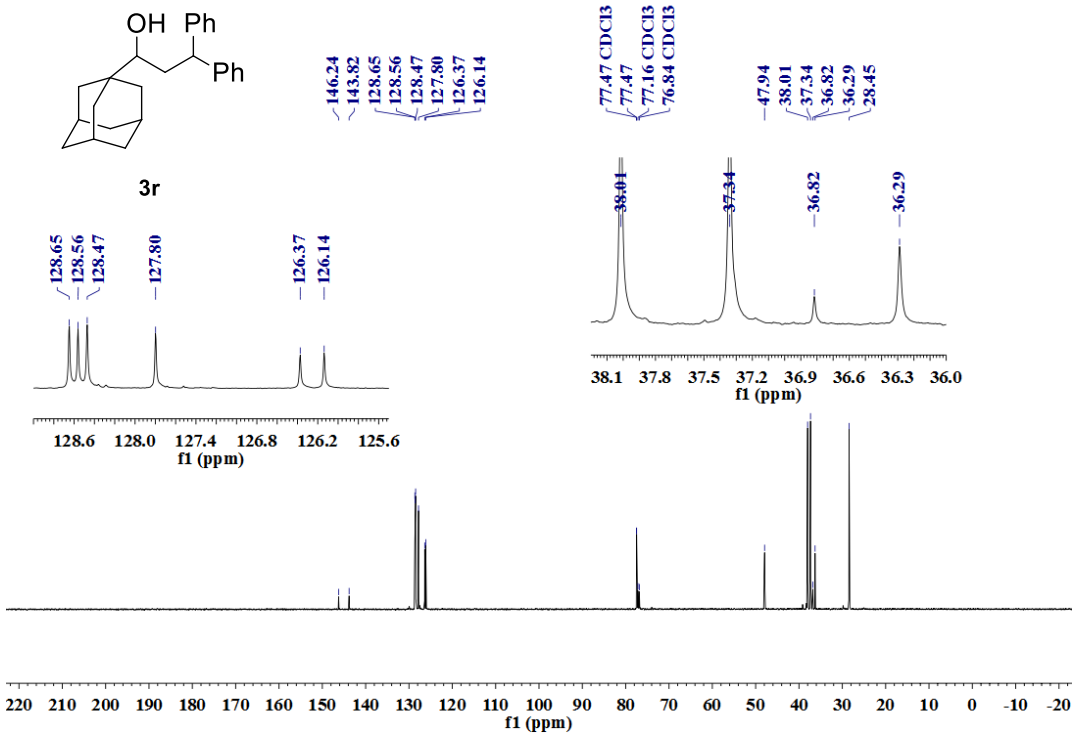

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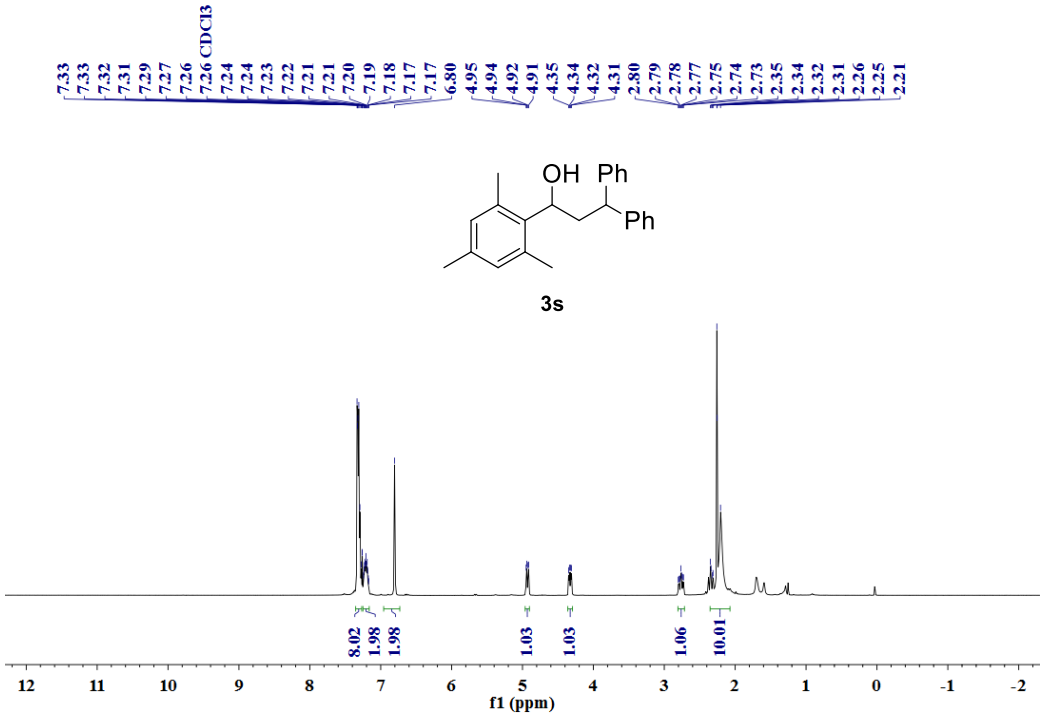

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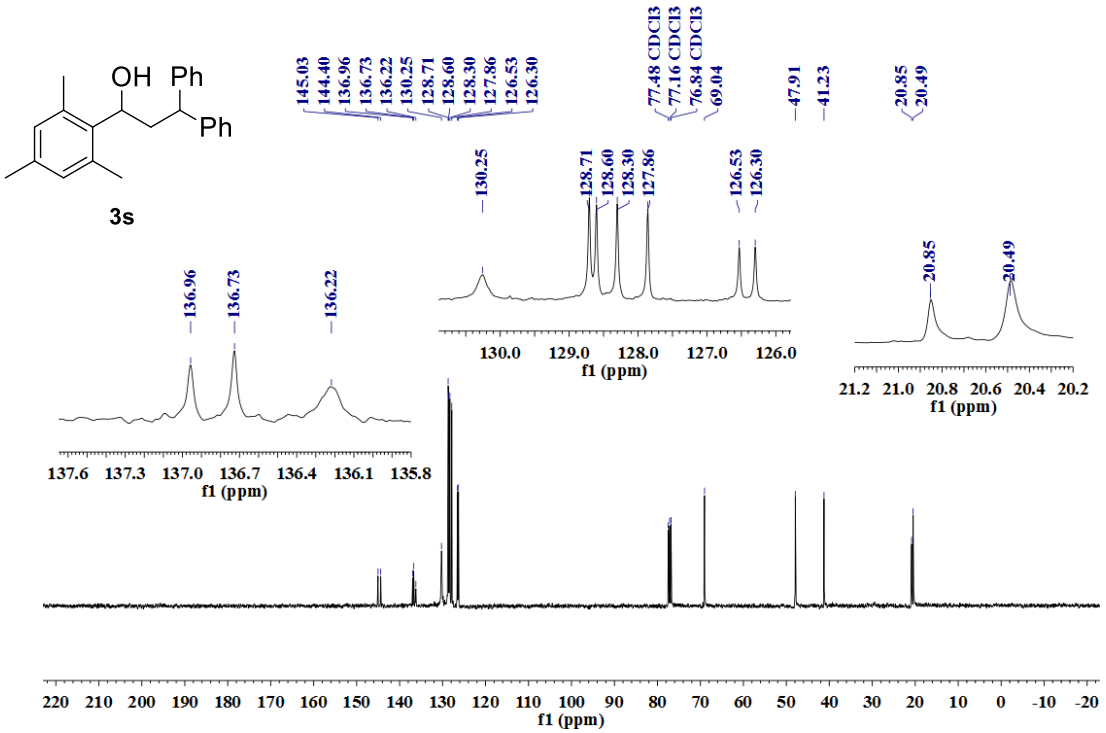

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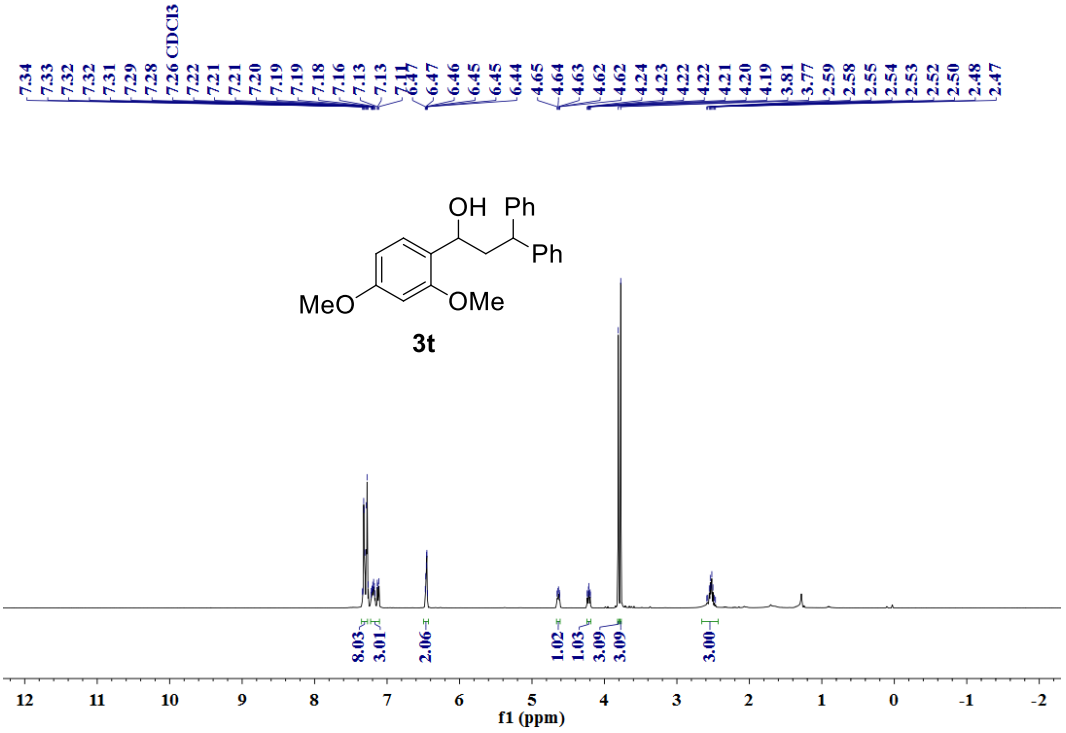

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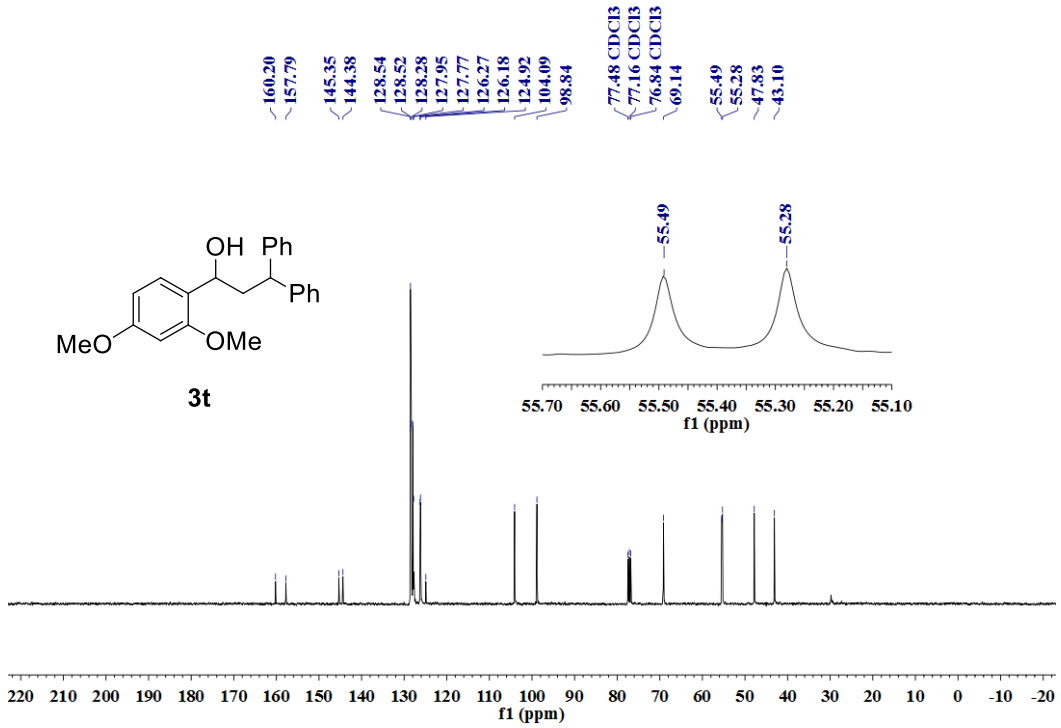

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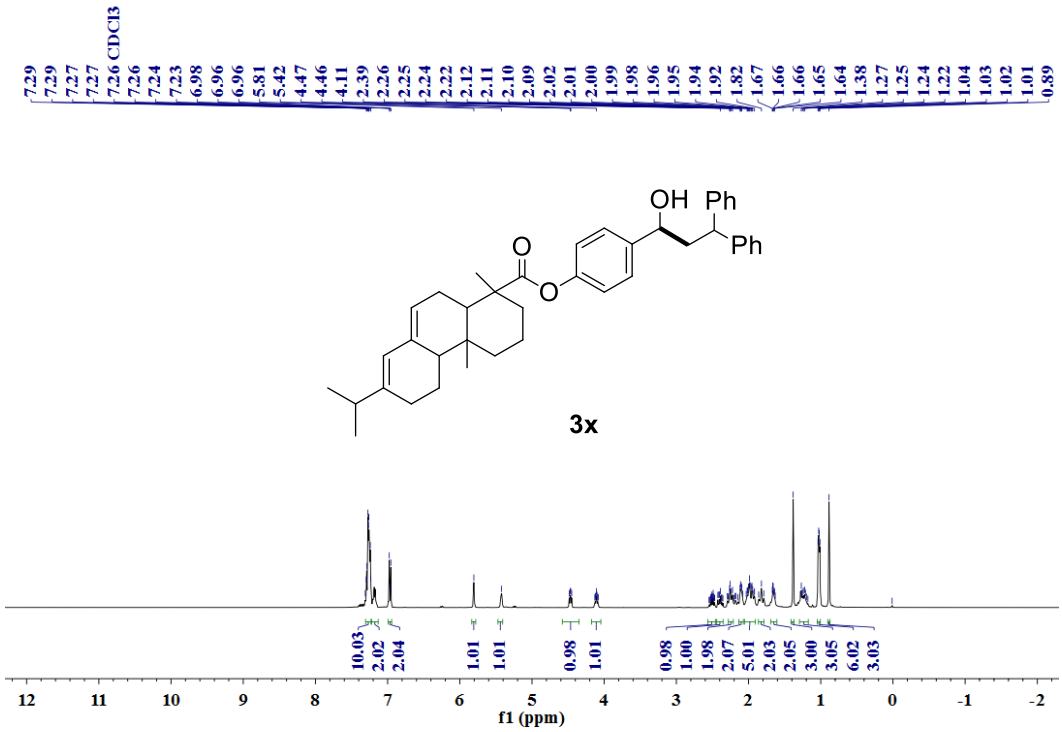

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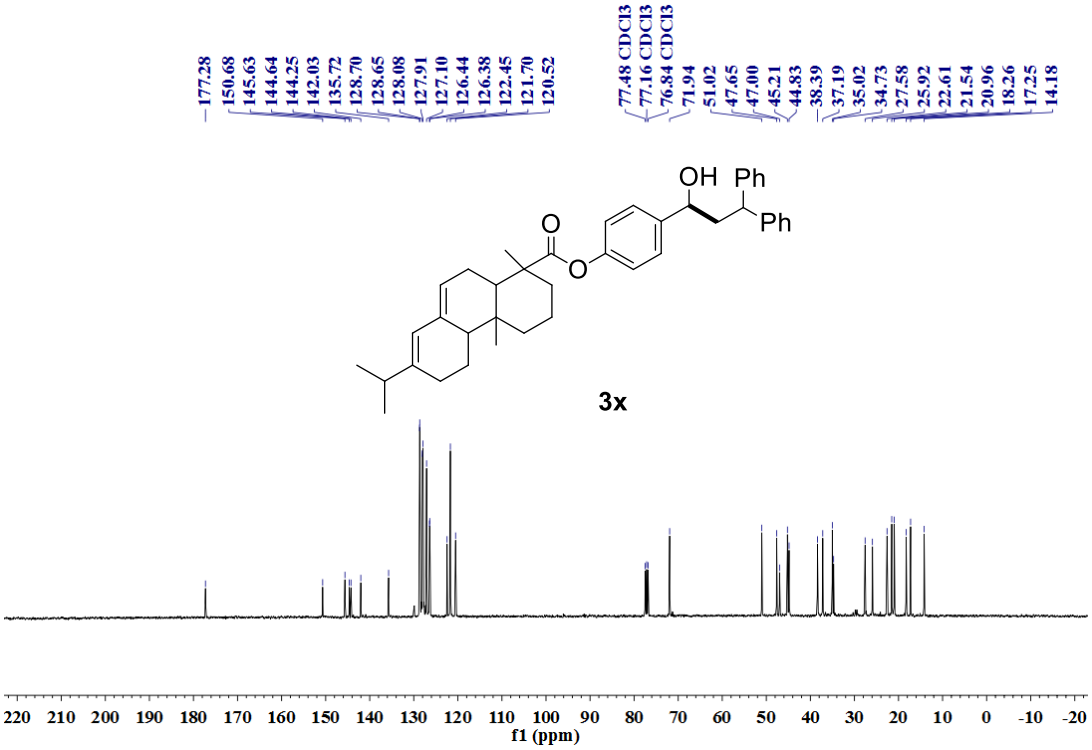

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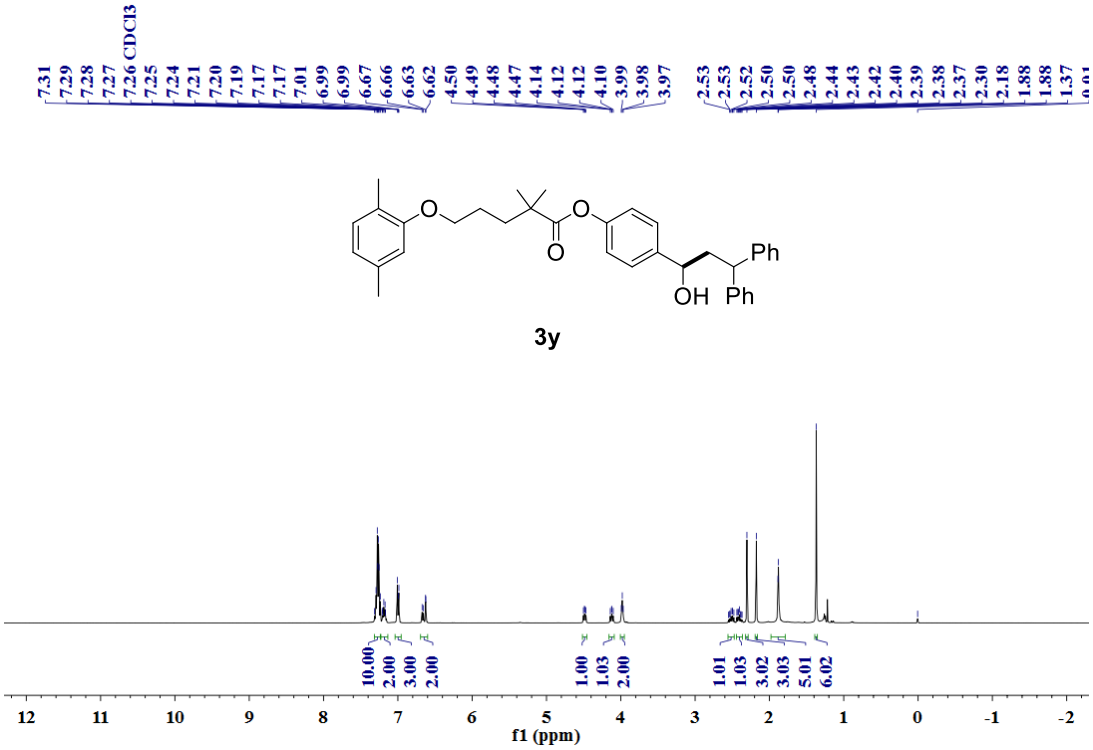

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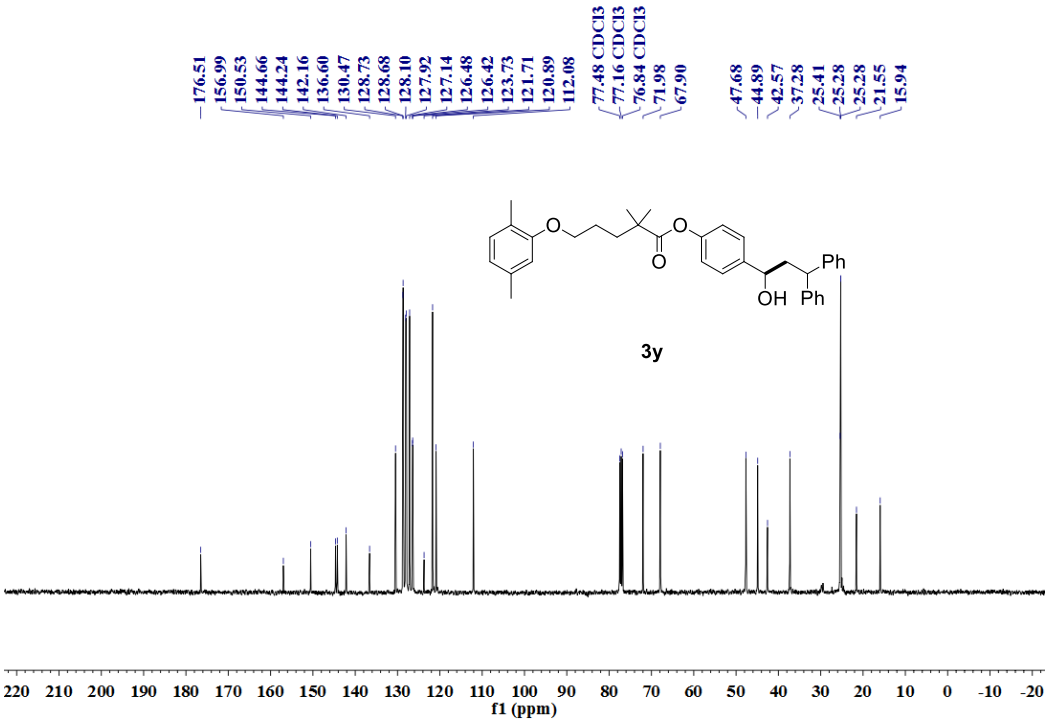

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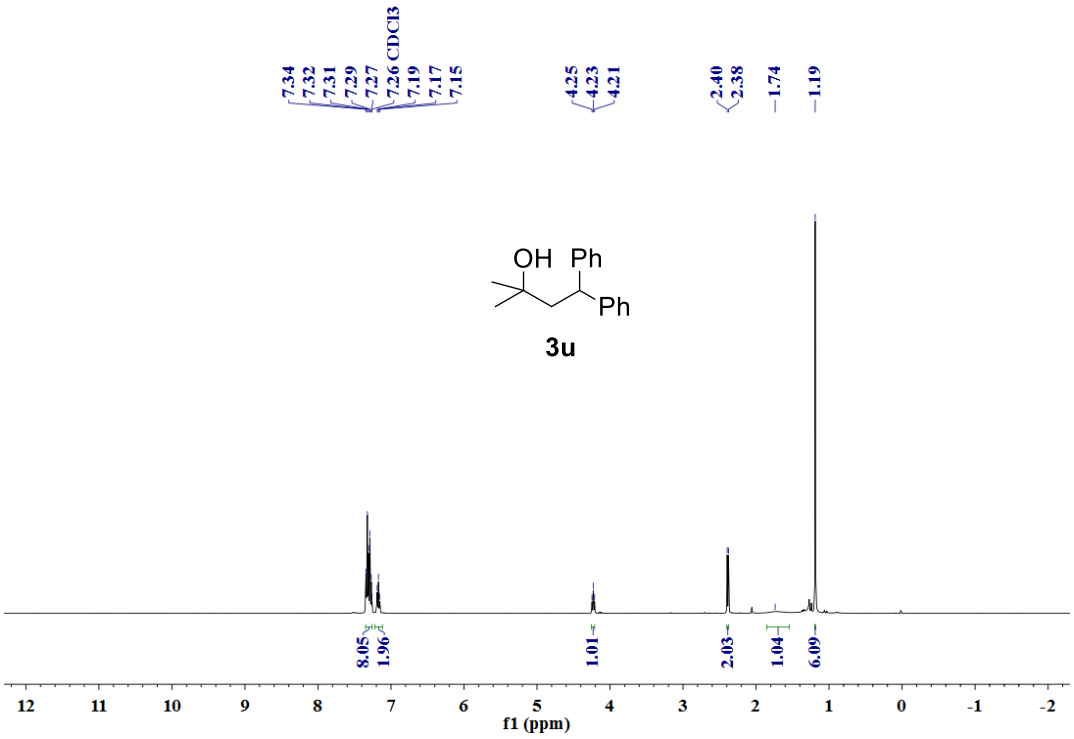

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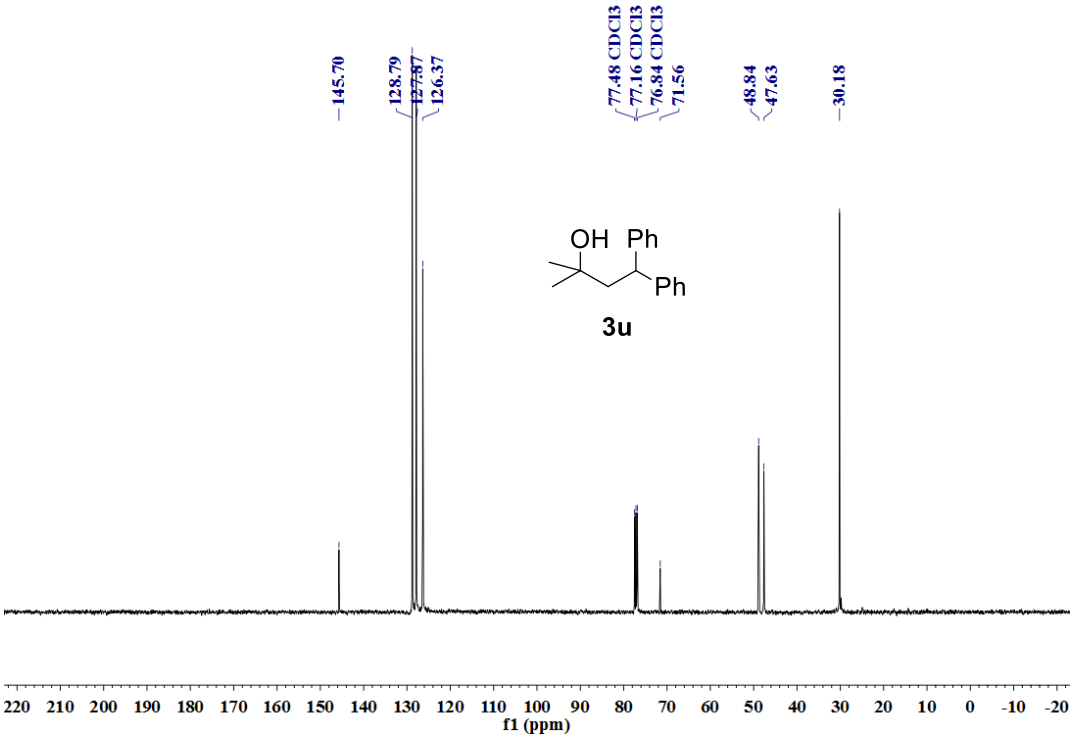

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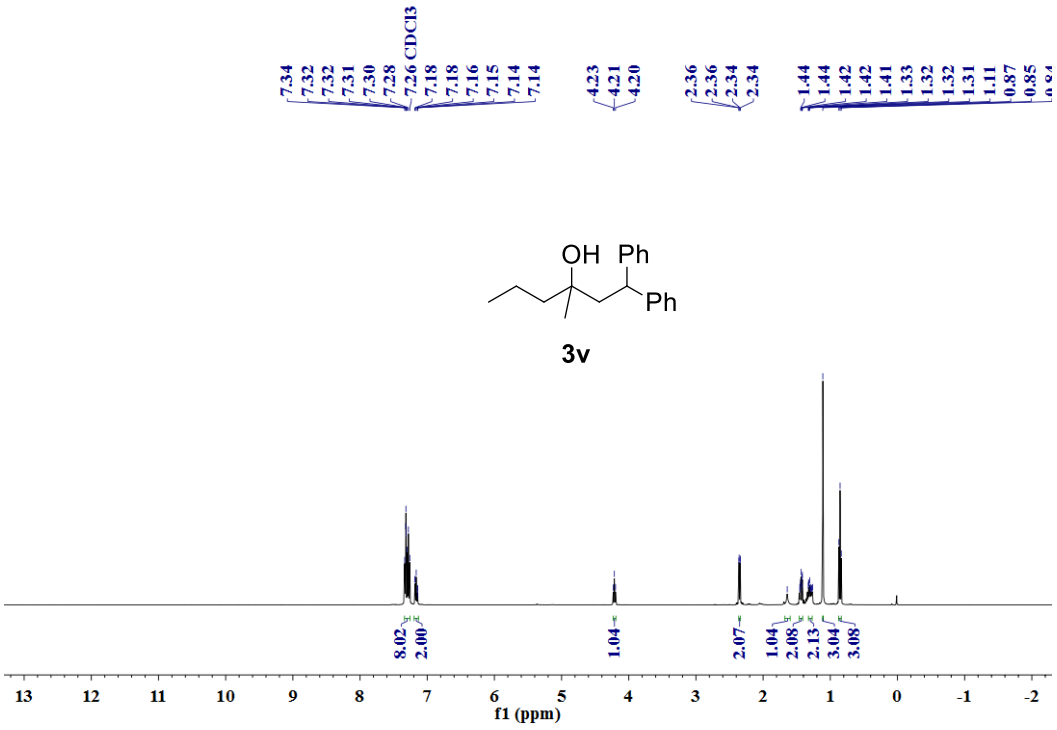

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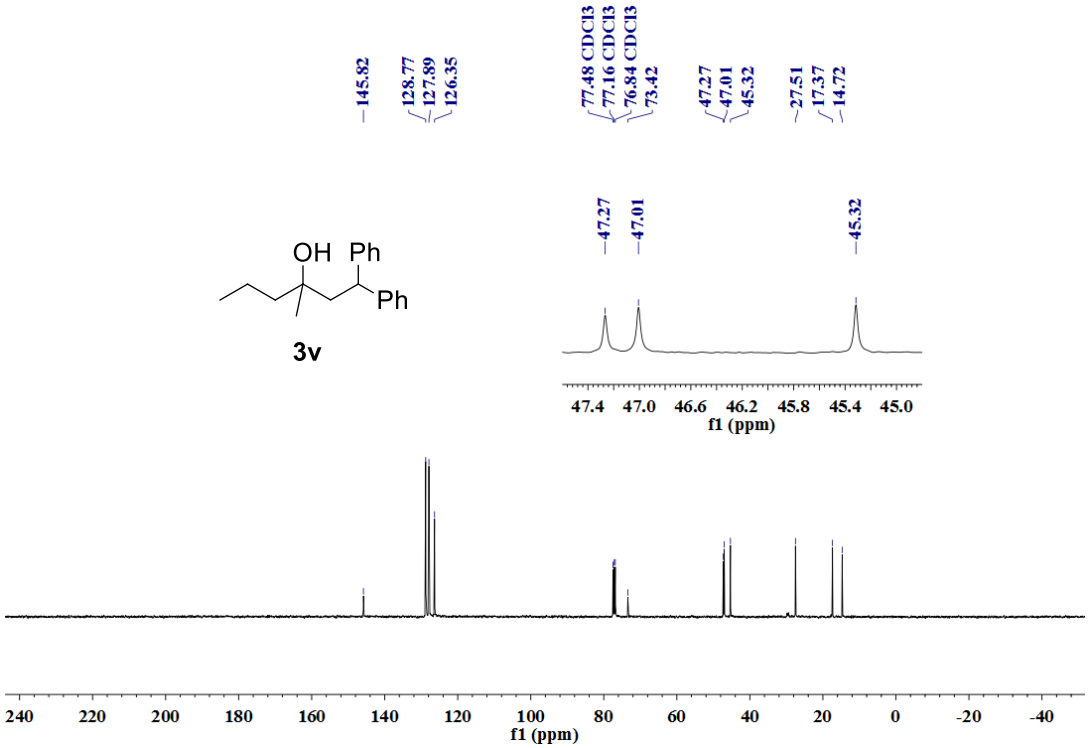

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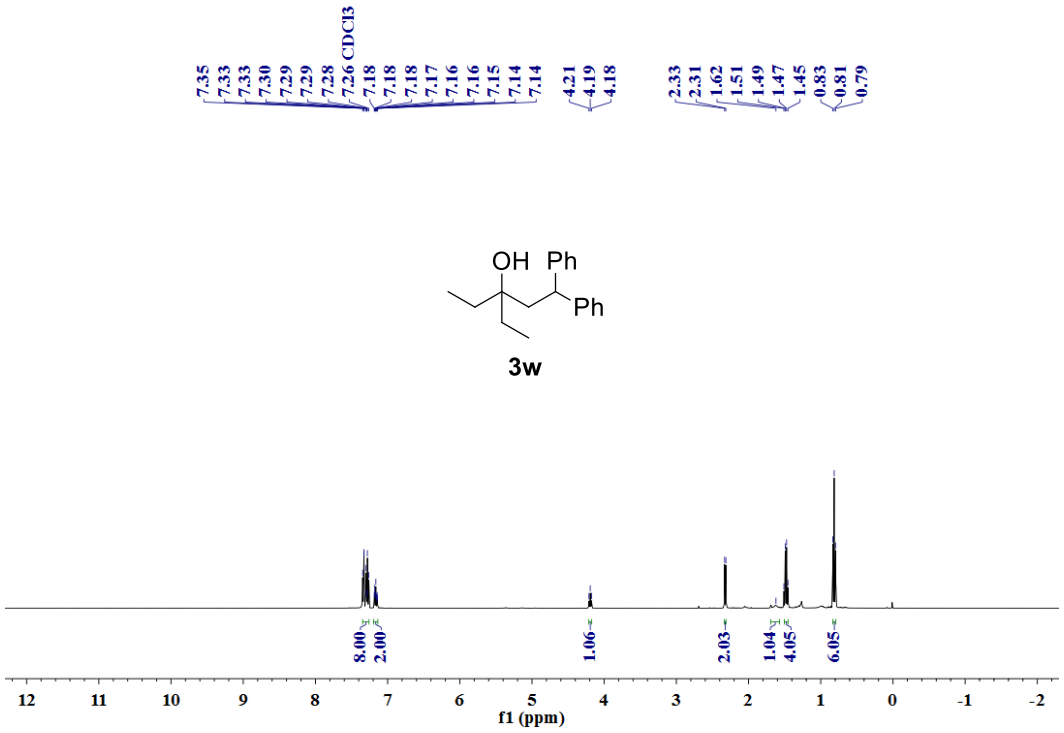

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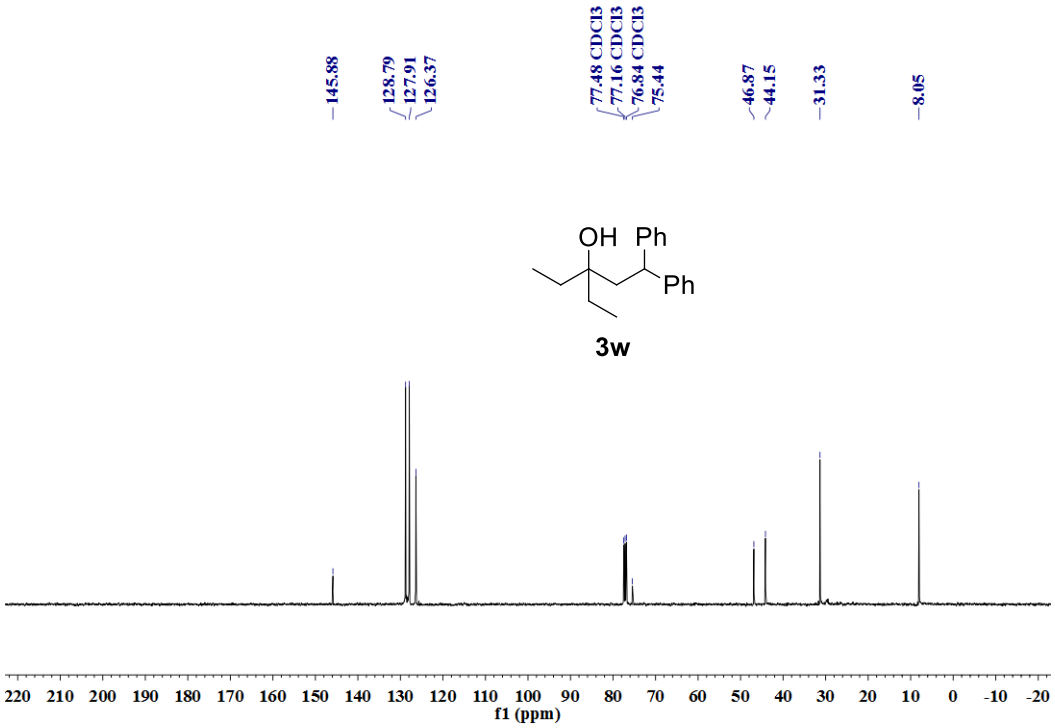

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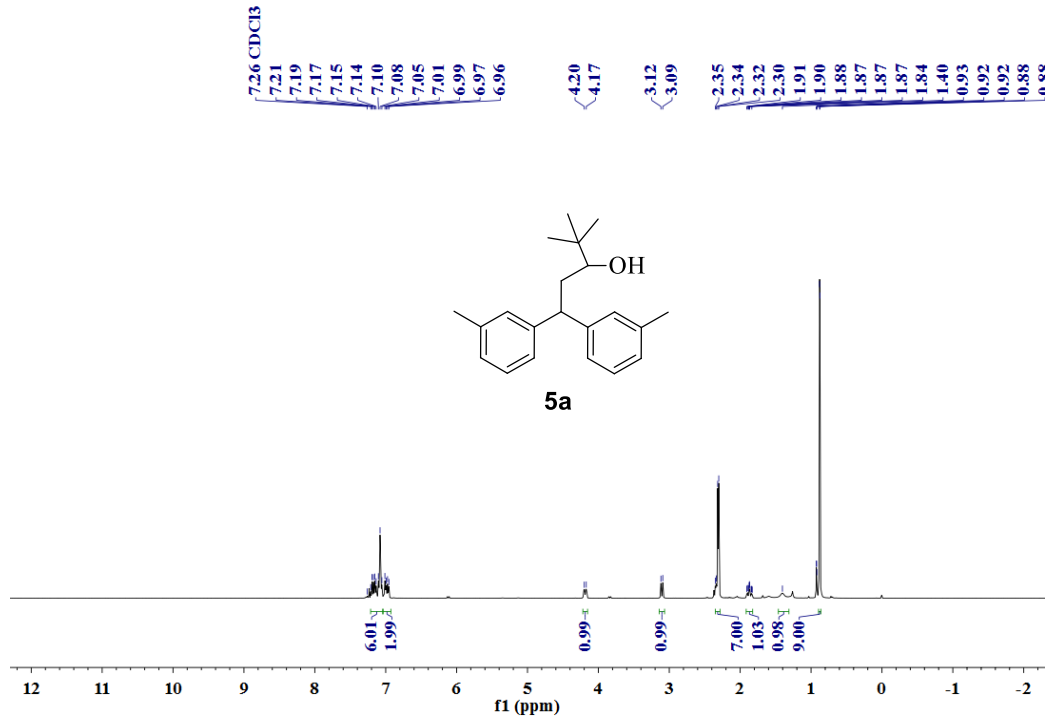

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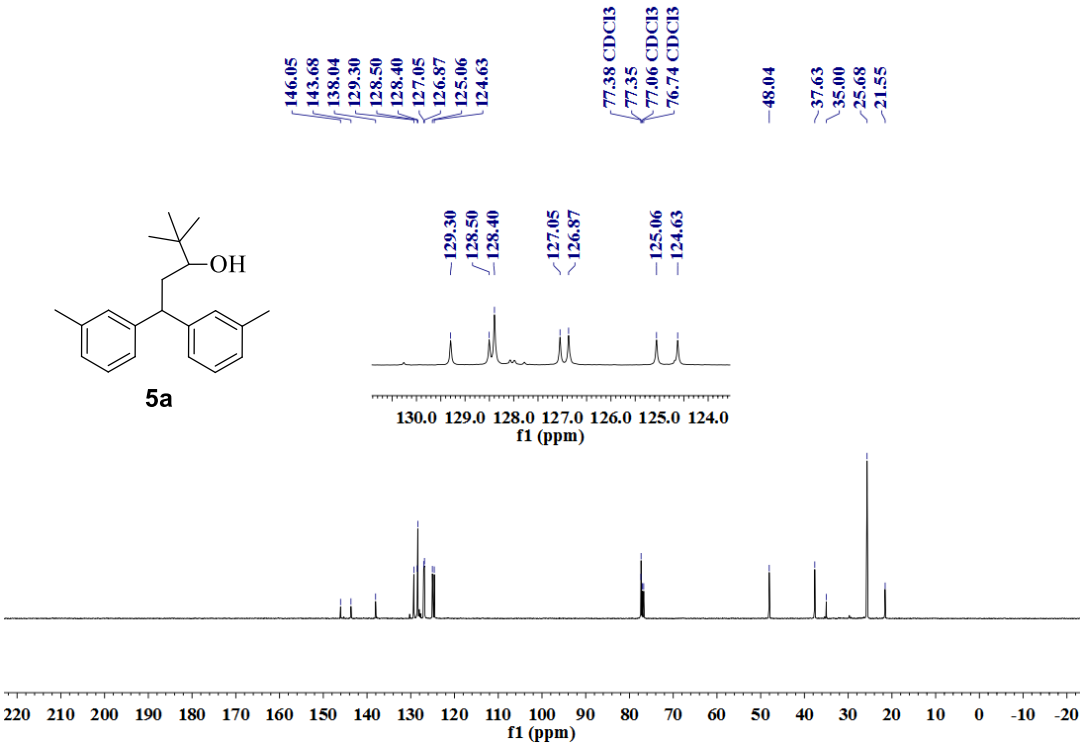

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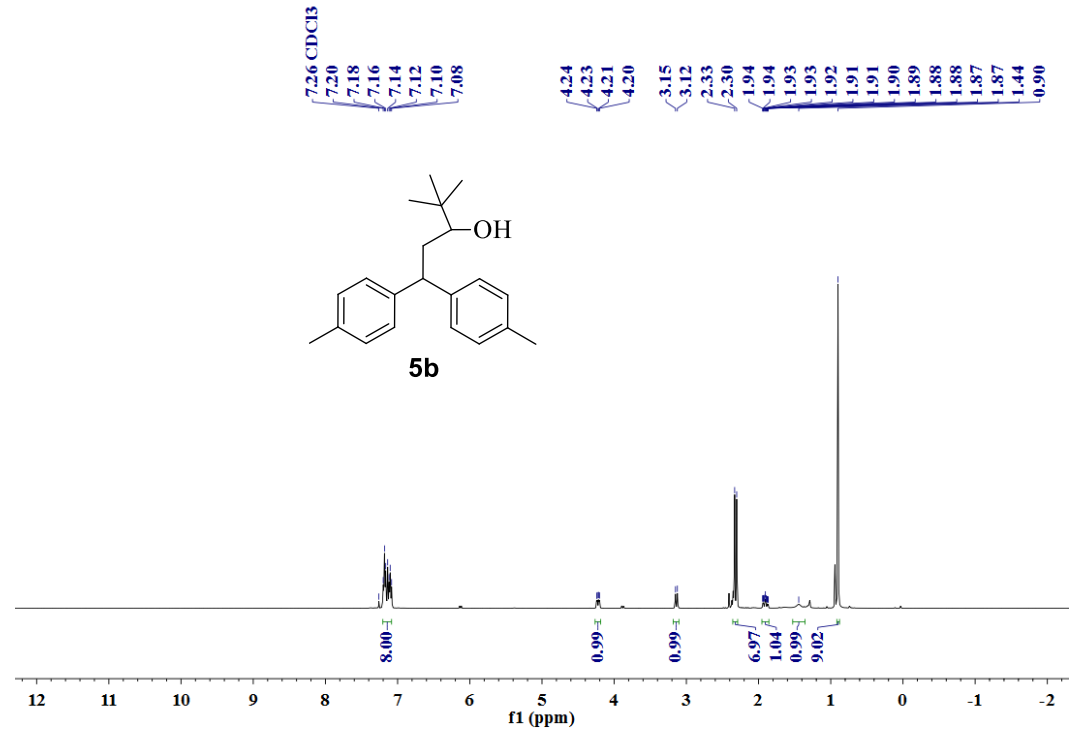

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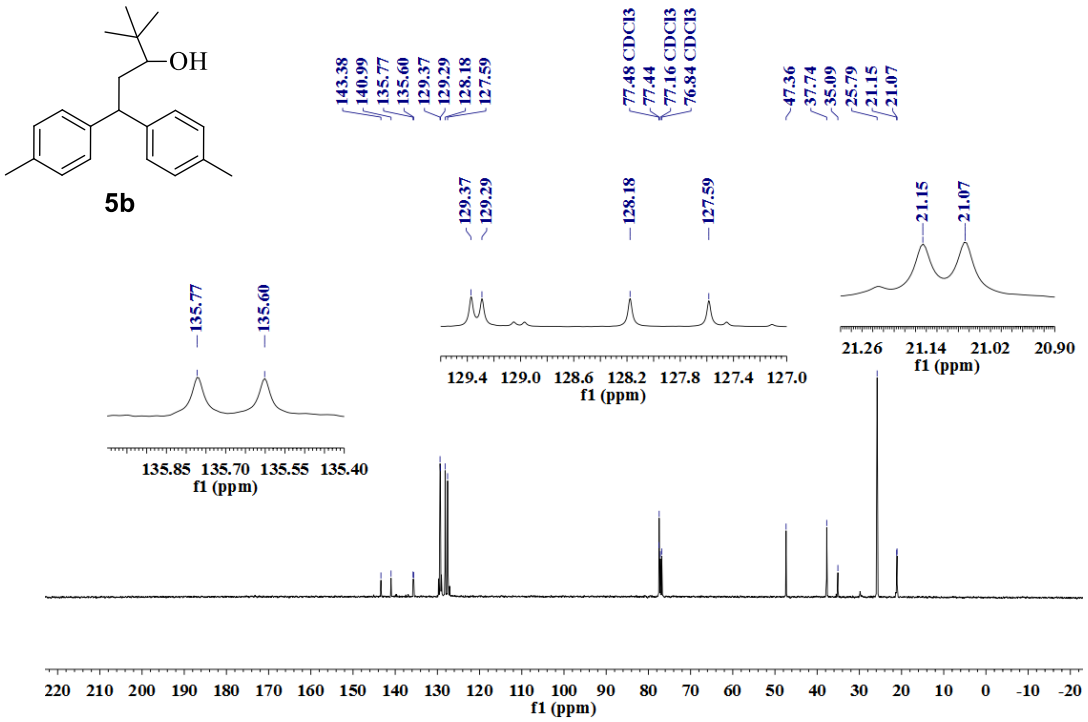

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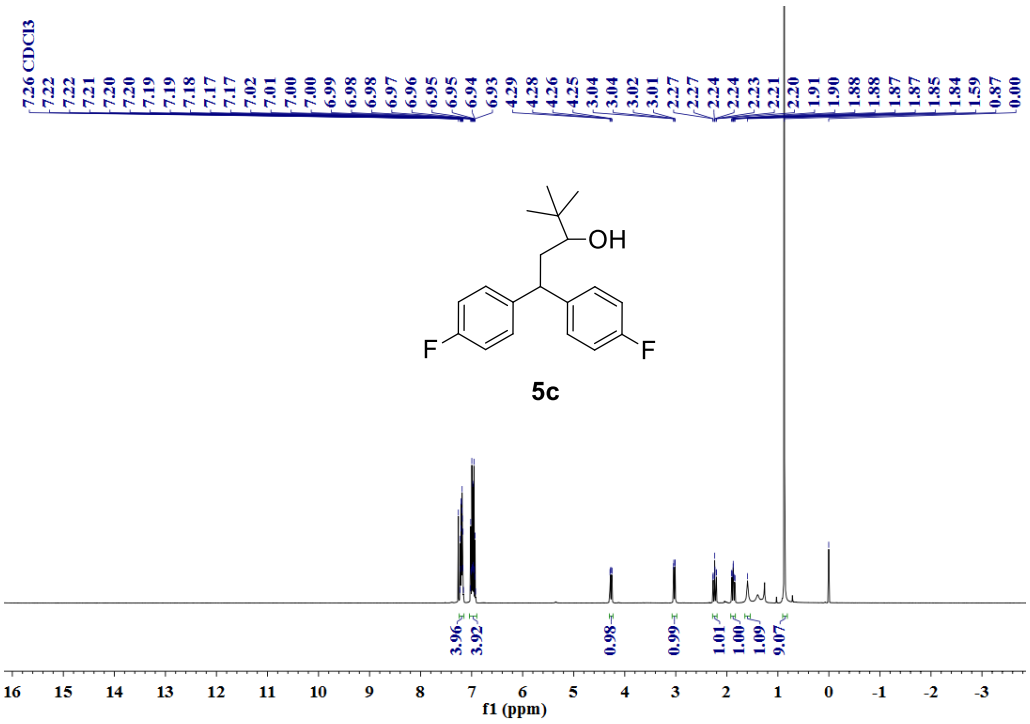

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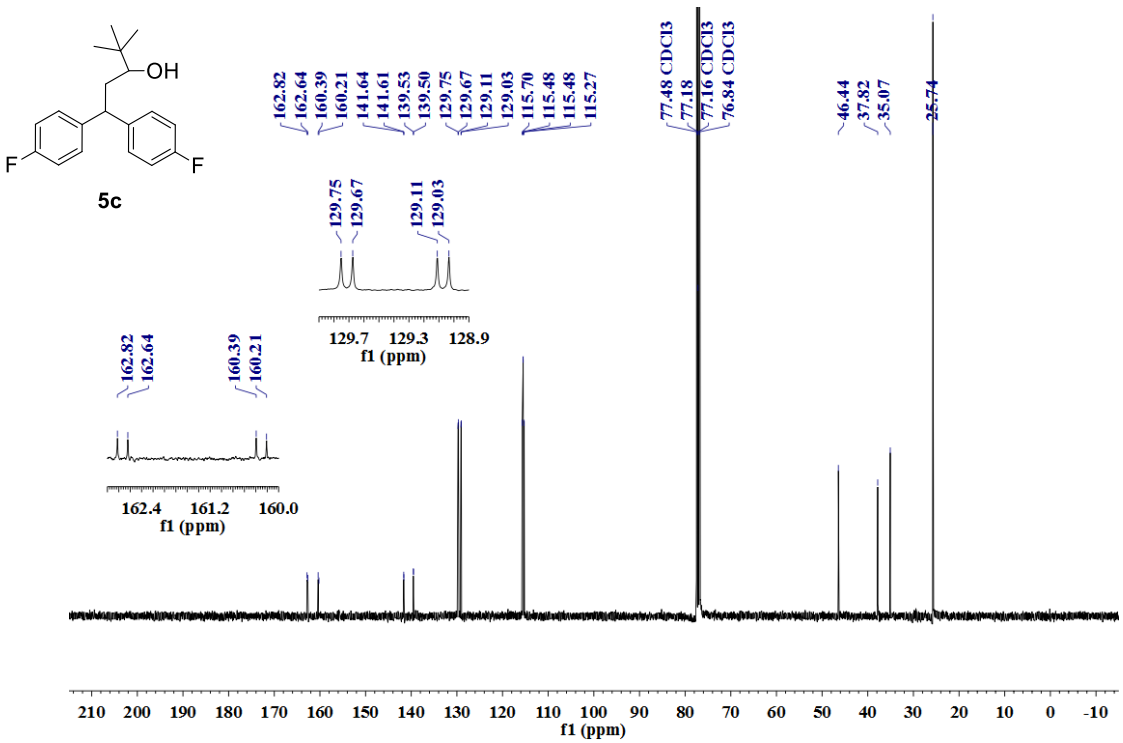

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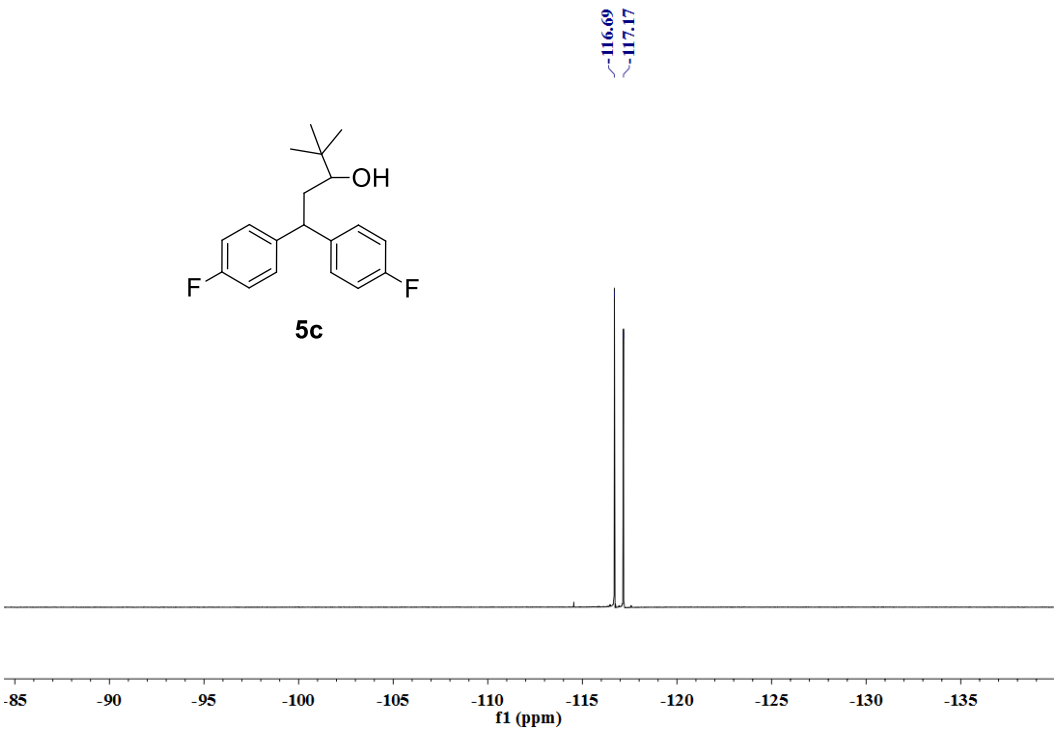
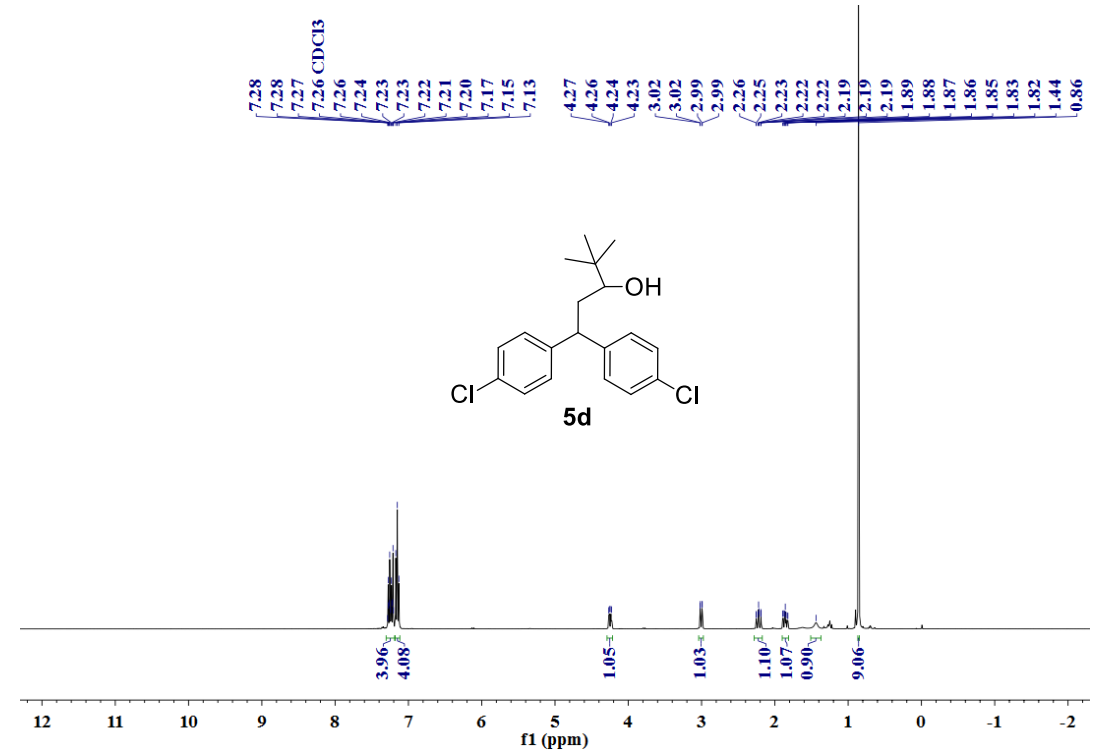
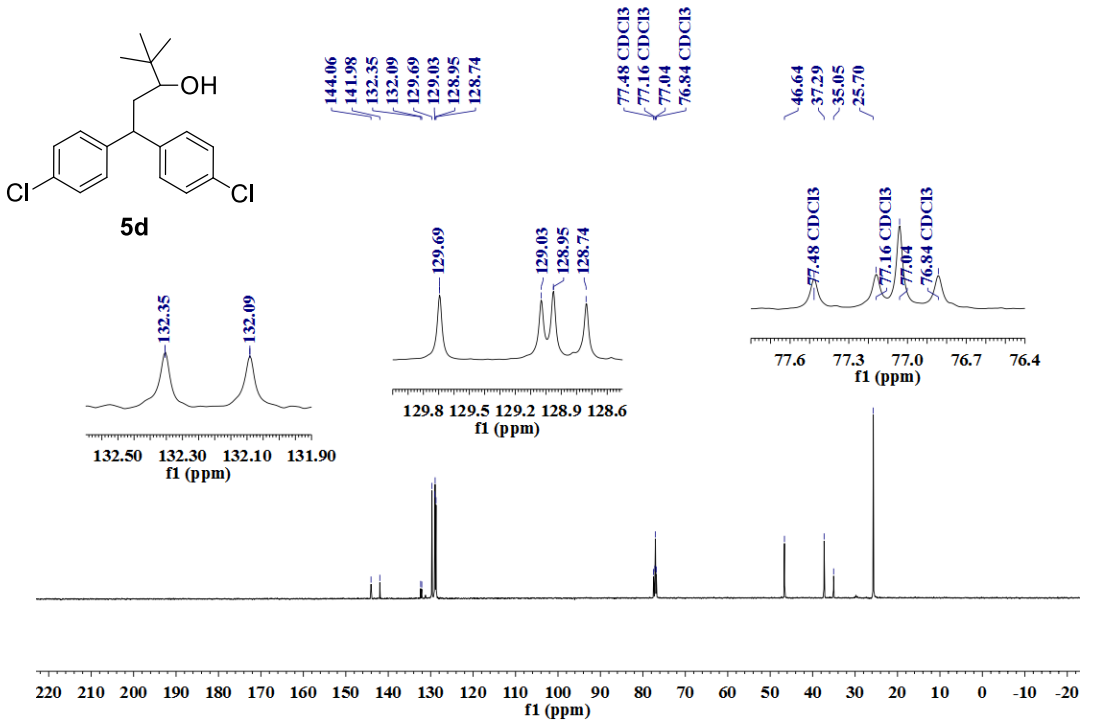


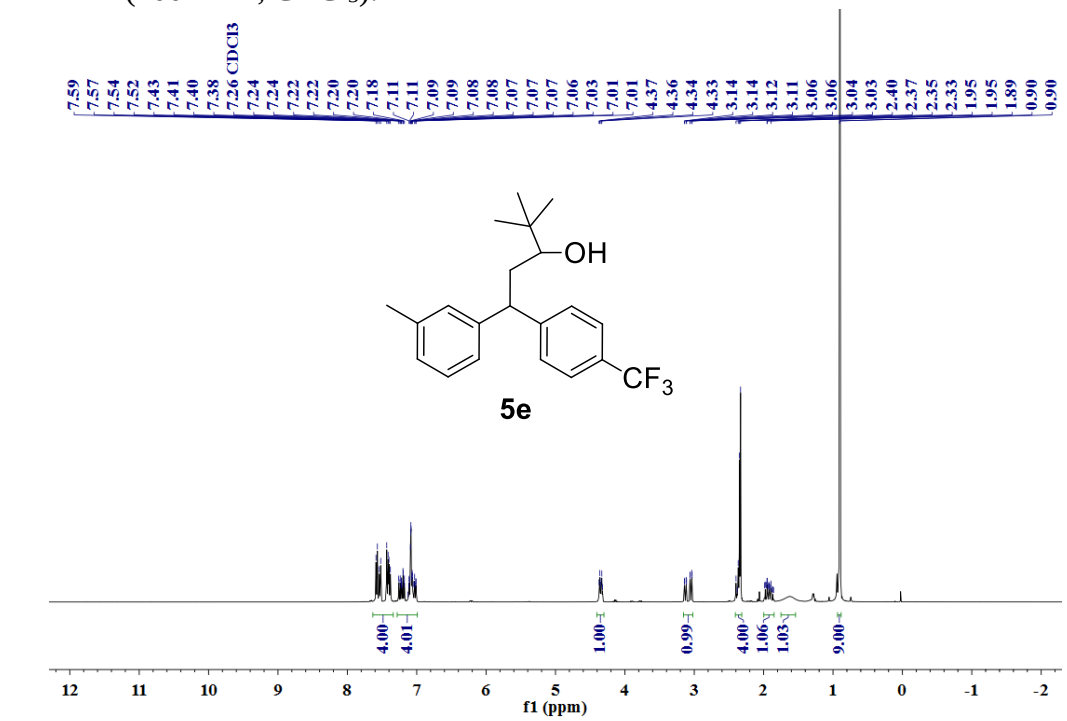
^{1}H NMR (400 MHz, $CDCl_3$):



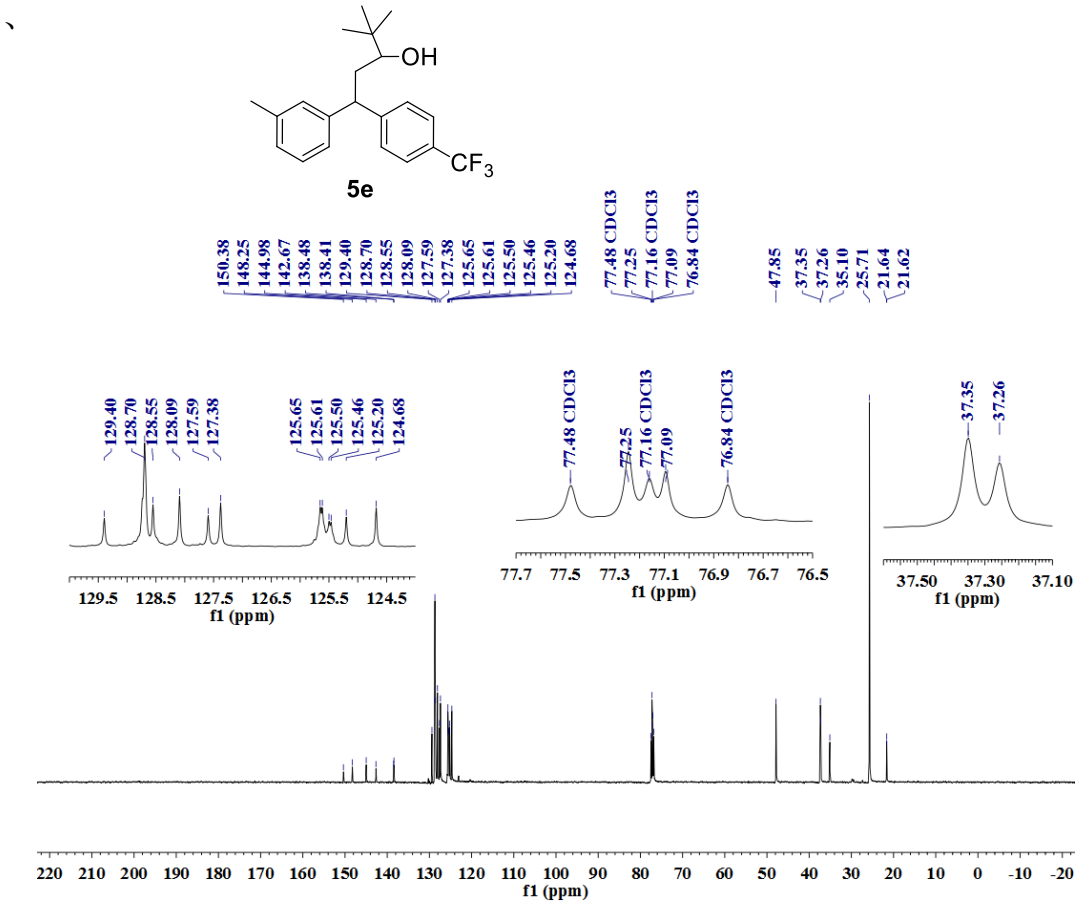
^{13}C NMR (100 MHz, $CDCl_3$):



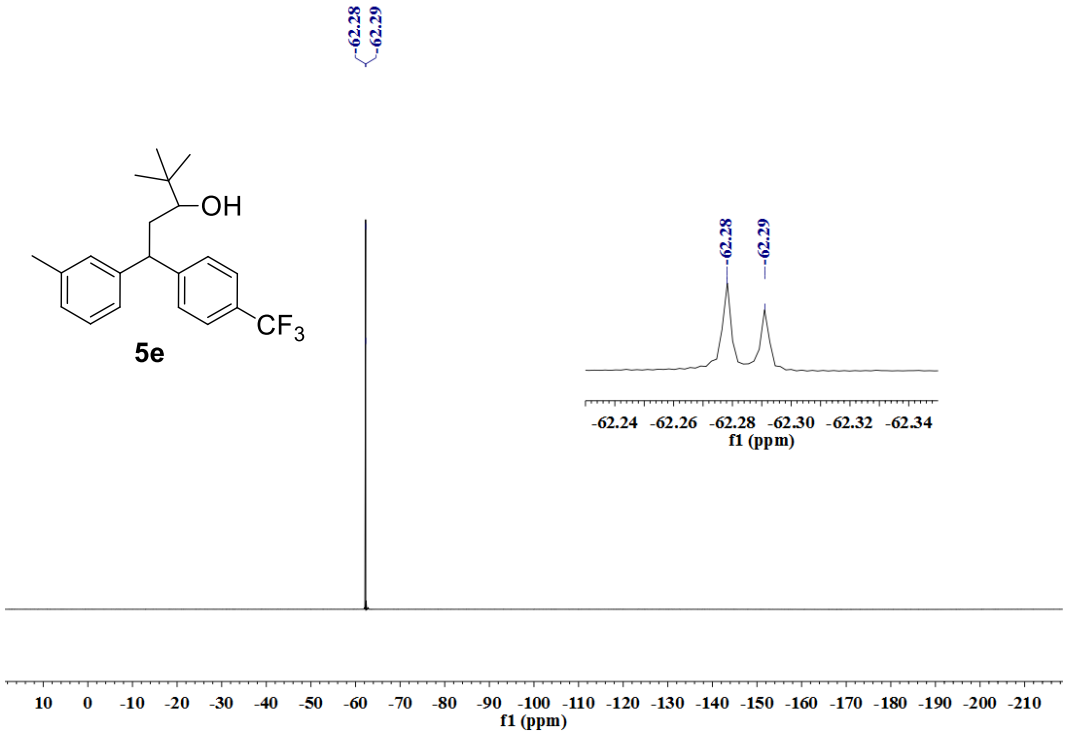
^{1}H NMR (400 MHz, $CDCl_3$):



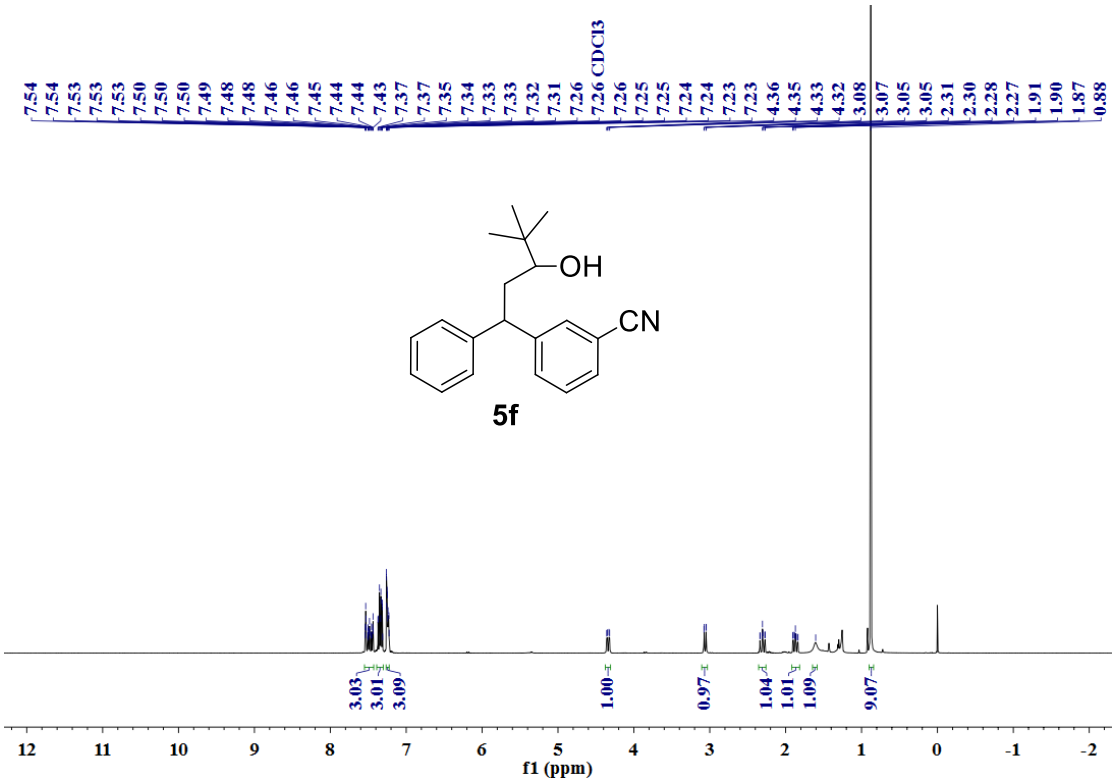
^{13}C NMR (100 MHz, $CDCl_3$):



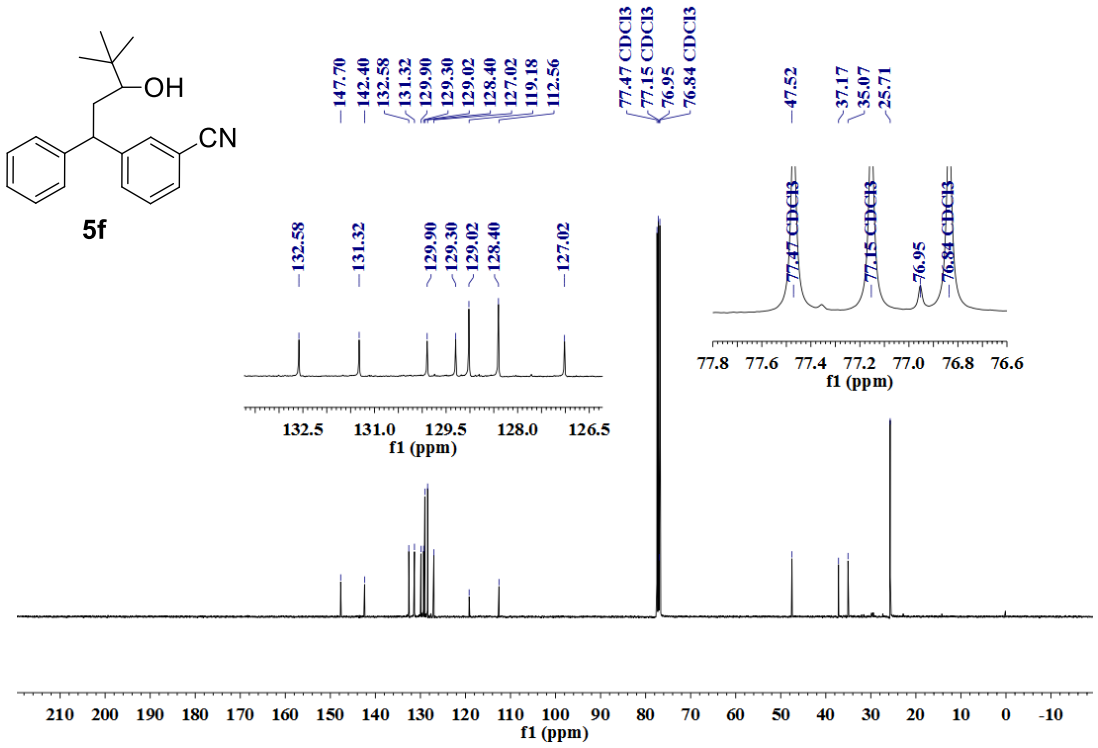
^{19}F NMR (376 MHz, $CDCl_3$):



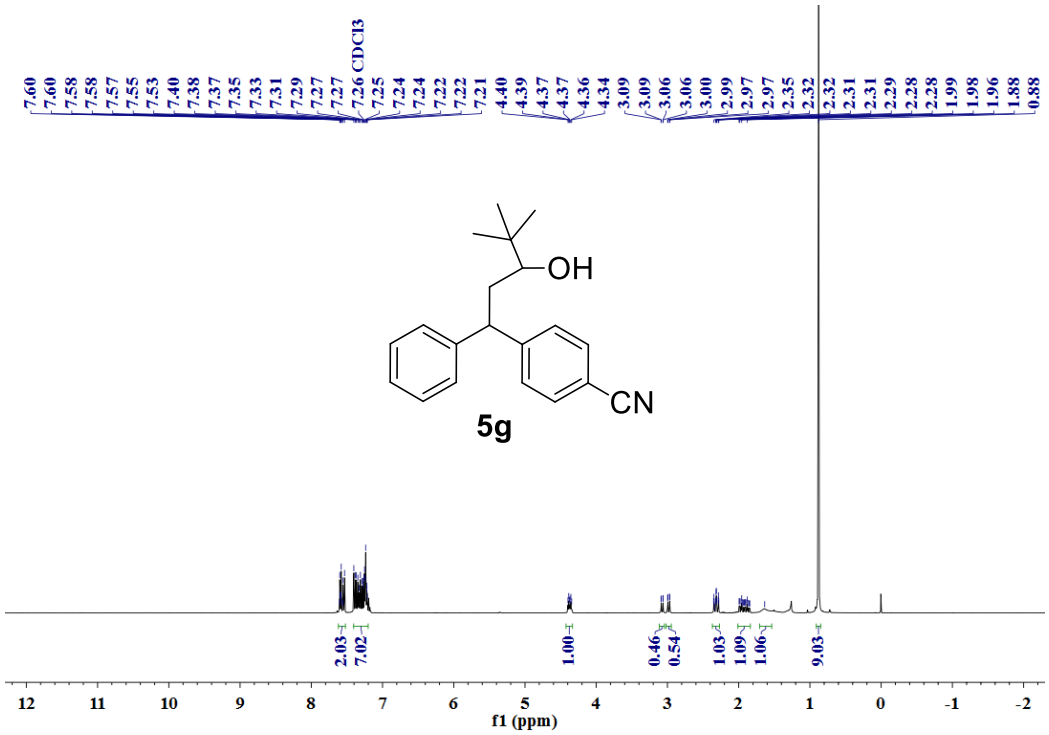
^{1}H NMR (400 MHz, $CDCl_3$):



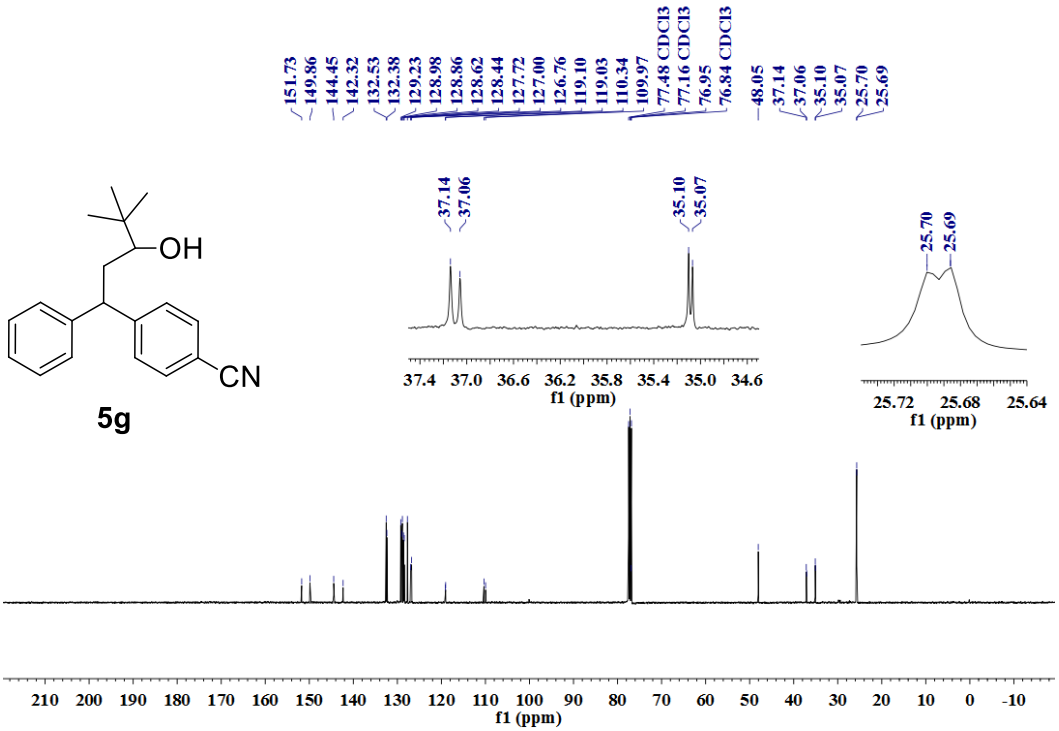
^{13}C NMR (100 MHz, $CDCl_3$):



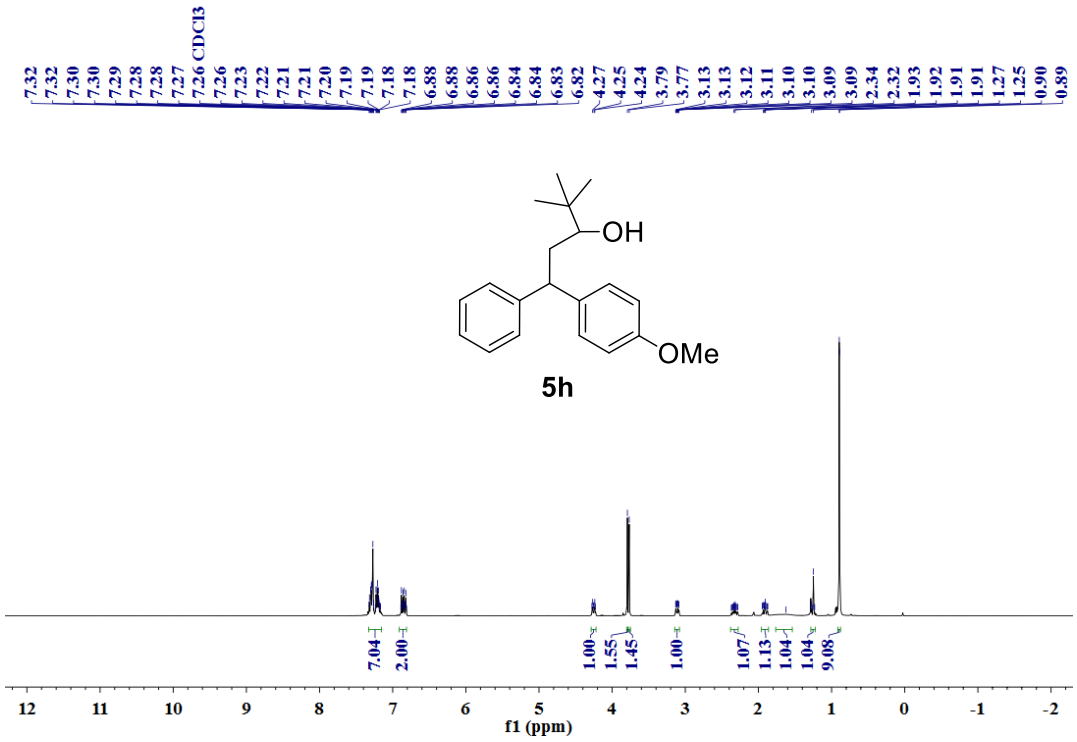
^{1}H NMR (400 MHz, $CDCl_3$):



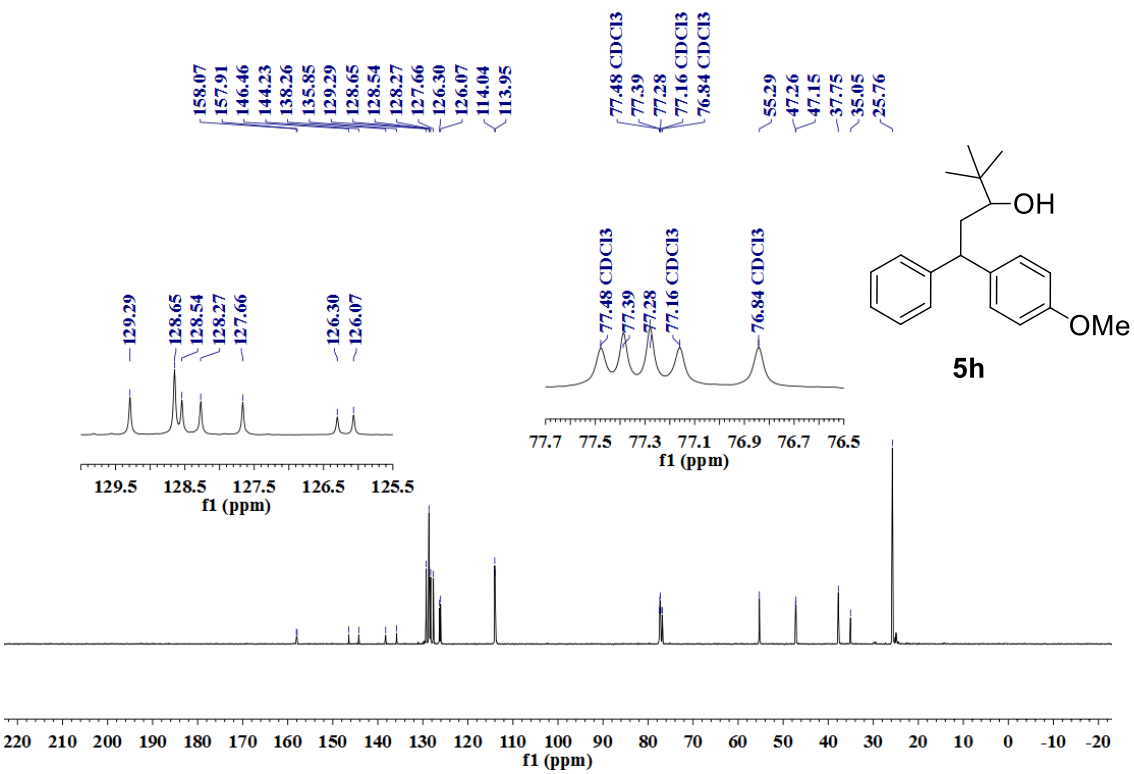
^{13}C NMR (100 MHz, $CDCl_3$):



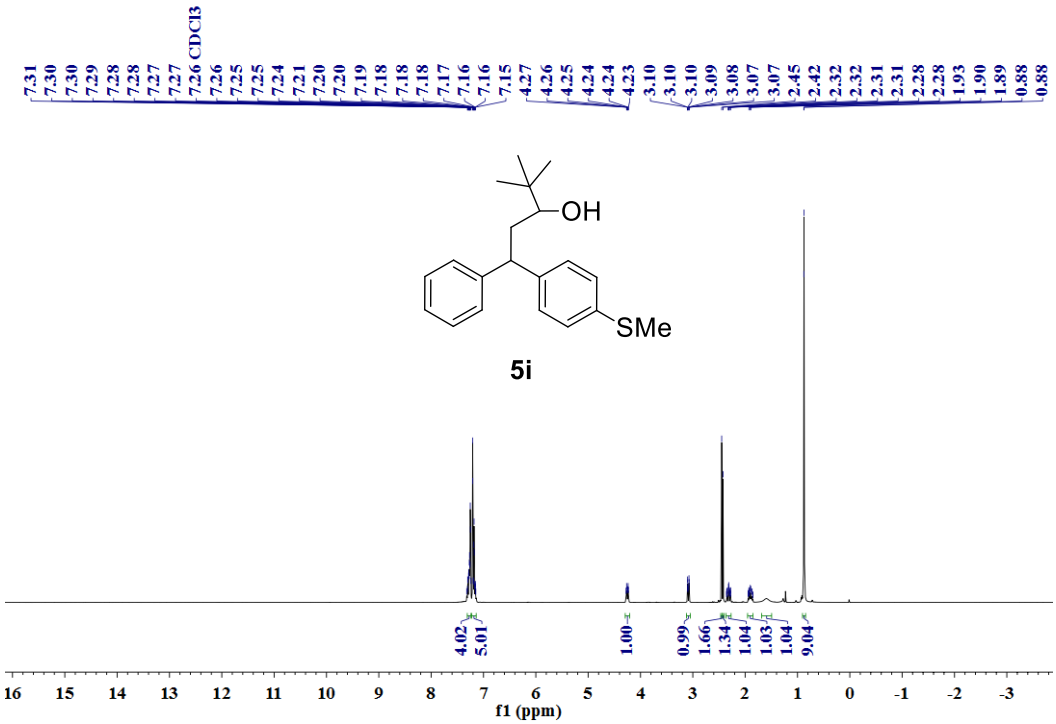
^{1}H NMR (400 MHz, $CDCl_3$):



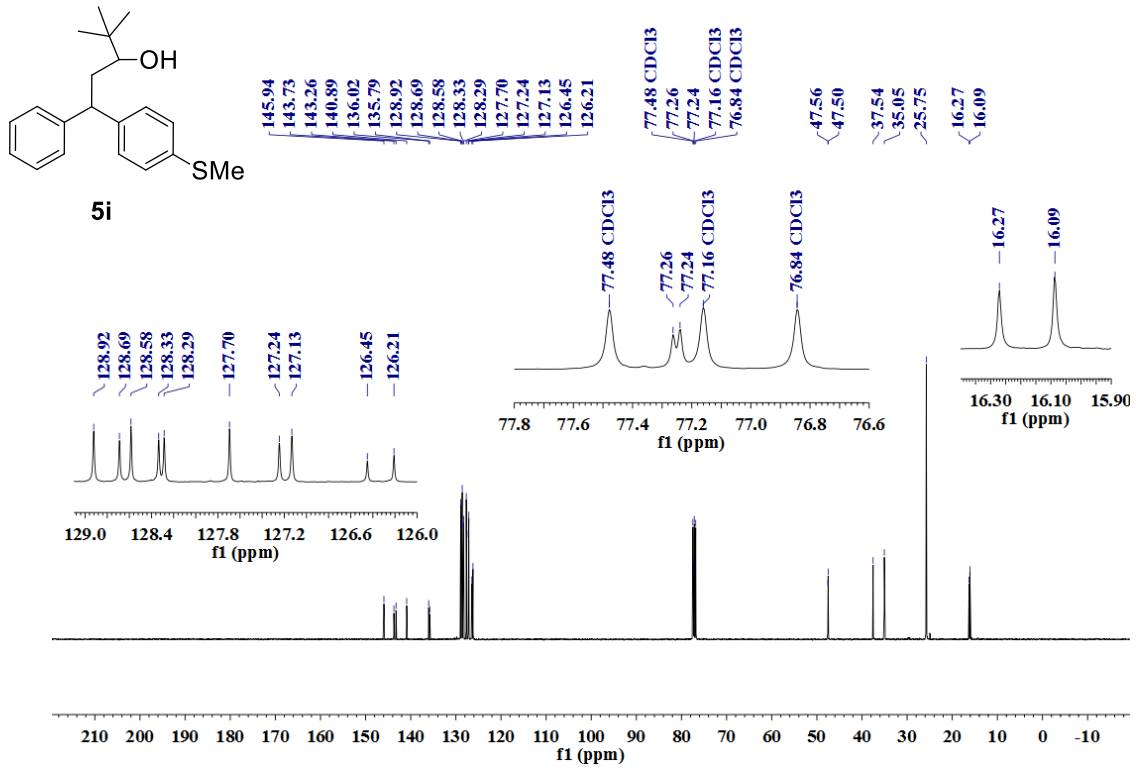
^{13}C NMR (100 MHz, $CDCl_3$):



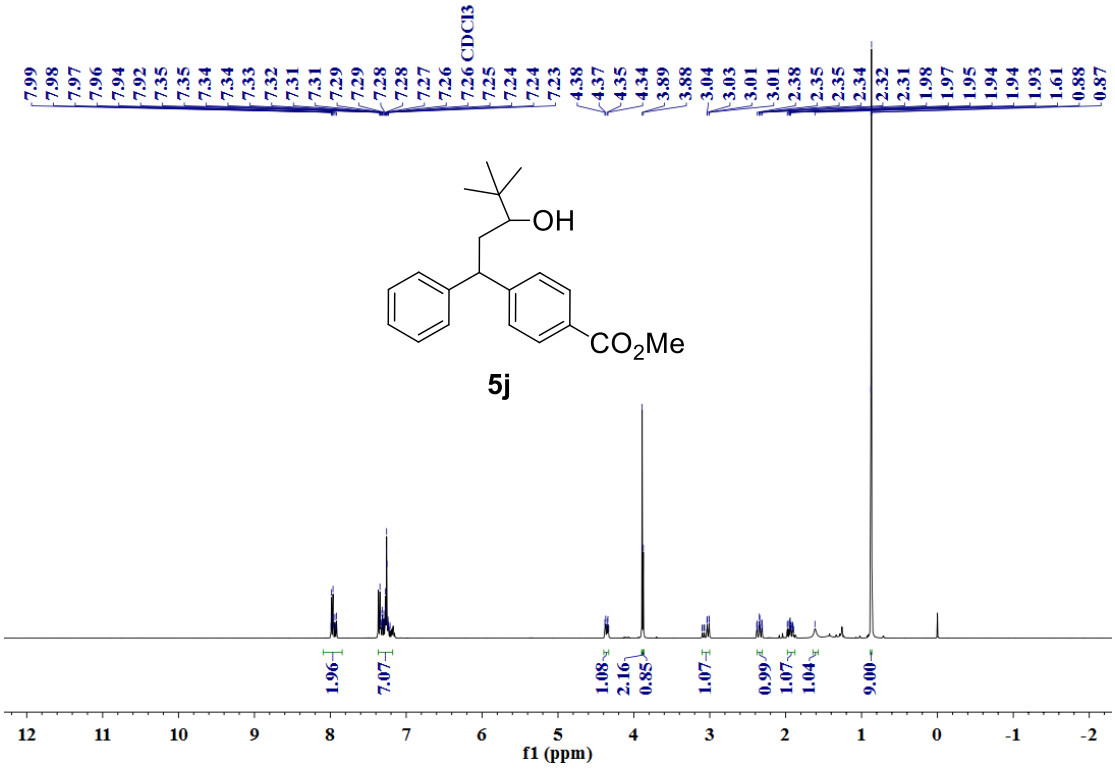
^{1}H NMR (400 MHz, $CDCl_3$):



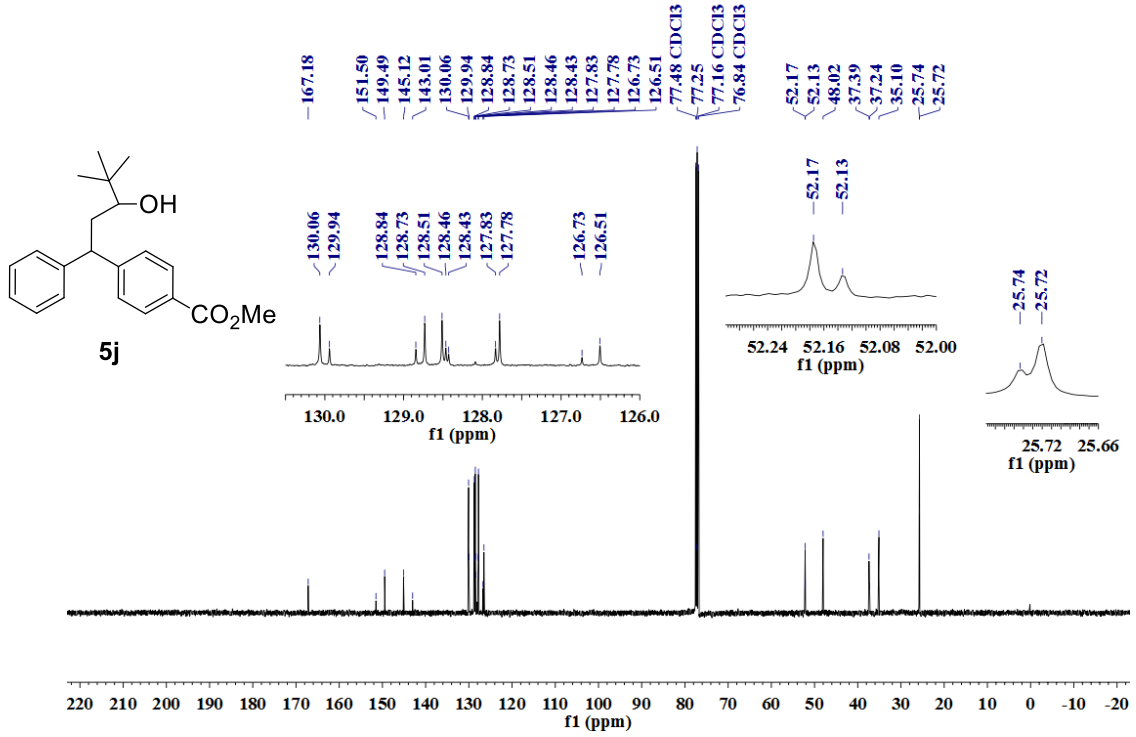
^{13}C NMR (100 MHz, $CDCl_3$):



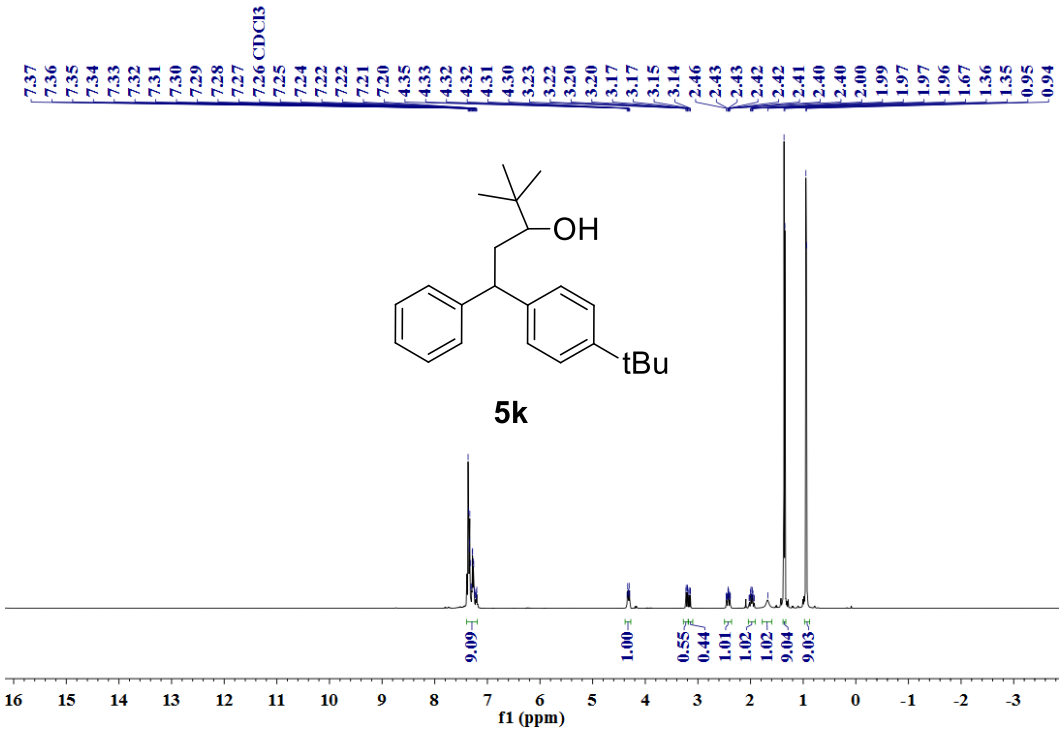
^{1}H NMR (400 MHz, $CDCl_3$):



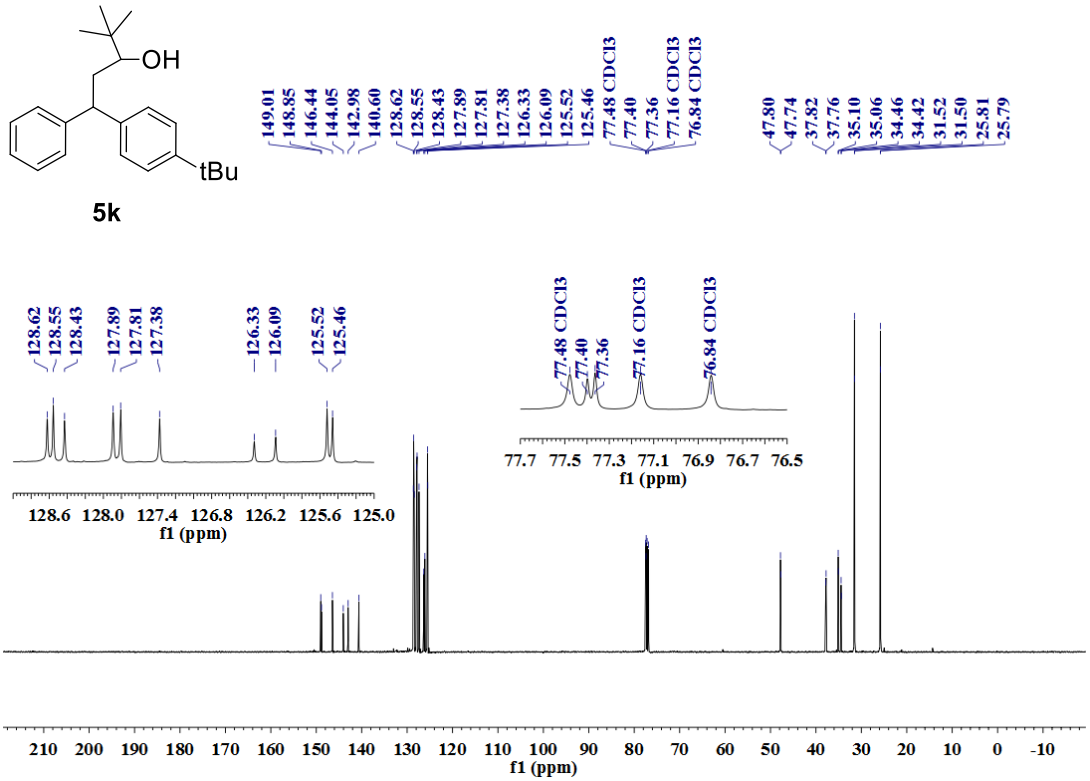
^{13}C NMR (100 MHz, $CDCl_3$):



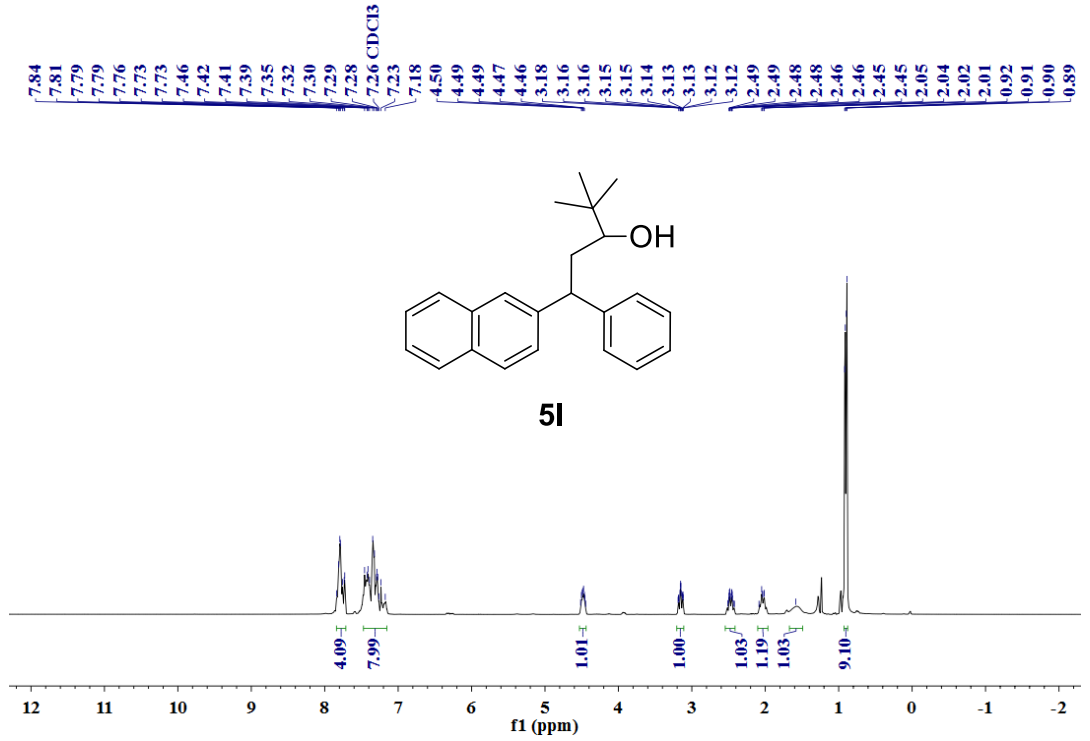
^{1}H NMR (400 MHz, $CDCl_3$):



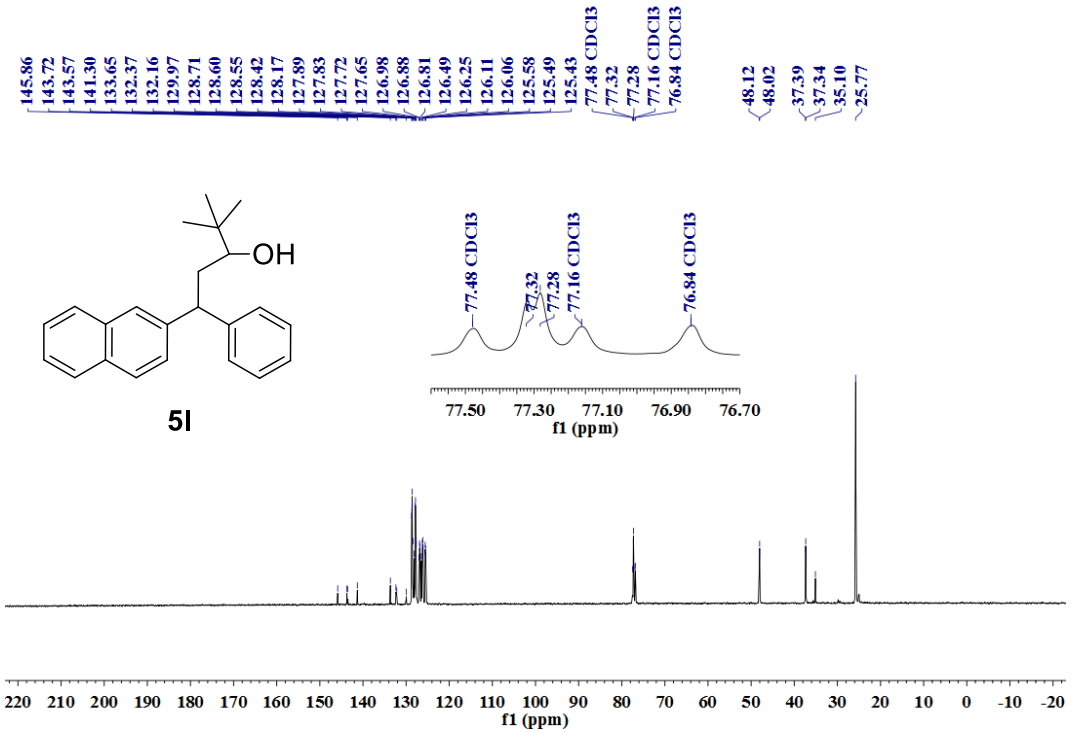
^{13}C NMR (100 MHz, $CDCl_3$):



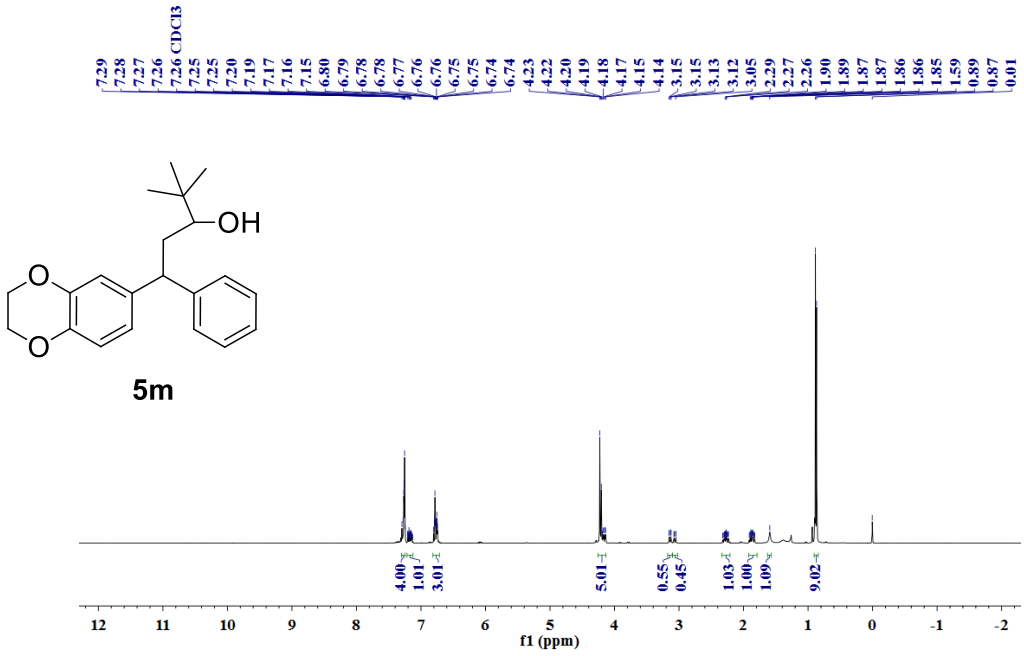
^{1}H NMR (400 MHz, $CDCl_3$):



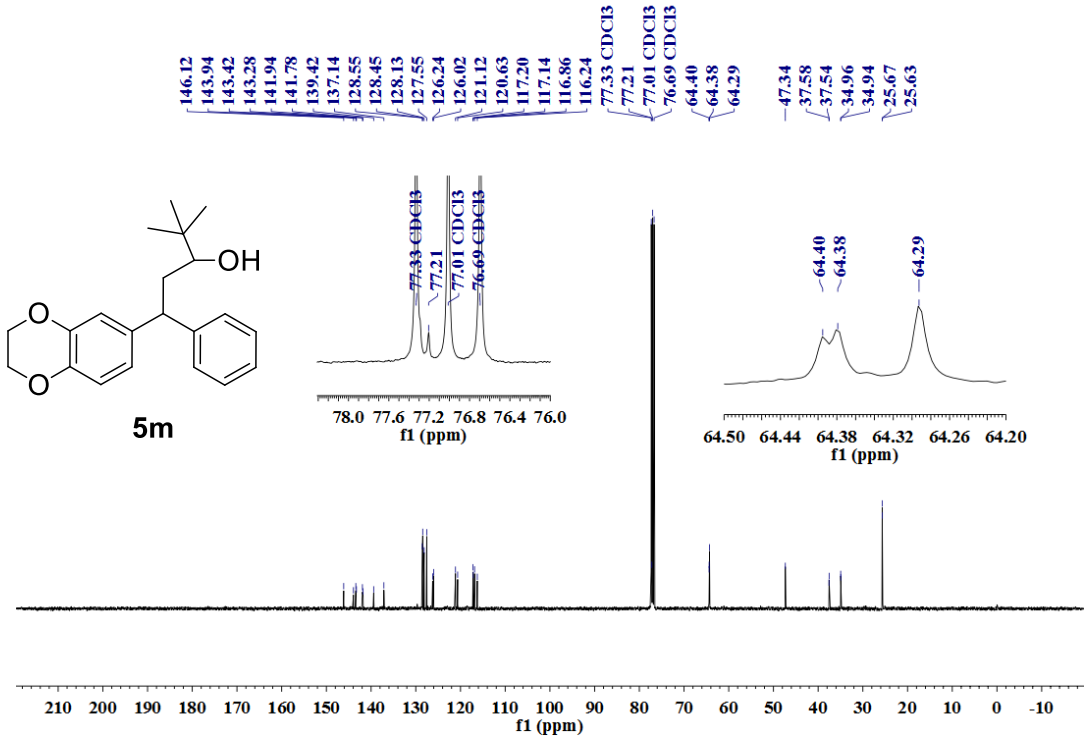
^{13}C NMR (100 MHz, $CDCl_3$):



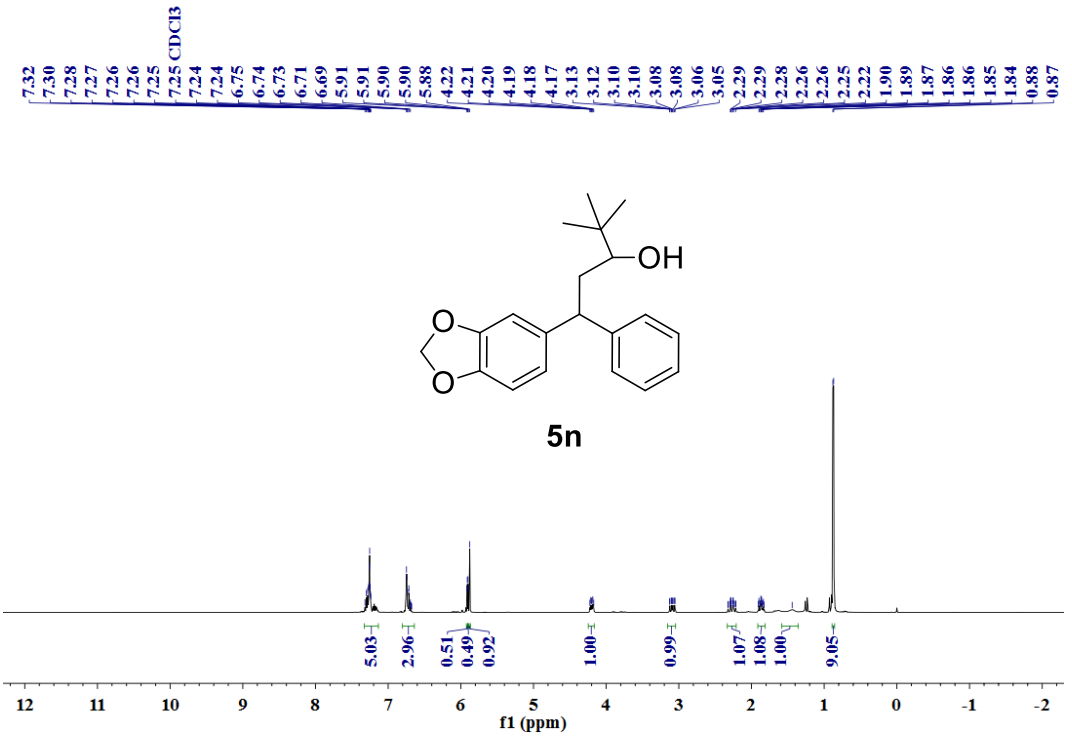
^{1}H NMR (400 MHz, $CDCl_3$):



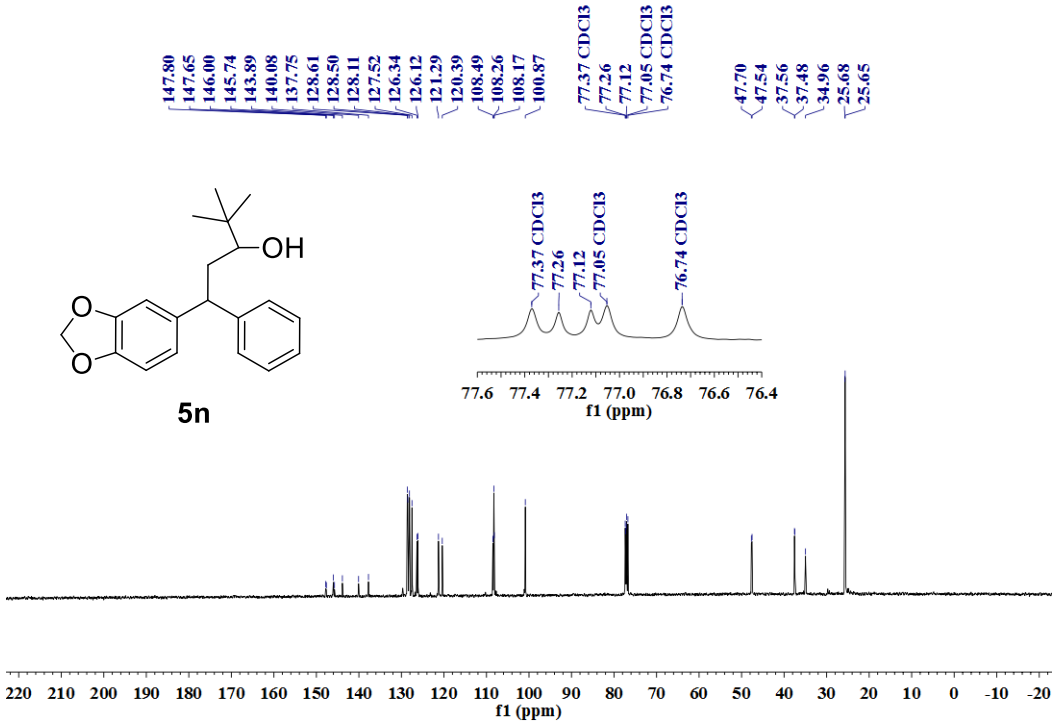
^{13}C NMR (100 MHz, $CDCl_3$):



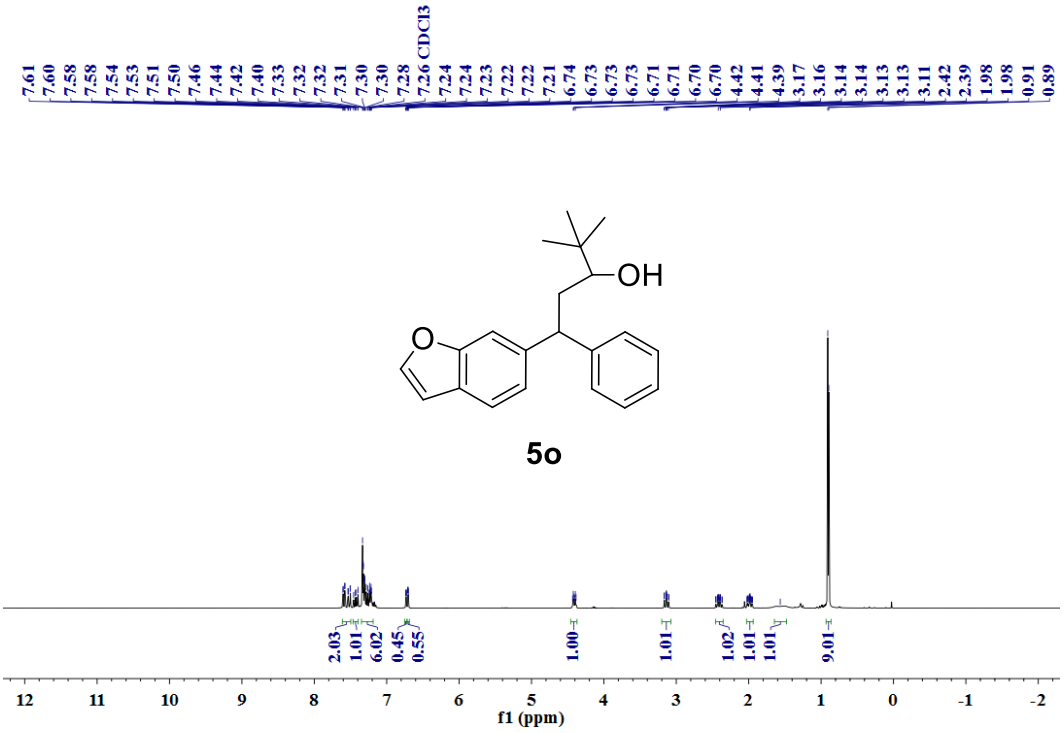
^{1}H NMR (400 MHz, $CDCl_3$):



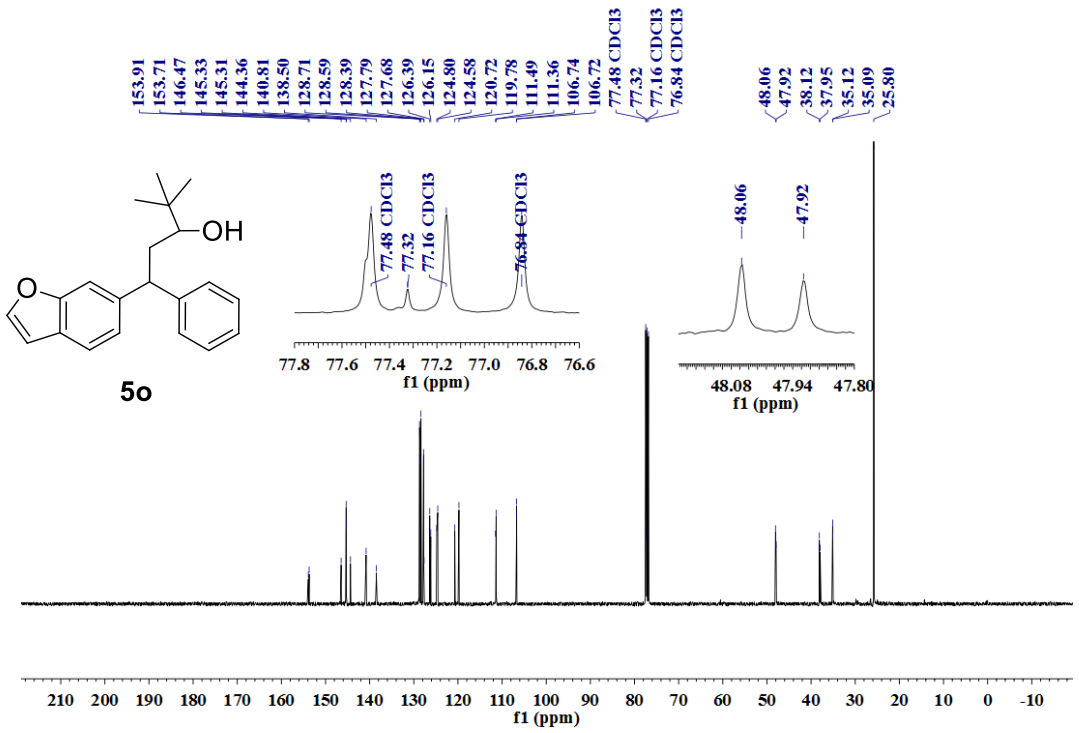
^{13}C NMR (100 MHz, $CDCl_3$):



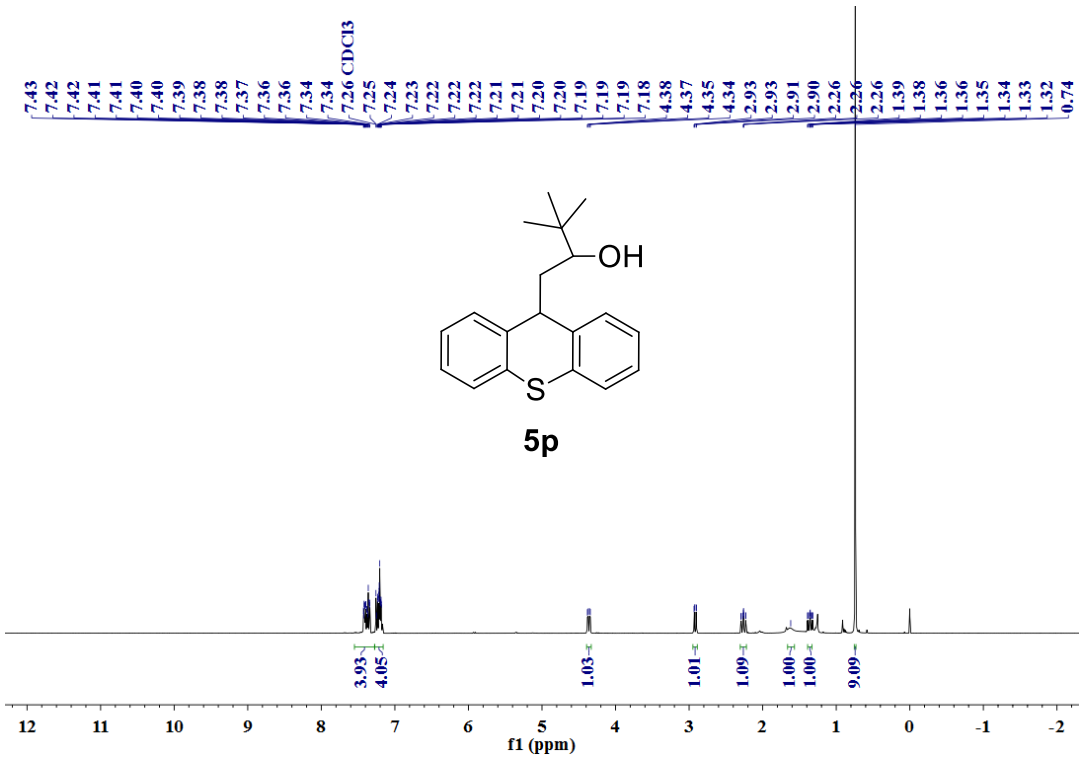
^{1}H NMR (400 MHz, $CDCl_3$):



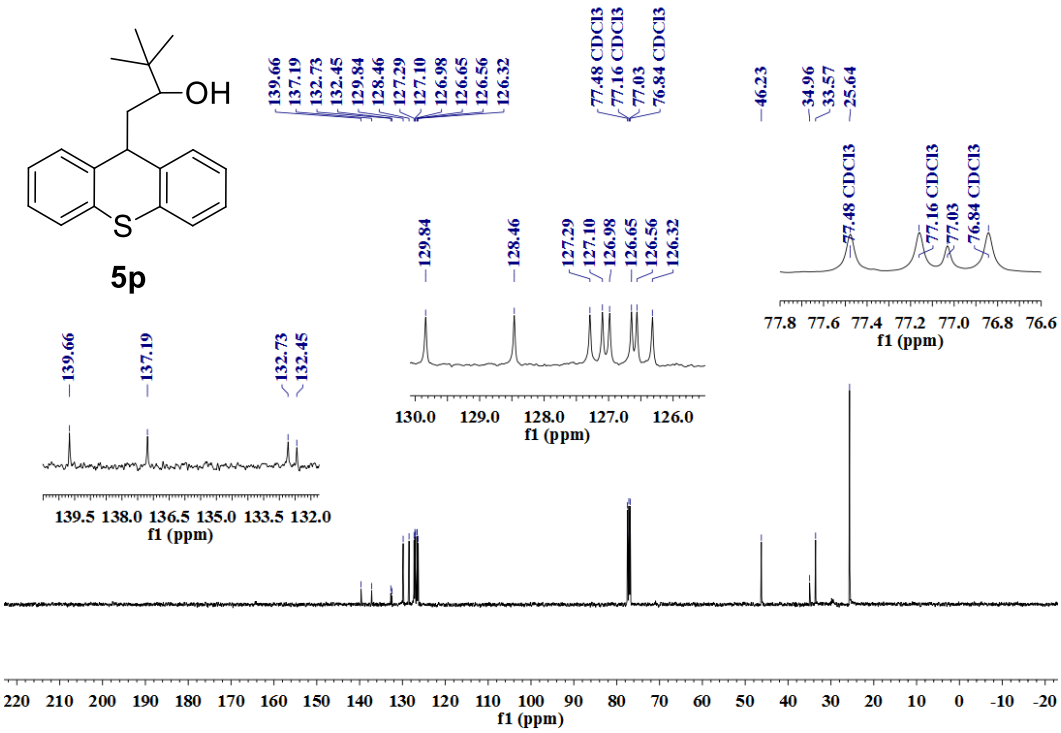
^{13}C NMR (100 MHz, $CDCl_3$):



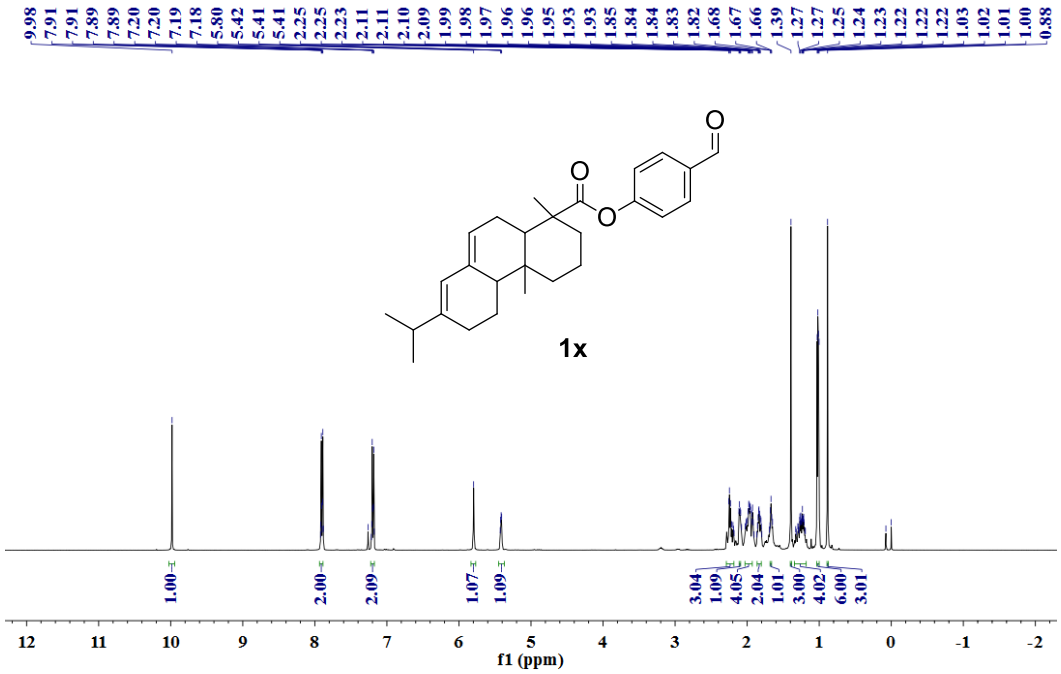
^{1}H NMR (400 MHz, $CDCl_3$):



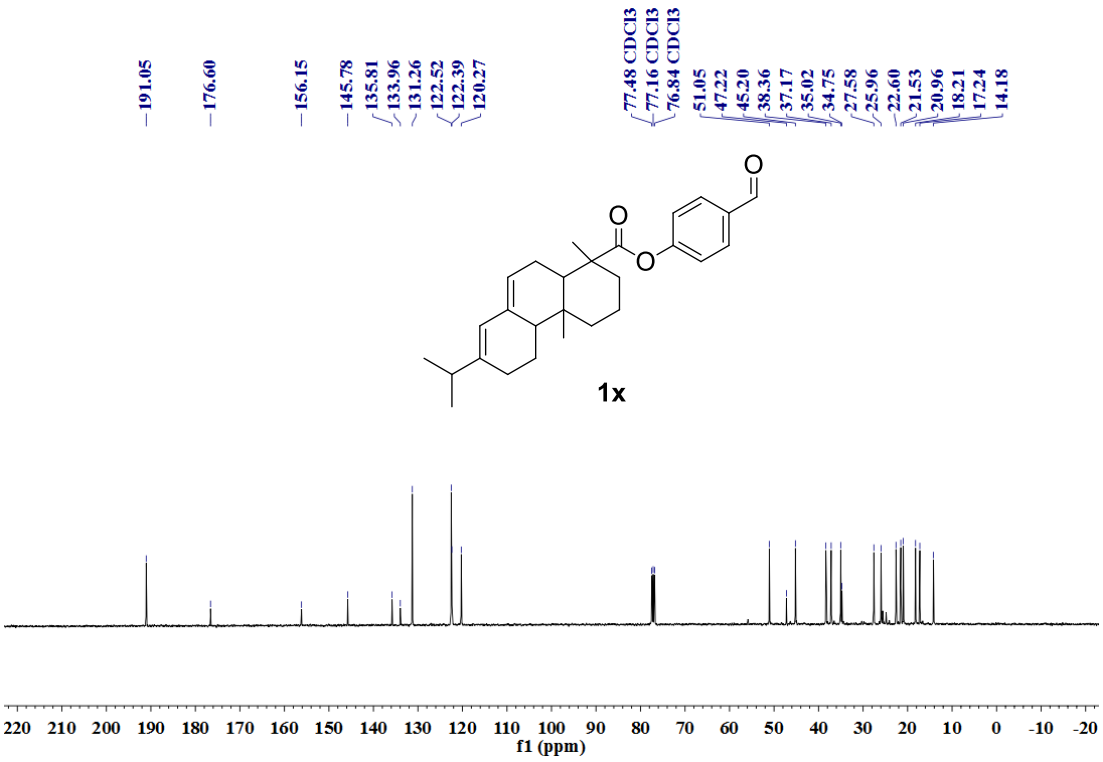
^{13}C NMR (100 MHz, $CDCl_3$):



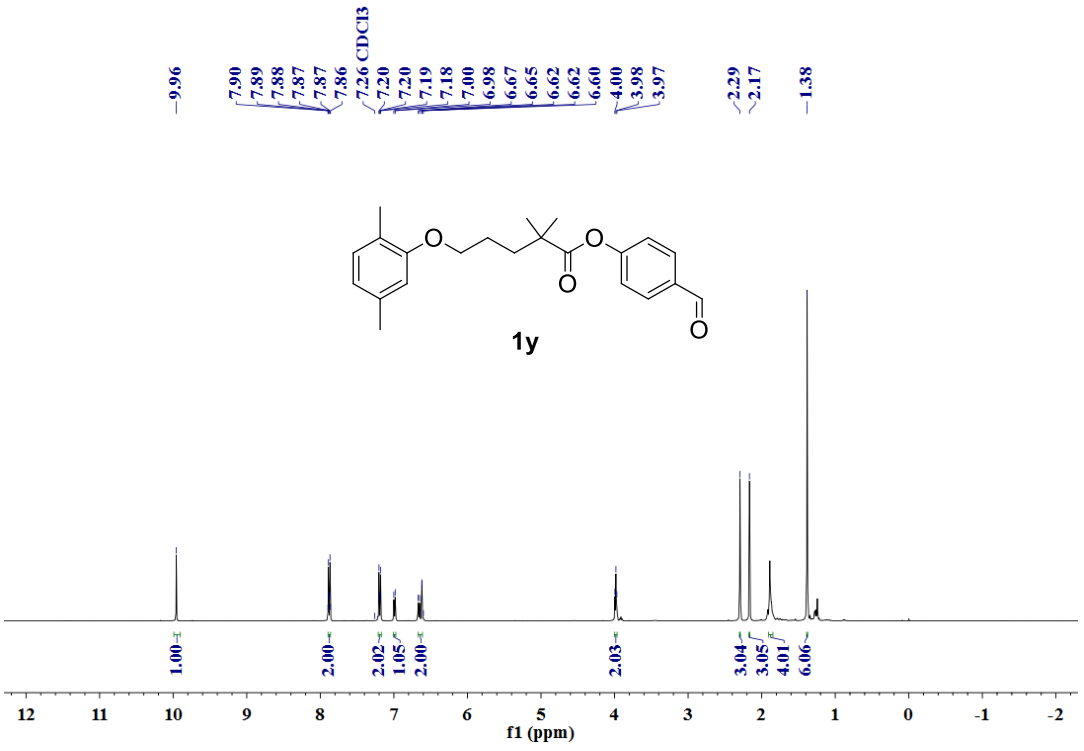
^{1}H NMR (400 MHz, $CDCl_3$):



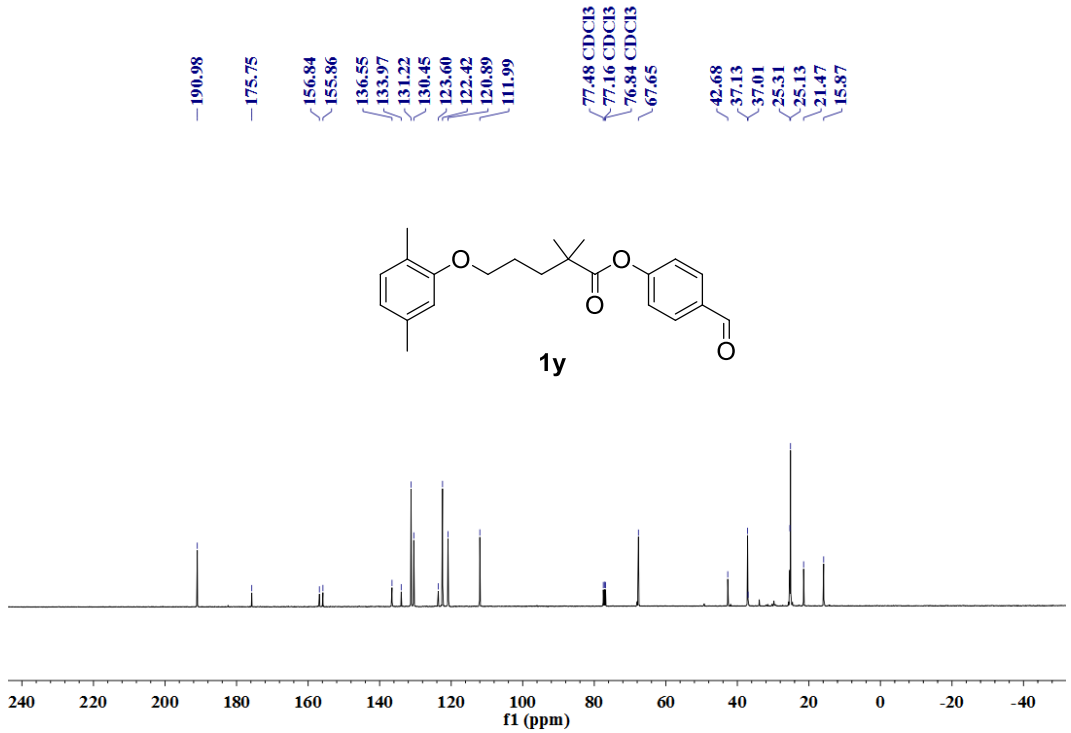
^{13}C NMR (100 MHz, $CDCl_3$):



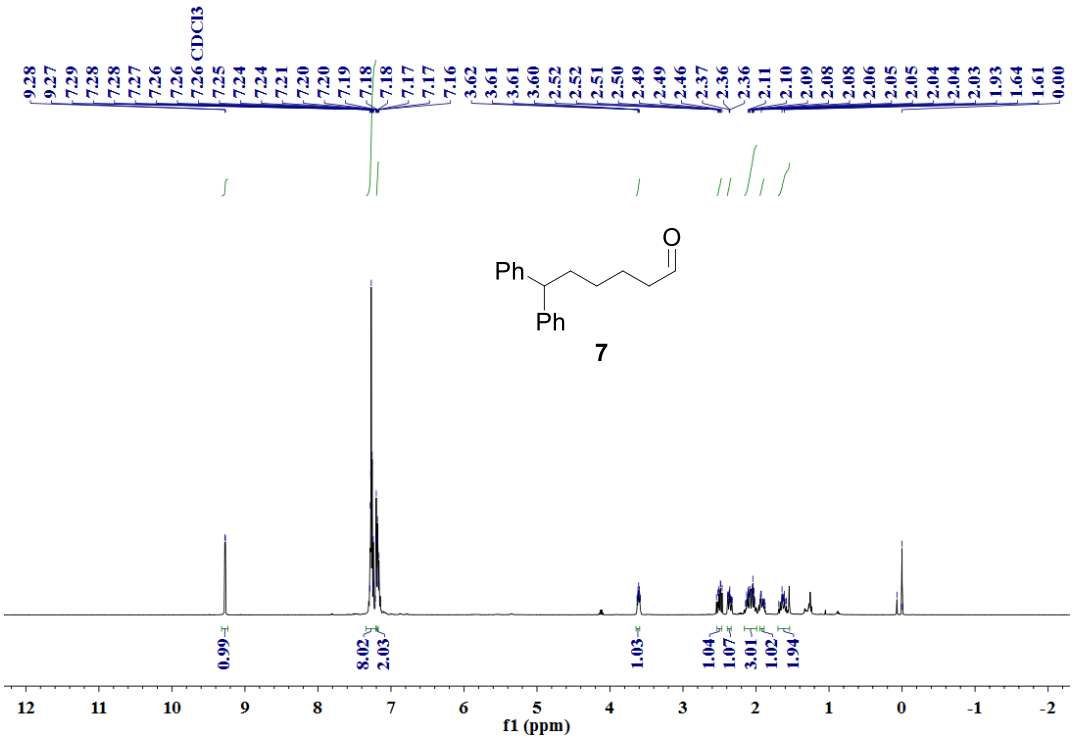
^{1}H NMR (400 MHz, $CDCl_3$):



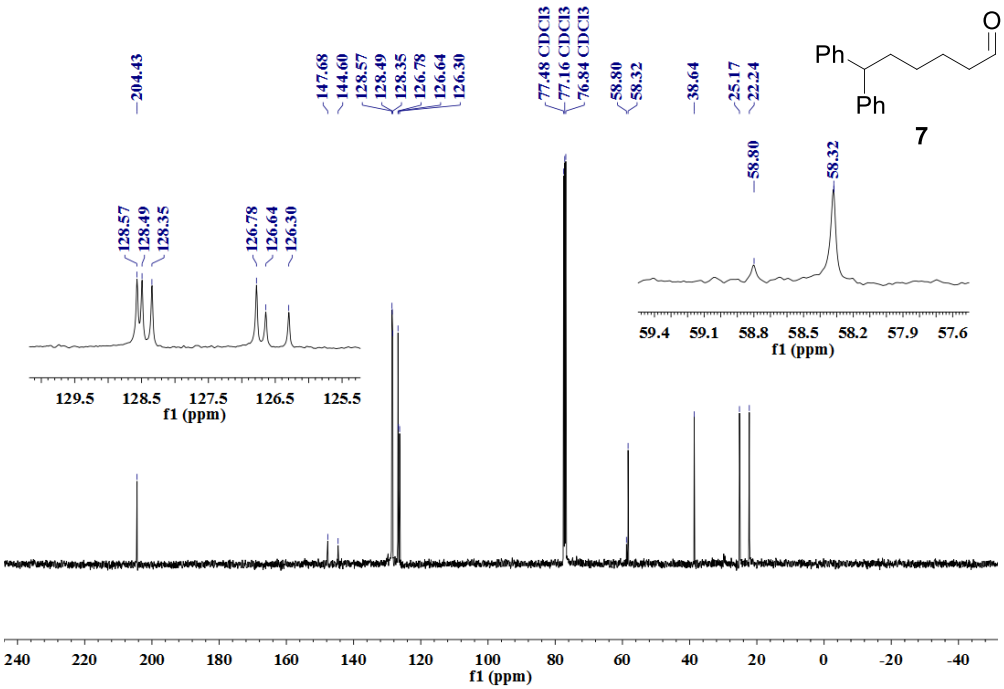
^{13}C NMR (100 MHz, $CDCl_3$):



^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (100 MHz, $CDCl_3$):


204.43
147.68
144.60
128.57
128.49
128.35
126.78
126.64
126.30
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
58.80
58.32
38.64
25.17
22.24
Ph
Ph
O
7
128.57
128.49
128.35
126.78
126.64
126.30
129.5 128.5 127.5 126.5 125.5
f1 (ppm)
58.80
58.32
59.4 59.1 58.8 58.5 58.2 57.9 57.6
f1 (ppm)
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40
f1 (ppm)

6. Cartesian Coordinates and Energies of the Optimized Structures

Geometry optimizations and characters of all the stationary points were calculated by using the M06-2X/6-31G(d,p) method. Single point energies (**Esol**, a.u.) are computed by using the M06-2X/cc-PVTZ method in solvent (benzene). The solvent effect was treated with the polarizable continuum model (PCM).

$B_2(pin)_2$

Thermal correction to Energy=	0.386465
Thermal correction to Enthalpy=	0.387410
Thermal correction to Gibbs Free Energy=	0.317567
Sum of electronic and zero-point Energies=	-821.850963
Sum of electronic and thermal Energies=	-821.830996
Sum of electronic and thermal Enthalpies=	-821.830052
Sum of electronic and thermal Free Energies=	-821.899895

Esol= -822.5113248

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.983276	0.771194	0.121489
2	6	0	-2.984383	-0.771015	-0.121353
3	5	0	-0.852630	-0.001146	-0.001172
4	8	0	-1.615951	1.126403	-0.175872
5	8	0	-1.616995	-1.127869	0.174082
6	6	0	-3.912037	-1.562033	0.786394
7	1	0	-4.950089	-1.244570	0.642717
8	1	0	-3.841497	-2.625233	0.543929
9	1	0	-3.646086	-1.432999	1.836509
10	6	0	-3.224889	1.141002	1.583859
11	1	0	-2.994717	2.200100	1.720257
12	1	0	-4.264423	0.966930	1.875690
13	1	0	-2.572777	0.560956	2.243098
14	6	0	-3.911205	1.563591	-0.784760
15	1	0	-4.949850	1.249842	-0.637302
16	1	0	-3.836318	2.626904	-0.544078
17	1	0	-3.649014	1.432196	-1.835515
18	6	0	-3.228464	-1.140701	-1.583324
19	1	0	-2.999304	-2.199988	-1.719944
20	1	0	-4.268319	-0.965896	-1.873614
21	1	0	-2.576895	-0.561216	-2.243598
22	6	0	2.983452	0.771111	-0.121515

23	6	0	2.984143	-0.771017	0.121527
24	5	0	0.852568	-0.001155	-0.001216
25	8	0	1.615711	1.126437	0.173941
26	8	0	1.617142	-1.127897	-0.175556
27	6	0	3.912892	-1.562442	-0.784723
28	1	0	4.951075	-1.246838	-0.637944
29	1	0	3.839932	-2.625747	-0.543420
30	1	0	3.649968	-1.432040	-1.835421
31	6	0	3.227186	1.140801	-1.583566
32	1	0	2.996968	2.199833	-1.720388
33	1	0	4.267205	0.966953	-1.873825
34	1	0	2.576192	0.560537	-2.243725
35	6	0	3.910139	1.563382	0.786105
36	1	0	4.948802	1.248510	0.641196
37	1	0	3.836826	2.626608	0.544553
38	1	0	3.645458	1.432902	1.836368
39	6	0	3.226521	-1.140176	1.583923
40	1	0	2.997361	-2.199443	1.720710
41	1	0	4.265992	-0.965058	1.875390
42	1	0	2.574093	-0.560516	2.243198

A

Thermal correction to Energy=	0.094380
Thermal correction to Enthalpy=	0.095324
Thermal correction to Gibbs Free Energy=	0.058181
Sum of electronic and zero-point Energies=	-340.300304
Sum of electronic and thermal Energies=	-340.294337
Sum of electronic and thermal Enthalpies=	-340.293393
Sum of electronic and thermal Free Energies=	-340.330537

Esol =-340.5096342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501787	1.140544	-0.000004
2	6	0	0.111946	1.203226	0.000009
3	6	0	-0.594341	0.000000	0.000000
4	6	0	0.111946	-1.203225	-0.000009
5	6	0	1.501788	-1.140543	0.000005
6	7	0	2.193304	0.000000	0.000000
7	1	0	2.087034	2.056307	0.000016

8	1	0	-0.408026	2.153948	0.000025
9	1	0	-0.408026	-2.153948	-0.000024
10	1	0	2.087034	-2.056307	-0.000016
11	6	0	-2.035592	0.000000	0.000000
12	7	0	-3.192093	0.000000	0.000000

TSA1

Thermal correction to Energy= 0.482657
Thermal correction to Enthalpy= 0.483601
Thermal correction to Gibbs Free Energy= 0.400950
Sum of electronic and zero-point Energies= -1162.162192
Sum of electronic and thermal Energies= -1162.136059
Sum of electronic and thermal Enthalpies= -1162.135115
Sum of electronic and thermal Free Energies= -1162.217766

Esol = -1163.0275948

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.194293	2.678111	-1.228755
2	6	0	1.093676	2.770858	1.186928
3	6	0	0.295763	1.621679	-1.174784
4	1	0	1.574670	3.043187	-2.175061
5	6	0	0.197281	1.710989	1.140186
6	1	0	1.397921	3.206114	2.131191
7	1	0	-0.064327	1.100571	-2.058550
8	1	0	-0.240699	1.260752	2.027184
9	7	0	-0.184142	1.169240	-0.015603
10	6	0	2.229823	-2.376356	-0.695364
11	6	0	2.451641	-1.749402	0.715450
12	5	0	0.322112	-1.352721	0.016833
13	8	0	1.003687	-1.745419	-1.115904
14	8	0	1.102291	-1.492622	1.150011
15	6	0	3.140087	-2.657074	1.721375
16	1	0	4.139954	-2.932987	1.370279
17	1	0	3.243695	-2.134633	2.675766
18	1	0	2.562803	-3.566784	1.892507
19	6	0	1.963897	-3.879298	-0.637226
20	1	0	1.602197	-4.209539	-1.613708
21	1	0	2.870070	-4.439617	-0.390133
22	1	0	1.195384	-4.105884	0.107286

23	6	0	3.318003	-2.068784	-1.711465
24	1	0	4.283989	-2.456262	-1.371452
25	1	0	3.073614	-2.545004	-2.664296
26	1	0	3.409512	-0.994383	-1.880737
27	6	0	3.156384	-0.393721	0.652405
28	1	0	3.086603	0.083133	1.633843
29	1	0	4.212545	-0.495297	0.387080
30	1	0	2.673798	0.260244	-0.083254
31	6	0	-3.246860	0.063641	-0.740925
32	6	0	-3.329644	-0.386871	0.753587
33	5	0	-1.162727	-0.509904	0.010567
34	8	0	-1.968912	-0.446715	-1.142847
35	8	0	-1.959055	-0.363609	1.171640
36	6	0	-4.143929	0.533225	1.651482
37	1	0	-5.180423	0.598630	1.304070
38	1	0	-4.149421	0.137174	2.670422
39	1	0	-3.718444	1.538231	1.679385
40	6	0	-3.246042	1.587192	-0.893509
41	1	0	-2.943397	1.836988	-1.914690
42	1	0	-4.241583	2.005138	-0.716488
43	1	0	-2.547104	2.059010	-0.198711
44	6	0	-4.313209	-0.537284	-1.646119
45	1	0	-5.316598	-0.271064	-1.296924
46	1	0	-4.190879	-0.151304	-2.661808
47	1	0	-4.226963	-1.624117	-1.683511
48	6	0	-3.819569	-1.828668	0.897463
49	1	0	-3.648865	-2.151989	1.927204
50	1	0	-4.885610	-1.924630	0.670926
51	1	0	-3.256048	-2.490203	0.233308
52	6	0	1.596273	3.258198	-0.021845
53	6	0	2.529706	4.356219	-0.024993
54	7	0	3.278020	5.237709	-0.027923

IntA1

Thermal correction to Energy=	0.484045
Thermal correction to Enthalpy=	0.484989
Thermal correction to Gibbs Free Energy=	0.400671
Sum of electronic and zero-point Energies=	-1162.163733
Sum of electronic and thermal Energies=	-1162.137111
Sum of electronic and thermal Enthalpies=	-1162.136167
Sum of electronic and thermal Free Energies=	-1162.220485

Esol =-1163.0304342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.564182	-1.186574	-1.318011
2	6	0	3.040021	-1.583877	0.114728
3	5	0	0.970734	-0.564433	0.226913
4	8	0	1.541906	-0.225350	-1.051420
5	8	0	1.822495	-1.536309	0.860176
6	6	0	3.619514	-2.987616	0.223431
7	1	0	4.482827	-3.107263	-0.439869
8	1	0	3.948594	-3.172176	1.249885
9	1	0	2.868141	-3.735855	-0.033065
10	6	0	1.914286	-2.361369	-2.052519
11	1	0	1.416549	-1.977567	-2.946446
12	1	0	2.649321	-3.113598	-2.354636
13	1	0	1.156009	-2.831743	-1.419912
14	6	0	3.636148	-0.546631	-2.188586
15	1	0	4.477849	-1.231292	-2.337002
16	1	0	3.215792	-0.305322	-3.168562
17	1	0	4.009939	0.376813	-1.741074
18	6	0	4.028699	-0.569930	0.700190
19	1	0	4.115261	-0.747449	1.775942
20	1	0	5.021528	-0.668318	0.250707
21	1	0	3.684723	0.456830	0.545868
22	6	0	-2.779898	-1.775052	-0.077920
23	6	0	-2.726029	-1.258757	1.393563
24	5	0	-0.703619	-0.946113	0.376126
25	8	0	-1.385592	-1.825376	-0.435618
26	8	0	-1.519007	-0.468692	1.392636
27	6	0	-3.897263	-0.382759	1.808923
28	1	0	-4.838332	-0.936807	1.730752
29	1	0	-3.771078	-0.069998	2.848678
30	1	0	-3.963306	0.512162	1.188436
31	6	0	-3.448140	-0.782725	-1.028820
32	1	0	-3.257325	-1.101321	-2.056074
33	1	0	-4.529322	-0.736485	-0.869822
34	1	0	-3.029379	0.219277	-0.899049
35	6	0	-3.386708	-3.158998	-0.248157
36	1	0	-4.423785	-3.171775	0.102985
37	1	0	-3.379630	-3.431798	-1.306279
38	1	0	-2.817967	-3.910850	0.300833
39	6	0	-2.517760	-2.384265	2.406310

40	1	0	-2.283548	-1.943531	3.378661
41	1	0	-3.413365	-3.002912	2.511490
42	1	0	-1.680923	-3.021864	2.107397
43	6	0	1.329500	2.062247	0.544055
44	6	0	1.389694	3.243578	1.267837
45	6	0	1.038823	1.938774	3.271606
46	6	0	0.985037	0.809387	2.471002
47	1	0	1.453104	2.005672	-0.532805
48	1	0	1.553099	4.191619	0.770727
49	1	0	0.925737	1.863811	4.345784
50	7	0	1.130270	0.886949	1.145721
51	1	0	0.828409	-0.189908	2.862240
52	6	0	1.242112	3.175529	2.654723
53	6	0	1.301436	4.377344	3.447562
54	7	0	1.349643	5.341760	4.083545

TSA2

Thermal correction to Energy=	0.579814
Thermal correction to Enthalpy=	0.580758
Thermal correction to Gibbs Free Energy=	0.481620
Sum of electronic and zero-point Energies=	-1502.477553
Sum of electronic and thermal Energies=	-1502.444229
Sum of electronic and thermal Enthalpies=	-1502.443285
Sum of electronic and thermal Free Energies=	-1502.542423

Esol = -1503.546605

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.917446	0.673667	2.796028
2	6	0	-3.013189	1.378864	0.760650
3	6	0	-0.710701	0.736051	2.117315
4	1	0	-1.952094	0.379297	3.837532
5	6	0	-1.763252	1.424998	0.161451
6	1	0	-3.906081	1.635109	0.203108
7	1	0	0.240497	0.473904	2.567389
8	1	0	-1.598559	1.720516	-0.870494
9	7	0	-0.653262	1.098565	0.831103
10	6	0	2.099765	-2.442771	1.336900
11	6	0	2.557334	-2.582890	-0.149121
12	5	0	1.178354	-0.765255	0.071392

13	8	0	0.975780	-1.553181	1.233717
14	8	0	2.220504	-1.298982	-0.691225
15	6	0	4.051247	-2.809488	-0.332880
16	1	0	4.372872	-3.725265	0.174444
17	1	0	4.276446	-2.911008	-1.397789
18	1	0	4.624656	-1.967106	0.057035
19	6	0	3.143977	-1.733343	2.200916
20	1	0	2.696122	-1.502224	3.171387
21	1	0	4.029322	-2.353709	2.367077
22	1	0	3.444813	-0.791537	1.731961
23	6	0	1.657341	-3.741108	1.993878
24	1	0	2.479634	-4.463735	2.017376
25	1	0	1.347929	-3.544925	3.024098
26	1	0	0.815060	-4.188240	1.461898
27	6	0	1.772379	-3.652260	-0.910493
28	1	0	1.961626	-3.526074	-1.979755
29	1	0	2.081133	-4.660313	-0.617608
30	1	0	0.698093	-3.551098	-0.740109
31	6	0	1.993877	2.938008	0.102065
32	6	0	1.681643	2.568603	-1.382414
33	5	0	0.854582	0.928586	0.020248
34	8	0	1.822677	1.687601	0.767092
35	8	0	0.638743	1.599529	-1.247927
36	6	0	1.180284	3.726805	-2.232904
37	1	0	1.925925	4.527367	-2.279409
38	1	0	0.991295	3.379605	-3.252563
39	1	0	0.250170	4.137526	-1.834073
40	6	0	0.993081	3.950159	0.669565
41	1	0	1.092333	3.964766	1.758470
42	1	0	1.177108	4.959763	0.289511
43	1	0	-0.035572	3.673129	0.420922
44	6	0	3.415116	3.426437	0.346184
45	1	0	3.634556	4.315210	-0.255203
46	1	0	3.537766	3.688085	1.400881
47	1	0	4.136976	2.645172	0.103196
48	6	0	2.867719	1.880444	-2.061901
49	1	0	2.530946	1.472111	-3.019079
50	1	0	3.690667	2.575901	-2.252693
51	1	0	3.226087	1.048799	-1.448292
52	6	0	-1.596509	-1.843269	-0.261674
53	6	0	-2.903559	-1.854183	-0.732883
54	6	0	-2.077949	-0.812489	-2.751115
55	6	0	-0.806871	-0.844072	-2.187055
56	1	0	-1.325457	-2.219787	0.722904

57	1	0	-3.714600	-2.253774	-0.135392
58	1	0	-2.241747	-0.396680	-3.738079
59	7	0	-0.582989	-1.348256	-0.972960
60	1	0	0.059540	-0.422717	-2.687480
61	6	0	-3.087079	0.992998	2.100889
62	6	0	-3.141814	-1.323641	-2.003868
63	6	0	-4.481335	-1.289255	-2.534334
64	7	0	-5.557595	-1.252307	-2.955999
65	6	0	-4.363911	0.918932	2.764124
66	7	0	-5.388246	0.853765	3.296632

IntA2

Thermal correction to Energy=	0.580853
Thermal correction to Enthalpy=	0.581798
Thermal correction to Gibbs Free Energy=	0.484598
Sum of electronic and zero-point Energies=	-1502.480483
Sum of electronic and thermal Energies=	-1502.447245
Sum of electronic and thermal Enthalpies=	-1502.446301
Sum of electronic and thermal Free Energies=	-1502.543500

Esol =-1503.5496756

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.785968	2.077328	-3.199423
2	6	0	-1.478111	3.434561	-1.323760
3	6	0	-0.811156	0.976705	-2.361448
4	1	0	-0.513848	1.970166	-4.241972
5	6	0	-1.485309	2.283218	-0.552796
6	1	0	-1.753003	4.389911	-0.893683
7	1	0	-0.558447	-0.027897	-2.680535
8	1	0	-1.765307	2.261216	0.496290
9	7	0	-1.152677	1.091564	-1.068662
10	6	0	2.464564	-1.144416	-1.325657
11	6	0	2.653904	-1.684267	0.127363
12	5	0	0.879440	-0.214157	0.074851
13	8	0	1.667296	0.025823	-1.121483
14	8	0	1.392519	-1.389664	0.726992
15	6	0	2.895626	-3.184006	0.219440
16	1	0	3.785650	-3.475310	-0.348571
17	1	0	3.048596	-3.468088	1.264333

18	1	0	2.033467	-3.734736	-0.160201
19	6	0	1.654503	-2.112844	-2.191126
20	1	0	1.409291	-1.612938	-3.133911
21	1	0	2.217016	-3.021053	-2.427536
22	1	0	0.720806	-2.380881	-1.685867
23	6	0	3.755454	-0.752524	-2.030095
24	1	0	4.425722	-1.613556	-2.122590
25	1	0	3.529305	-0.388790	-3.036347
26	1	0	4.275603	0.041247	-1.490279
27	6	0	3.752523	-0.927657	0.881230
28	1	0	3.667002	-1.158977	1.946654
29	1	0	4.751861	-1.216843	0.541892
30	1	0	3.645156	0.153599	0.751849
31	6	0	-2.653901	-1.684274	-0.127363
32	6	0	-2.464566	-1.144417	1.325656
33	5	0	-0.879441	-0.214160	-0.074852
34	8	0	-1.392515	-1.389671	-0.726988
35	8	0	-1.667301	0.025823	1.121479
36	6	0	-3.755460	-0.752524	2.030088
37	1	0	-4.425727	-1.613557	2.122584
38	1	0	-3.529315	-0.388786	3.036339
39	1	0	-4.275608	0.041243	1.490267
40	6	0	-3.752518	-0.927670	-0.881236
41	1	0	-3.666995	-1.158995	-1.946658
42	1	0	-4.751857	-1.216855	-0.541898
43	1	0	-3.645153	0.153587	-0.751860
44	6	0	-2.895619	-3.184014	-0.219434
45	1	0	-3.785645	-3.475318	0.348576
46	1	0	-3.048586	-3.468101	-1.264326
47	1	0	-2.033461	-3.734740	0.160212
48	6	0	-1.654507	-2.112840	2.191132
49	1	0	-1.409301	-1.612931	3.133917
50	1	0	-2.217018	-3.021050	2.427541
51	1	0	-0.720806	-2.380875	1.685878
52	6	0	1.485240	2.283242	0.552778
53	6	0	1.478039	3.434581	1.323747
54	6	0	0.786040	2.077314	3.199439
55	6	0	0.811226	0.976696	2.361458
56	1	0	1.765185	2.261255	-0.496323
57	1	0	1.752874	4.389943	0.893661
58	1	0	0.513976	1.970137	4.242001
59	7	0	1.152677	1.091574	1.068655
60	1	0	0.558570	-0.027917	2.680553
61	6	0	-1.119013	3.328360	-2.669800

62	6	0	1.119012	3.328361	2.669805
63	6	0	1.093294	4.500118	3.505630
64	7	0	1.069615	5.443517	4.174314
65	6	0	-1.093296	4.500122	-3.505618
66	7	0	-1.069618	5.443525	-4.174297

TSA3

Thermal correction to Energy= 0.579963
Thermal correction to Enthalpy= 0.580908
Thermal correction to Gibbs Free Energy= 0.486567
Sum of electronic and zero-point Energies= -1502.476367
Sum of electronic and thermal Energies= -1502.443837
Sum of electronic and thermal Enthalpies= -1502.442893
Sum of electronic and thermal Free Energies= -1502.537234

Esol = -1503.5444016

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.566661	-2.219168	-2.353764
2	6	0	3.001715	-0.386039	-1.721474
3	6	0	0.483144	-1.464516	-1.990711
4	1	0	1.421705	-3.212790	-2.759502
5	6	0	1.872929	0.327127	-1.360330
6	1	0	3.979190	0.071265	-1.620944
7	1	0	-0.540800	-1.802887	-2.081787
8	1	0	1.902805	1.351022	-1.004286
9	7	0	0.627241	-0.202029	-1.487298
10	6	0	-1.636264	-2.525140	1.100568
11	6	0	-2.267003	-1.459973	2.057514
12	5	0	-0.575689	-0.506082	0.874350
13	8	0	-0.396537	-1.904079	0.715806
14	8	0	-1.824659	-0.220721	1.480867
15	6	0	-3.786368	-1.461023	2.094233
16	1	0	-4.169133	-2.434474	2.418070
17	1	0	-4.136690	-0.703862	2.800913
18	1	0	-4.195139	-1.226583	1.109596
19	6	0	-2.471455	-2.740514	-0.160278
20	1	0	-1.895437	-3.361157	-0.854086
21	1	0	-3.405527	-3.264522	0.062524
22	1	0	-2.695098	-1.784101	-0.642527
23	6	0	-1.323080	-3.858854	1.762939

24	1	0	-2.233856	-4.313786	2.165951
25	1	0	-0.898866	-4.543831	1.024107
26	1	0	-0.600180	-3.739348	2.571575
27	6	0	-1.693048	-1.542651	3.473138
28	1	0	-2.002967	-0.653899	4.028779
29	1	0	-2.048926	-2.428914	4.006420
30	1	0	-0.598874	-1.568501	3.447790
31	6	0	-2.267085	1.459904	-2.057537
32	6	0	-1.636340	2.525070	-1.100584
33	5	0	-0.575674	0.506047	-0.874445
34	8	0	-1.824593	0.220639	-1.481031
35	8	0	-0.396591	1.904041	-0.715851
36	6	0	-1.323170	3.858805	-1.762914
37	1	0	-2.233988	4.313871	-2.165680
38	1	0	-0.898730	4.543657	-1.024097
39	1	0	-0.600451	3.739320	-2.571713
40	6	0	-1.693298	1.542697	-3.473218
41	1	0	-2.003255	0.653975	-4.028884
42	1	0	-2.049259	2.428988	-4.006400
43	1	0	-0.599120	1.568568	-3.447986
44	6	0	-3.786458	1.460858	-2.094070
45	1	0	-4.169335	2.434431	-2.417411
46	1	0	-4.136840	0.703997	-2.801041
47	1	0	-4.195058	1.225950	-1.109472
48	6	0	-2.471530	2.740419	0.160270
49	1	0	-1.895585	3.361174	0.854039
50	1	0	-3.405674	3.264293	-0.062547
51	1	0	-2.695058	1.784004	0.642567
52	6	0	1.872884	-0.327067	1.360350
53	6	0	3.001629	0.386144	1.721528
54	6	0	1.566483	2.219213	2.353775
55	6	0	0.483007	1.464516	1.990688
56	1	0	1.902816	-1.350965	1.004321
57	1	0	3.979124	-0.071122	1.621025
58	1	0	1.421472	3.212828	2.759512
59	7	0	0.627168	0.202040	1.487266
60	1	0	-0.540953	1.802843	2.081750
61	6	0	2.864303	-1.683561	-2.216406
62	6	0	2.864152	1.683663	2.216450
63	6	0	4.015367	2.452221	2.586377
64	7	0	4.945345	3.075711	2.882736
65	6	0	4.015556	-2.452071	-2.586318
66	7	0	4.945555	-3.075531	-2.882672

IntA3

Thermal correction to Energy= 0.584419
Thermal correction to Enthalpy= 0.585364
Thermal correction to Gibbs Free Energy= 0.490141
Sum of electronic and zero-point Energies= -1502.542337
Sum of electronic and thermal Energies= -1502.509748
Sum of electronic and thermal Enthalpies= -1502.508803
Sum of electronic and thermal Free Energies= -1502.604026

Esol =-1503.6203191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192411	2.918531	-0.064897
2	6	0	-2.265922	0.855173	-0.809719
3	6	0	0.017750	2.368775	-0.277069
4	1	0	-1.294106	3.935734	0.285978
5	6	0	-0.963968	0.155567	-0.535331
6	1	0	-3.108999	0.298453	-1.202832
7	1	0	0.943598	2.920113	-0.155419
8	1	0	-0.825382	-0.704150	-1.197988
9	7	0	0.159565	1.068443	-0.739529
10	6	0	2.399557	1.473403	2.999795
11	6	0	3.261204	0.164621	3.064959
12	5	0	1.355574	-0.217096	1.924984
13	8	0	1.116824	0.979379	2.547387
14	8	0	2.653518	-0.658825	2.042750
15	6	0	4.730203	0.352394	2.728815
16	1	0	5.203630	1.030687	3.445580
17	1	0	5.241980	-0.611951	2.779209
18	1	0	4.855815	0.760237	1.724315
19	6	0	2.902889	2.461933	1.953014
20	1	0	2.161819	3.258607	1.847194
21	1	0	3.850140	2.914096	2.260405
22	1	0	3.037030	1.980959	0.978552
23	6	0	2.204511	2.169772	4.336803
24	1	0	3.168698	2.482964	4.749644
25	1	0	1.587649	3.060427	4.195053
26	1	0	1.705452	1.519598	5.056463
27	6	0	3.103367	-0.584015	4.386124
28	1	0	3.560946	-1.571143	4.287754

29	1	0	3.590226	-0.052629	5.208039
30	1	0	2.046465	-0.719593	4.633978
31	6	0	3.437111	0.737400	-2.235186
32	6	0	2.920858	-0.742810	-2.268869
33	5	0	1.387095	0.608614	-1.308586
34	8	0	2.540299	1.358174	-1.285844
35	8	0	1.515940	-0.590416	-1.958684
36	6	0	3.048389	-1.425081	-3.620960
37	1	0	4.098781	-1.477570	-3.924679
38	1	0	2.660603	-2.444120	-3.551800
39	1	0	2.484311	-0.896130	-4.390246
40	6	0	3.244598	1.463657	-3.564159
41	1	0	3.432844	2.529066	-3.413381
42	1	0	3.933457	1.090845	-4.326623
43	1	0	2.220376	1.345188	-3.929846
44	6	0	4.862980	0.902059	-1.738421
45	1	0	5.560985	0.379437	-2.400079
46	1	0	5.127288	1.962522	-1.729988
47	1	0	4.977590	0.508020	-0.726818
48	6	0	3.535918	-1.608327	-1.173878
49	1	0	3.005454	-2.564025	-1.150468
50	1	0	4.592618	-1.807509	-1.373236
51	1	0	3.442695	-1.134676	-0.190851
52	6	0	-0.955623	-0.376781	0.938995
53	6	0	-2.050984	-1.391630	1.116033
54	6	0	-0.422711	-3.103837	0.499804
55	6	0	0.582379	-2.261421	0.802488
56	1	0	-1.099686	0.484114	1.599023
57	1	0	-3.038408	-1.073711	1.430537
58	1	0	-0.228543	-4.112452	0.163155
59	7	0	0.345422	-0.969108	1.248629
60	1	0	1.625171	-2.557081	0.771565
61	6	0	-2.367400	2.159121	-0.486852
62	6	0	-1.785168	-2.675900	0.809525
63	6	0	-2.822166	-3.673264	0.881555
64	7	0	-3.644721	-4.486049	0.926494
65	6	0	-3.619896	2.853224	-0.643575
66	7	0	-4.621534	3.422403	-0.752386

TSA4

Thermal correction to Energy= 0.580769

Thermal correction to Enthalpy= 0.581713

Thermal correction to Gibbs Free Energy= 0.485500

Sum of electronic and zero-point Energies= -1502.501972
Sum of electronic and thermal Energies= -1502.469157
Sum of electronic and thermal Enthalpies= -1502.468213
Sum of electronic and thermal Free Energies= -1502.564426

Esol = -1503.5796455

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.813266	-0.721878	-3.081922
2	6	0	3.295701	0.440979	-1.557725
3	6	0	0.752098	-0.205929	-2.431409
4	1	0	1.657925	-1.363977	-3.939803
5	6	0	2.185340	0.850480	-0.820900
6	1	0	4.281445	0.718931	-1.199876
7	1	0	-0.269332	-0.373921	-2.743638
8	1	0	2.255235	1.600607	-0.042401
9	7	0	0.895381	0.642158	-1.326602
10	6	0	-1.468480	-2.858782	-0.354684
11	6	0	-2.248458	-2.351226	0.909340
12	5	0	-0.239303	-1.350731	0.795476
13	8	0	-0.128427	-2.359375	-0.120751
14	8	0	-1.513982	-1.157179	1.274434
15	6	0	-3.697073	-1.974706	0.652669
16	1	0	-4.266287	-2.848325	0.320038
17	1	0	-4.147312	-1.605991	1.578162
18	1	0	-3.773524	-1.195051	-0.106838
19	6	0	-1.977210	-2.236513	-1.649976
20	1	0	-1.272880	-2.479213	-2.449970
21	1	0	-2.957412	-2.640495	-1.918846
22	1	0	-2.054468	-1.148492	-1.561217
23	6	0	-1.398097	-4.371605	-0.487604
24	1	0	-2.404166	-4.794108	-0.573899
25	1	0	-0.839655	-4.630824	-1.390092
26	1	0	-0.895825	-4.825681	0.367551
27	6	0	-2.143244	-3.306615	2.095937
28	1	0	-2.537030	-2.808968	2.985026
29	1	0	-2.715573	-4.221966	1.924615
30	1	0	-1.100792	-3.577540	2.288463
31	6	0	-2.248562	2.351353	-0.909353
32	6	0	-1.468470	2.858989	0.354541
33	5	0	-0.239335	1.350993	-0.795679

34	8	0	-1.514081	1.157298	-1.274411
35	8	0	-0.128361	2.359854	0.120304
36	6	0	-1.398406	4.371808	0.487566
37	1	0	-2.404561	4.794080	0.573985
38	1	0	-0.839930	4.631101	1.390011
39	1	0	-0.896324	4.826038	-0.367620
40	6	0	-2.143488	3.306673	-2.096015
41	1	0	-2.537277	2.808932	-2.985051
42	1	0	-2.715899	4.221978	-1.924716
43	1	0	-1.101073	3.577692	-2.288609
44	6	0	-3.697145	1.974840	-0.652491
45	1	0	-4.266279	2.848462	-0.319727
46	1	0	-4.147546	1.606182	-1.577928
47	1	0	-3.773493	1.195158	0.106996
48	6	0	-1.976771	2.236381	1.649835
49	1	0	-1.272196	2.478927	2.449658
50	1	0	-2.956946	2.640158	1.919107
51	1	0	-2.053919	1.148372	1.560703
52	6	0	2.185402	-0.850334	0.820800
53	6	0	3.295764	-0.440941	1.557669
54	6	0	1.813352	0.721461	3.082233
55	6	0	0.752175	0.205697	2.431587
56	1	0	2.255266	-1.600335	0.042176
57	1	0	4.281503	-0.718761	1.199703
58	1	0	1.658020	1.363261	3.940340
59	7	0	0.895449	-0.642038	1.326499
60	1	0	-0.269244	0.373517	2.743953
61	6	0	3.152845	-0.376288	-2.666508
62	6	0	3.152924	0.376058	2.666655
63	6	0	4.284493	0.862746	3.380465
64	7	0	5.199866	1.266103	3.969703
65	6	0	4.284359	-0.863040	-3.380257
66	7	0	5.199719	-1.266481	-3.969456

IntA4

Thermal correction to Energy=	0.288834
Thermal correction to Enthalpy=	0.289778
Thermal correction to Gibbs Free Energy=	0.227912
Sum of electronic and zero-point Energies=	-751.250341
Sum of electronic and thermal Energies=	-751.233933
Sum of electronic and thermal Enthalpies=	-751.232989
Sum of electronic and thermal Free Energies=	-751.294855

Esol = -751.7913445

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659096	1.185973	-0.180389
2	6	0	3.014411	1.204109	-0.183755
3	6	0	3.757894	-0.000017	-0.000053
4	6	0	3.014407	-1.204136	0.183668
5	6	0	1.659092	-1.185990	0.180337
6	7	0	0.942727	-0.000006	-0.000016
7	1	0	1.051679	2.071756	-0.314909
8	1	0	3.531257	2.145335	-0.327519
9	1	0	3.531249	-2.145366	0.327418
10	1	0	1.051672	-2.071769	0.314874
11	6	0	5.172422	-0.000022	-0.000072
12	7	0	6.335976	-0.000025	-0.000087
13	5	0	-0.497292	0.000000	0.000005
14	8	0	-1.235849	-1.129146	0.227042
15	8	0	-1.235845	1.129154	-0.227011
16	6	0	-2.601367	-0.776254	-0.104468
17	6	0	-2.601356	0.776276	0.104543
18	6	0	-3.542222	-1.540887	0.809991
19	1	0	-4.576183	-1.223153	0.642282
20	1	0	-3.473353	-2.609868	0.594657
21	1	0	-3.290618	-1.385312	1.859912
22	6	0	-2.822209	-1.174404	-1.561111
23	1	0	-2.597029	-2.237333	-1.673512
24	1	0	-3.857039	-1.002112	-1.868613
25	1	0	-2.161107	-0.609992	-2.225328
26	6	0	-3.542231	1.540919	-0.809886
27	1	0	-4.576192	1.223209	-0.642133
28	1	0	-3.473330	2.609901	-0.594564
29	1	0	-3.290672	1.385330	-1.859815
30	6	0	-2.822149	1.174428	1.561193
31	1	0	-2.596958	2.237355	1.673587
32	1	0	-3.856970	1.002143	1.868728
33	1	0	-2.161030	0.610012	2.225389

B: 4-(4-pyridinyl)benzonitrile

Thermal correction to Energy= 0.180854

Thermal correction to Enthalpy= 0.181798

Thermal correction to Gibbs Free Energy= 0.133081
Sum of electronic and zero-point Energies= -571.188782
Sum of electronic and thermal Energies= -571.178245
Sum of electronic and thermal Enthalpies= -571.177301
Sum of electronic and thermal Free Energies= -571.226018

Esol = -571.5545936

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.072497	-0.693676	-0.377266
2	6	0	1.125867	0.696151	-0.394840
3	6	0	-1.125826	0.695811	0.392822
4	6	0	-1.072641	-0.693997	0.373539
5	7	0	-0.000119	-1.392921	-0.002300
6	1	0	1.938313	-1.274689	-0.686192
7	1	0	2.023018	1.202278	-0.736525
8	1	0	-2.022906	1.201635	0.735141
9	1	0	-1.938531	-1.275276	0.681755
10	6	0	0.000070	1.423185	-0.000560
11	6	0	0.000168	2.905975	0.000379
12	6	0	1.144225	3.616519	0.382208
13	6	0	-1.143809	3.617149	-0.380532
14	6	0	1.150084	5.003510	0.385946
15	1	0	2.028635	3.074768	0.702292
16	6	0	-1.149512	5.004143	-0.382468
17	1	0	-2.028281	3.075911	-0.701318
18	6	0	0.000323	5.701071	0.002203
19	1	0	2.034182	5.552988	0.689605
20	1	0	-2.033548	5.554116	-0.685405
21	6	0	0.000389	7.140436	0.003208
22	7	0	0.000459	8.297595	0.004063

TSB1

Thermal correction to Energy= 0.569359
Thermal correction to Enthalpy= 0.570303
Thermal correction to Gibbs Free Energy= 0.476528
Sum of electronic and zero-point Energies= -1393.052164
Sum of electronic and thermal Energies= -1393.021374
Sum of electronic and thermal Enthalpies= -1393.020430
Sum of electronic and thermal Free Energies= -1393.114205

Esol = -1394.0745723

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.462530	-0.536241	-1.240776
2	6	0	-1.444714	-0.981093	1.116228
3	6	0	-0.075034	-0.541531	-1.206450
4	1	0	-1.983265	-0.382873	-2.179865
5	6	0	-0.056687	-0.969022	1.060892
6	1	0	-1.950230	-1.127610	2.064688
7	1	0	0.535700	-0.361170	-2.087605
8	1	0	0.572583	-1.115826	1.935570
9	7	0	0.601766	-0.758662	-0.077967
10	6	0	1.487796	3.352821	-0.615182
11	6	0	1.051716	3.097004	0.860931
12	5	0	2.170400	1.283280	0.061869
13	8	0	1.856792	2.032259	-1.056025
14	8	0	1.852597	1.956981	1.224608
15	6	0	1.339223	4.238611	1.822800
16	1	0	0.807065	5.145074	1.516063
17	1	0	1.001996	3.965323	2.825762
18	1	0	2.407296	4.455167	1.870263
19	6	0	2.735871	4.227416	-0.721064
20	1	0	3.106743	4.185423	-1.747768
21	1	0	2.520866	5.269332	-0.466960
22	1	0	3.523120	3.858181	-0.057957
23	6	0	0.389694	3.884135	-1.523820
24	1	0	0.014387	4.845429	-1.157960
25	1	0	0.788512	4.032238	-2.530480
26	1	0	-0.442774	3.180422	-1.586913
27	6	0	-0.409551	2.660186	0.976501
28	1	0	-0.583120	2.284143	1.988035
29	1	0	-1.096810	3.489839	0.786847
30	1	0	-0.630981	1.853143	0.269388
31	6	0	3.535940	-2.279132	-0.825444
32	6	0	3.874709	-2.136498	0.694759
33	5	0	2.604506	-0.361834	-0.002723
34	8	0	3.103917	-0.955568	-1.169336
35	8	0	2.972637	-1.111048	1.130998
36	6	0	3.640039	-3.393575	1.520209
37	1	0	4.263816	-4.218490	1.160155
38	1	0	3.900828	-3.197754	2.563607

39	1	0	2.593476	-3.701887	1.482337
40	6	0	2.385456	-3.254837	-1.085980
41	1	0	2.045666	-3.124165	-2.117297
42	1	0	2.707022	-4.292472	-0.955015
43	1	0	1.541517	-3.065702	-0.419298
44	6	0	4.721073	-2.645405	-1.708538
45	1	0	5.153248	-3.603881	-1.402243
46	1	0	4.388692	-2.735533	-2.746158
47	1	0	5.494814	-1.877684	-1.665503
48	6	0	5.292742	-1.613078	0.929590
49	1	0	5.391551	-1.336945	1.982109
50	1	0	6.051169	-2.364125	0.689707
51	1	0	5.475086	-0.721041	0.323816
52	6	0	-2.174362	-0.757579	-0.055542
53	6	0	-3.656411	-0.743978	-0.042141
54	6	0	-4.368331	-1.651339	0.750867
55	6	0	-4.363147	0.179495	-0.821264
56	6	0	-5.755400	-1.642197	0.765946
57	1	0	-3.829604	-2.386443	1.340217
58	6	0	-5.750085	0.200143	-0.811131
59	1	0	-3.819181	0.904470	-1.418491
60	6	0	-6.449402	-0.713730	-0.016407
61	1	0	-6.307049	-2.351616	1.372483
62	1	0	-6.297391	0.921907	-1.406955
63	6	0	-7.888634	-0.698091	-0.003141
64	7	0	-9.045572	-0.685338	0.007491

IntB1

Thermal correction to Energy=	0.570737
Thermal correction to Enthalpy=	0.571681
Thermal correction to Gibbs Free Energy=	0.477369
Sum of electronic and zero-point Energies=	-1393.054236
Sum of electronic and thermal Energies=	-1393.023229
Sum of electronic and thermal Enthalpies=	-1393.022285
Sum of electronic and thermal Free Energies=	-1393.116597

Esol = -1394.0781288

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.147805	1.966982	-3.254207
2	6	0	-1.548411	3.249566	-1.269754
3	6	0	-1.073487	0.835521	-2.461151
4	1	0	-1.043317	1.878620	-4.329742
5	6	0	-1.464198	2.073161	-0.541041
6	1	0	-1.714248	4.190597	-0.757040
7	1	0	-0.892411	-0.157738	-2.857904
8	1	0	-1.585663	2.017207	0.536233
9	7	0	-1.226089	0.900735	-1.135351
10	6	0	2.677235	-1.179976	-1.448397
11	6	0	2.750906	-1.711282	0.017020
12	5	0	0.661106	-0.895982	-0.406773
13	8	0	1.464343	-0.401625	-1.426478
14	8	0	1.361699	-1.779066	0.387604
15	6	0	3.373851	-3.090398	0.165606
16	1	0	4.409262	-3.086274	-0.190958
17	1	0	3.375215	-3.377820	1.220014
18	1	0	2.810946	-3.841194	-0.391028
19	6	0	2.469534	-2.297015	-2.470753
20	1	0	2.221932	-1.848372	-3.436371
21	1	0	3.369333	-2.907184	-2.590593
22	1	0	1.640362	-2.943796	-2.170086
23	6	0	3.836046	-0.288609	-1.865876
24	1	0	4.783377	-0.834375	-1.805785
25	1	0	3.694350	0.036707	-2.899982
26	1	0	3.899925	0.598393	-1.233768
27	6	0	3.419135	-0.721955	0.970924
28	1	0	3.246914	-1.055624	1.996829
29	1	0	4.497374	-0.658272	0.797518
30	1	0	2.983827	0.275193	0.858782
31	6	0	-3.046788	-1.623823	-0.060154
32	6	0	-2.536555	-1.219407	1.359190
33	5	0	-1.016619	-0.531579	-0.233559
34	8	0	-1.858117	-1.532946	-0.843984
35	8	0	-1.564460	-0.217475	1.065150
36	6	0	-3.601866	-0.629323	2.272087
37	1	0	-4.411328	-1.347494	2.441643
38	1	0	-3.157894	-0.380447	3.239935
39	1	0	-4.025203	0.283028	1.846331
40	6	0	-4.085956	-0.637253	-0.604072
41	1	0	-4.203493	-0.810948	-1.677579
42	1	0	-5.059497	-0.768116	-0.121312
43	1	0	-3.765508	0.398035	-0.455005
44	6	0	-3.585336	-3.044535	-0.158126

45	1	0	-4.419264	-3.196457	0.535828
46	1	0	-3.945704	-3.233803	-1.173381
47	1	0	-2.800854	-3.769202	0.065644
48	6	0	-1.818355	-2.375851	2.058698
49	1	0	-1.296592	-1.979747	2.933566
50	1	0	-2.515556	-3.153200	2.386393
51	1	0	-1.072134	-2.816976	1.391635
52	6	0	-1.380606	3.210445	-2.657095
53	6	0	-1.429583	4.446477	-3.473057
54	6	0	-2.365151	5.450478	-3.199801
55	6	0	-0.527720	4.622451	-4.528662
56	6	0	-2.404923	6.606120	-3.966925
57	1	0	-3.083971	5.312357	-2.398256
58	6	0	-0.554325	5.776646	-5.297220
59	1	0	0.218925	3.860444	-4.728624
60	6	0	-1.496606	6.771003	-5.017404
61	1	0	-3.137314	7.379741	-3.764936
62	1	0	0.152589	5.918678	-6.106879
63	6	0	-1.530876	7.969430	-5.814069
64	7	0	-1.557477	8.931847	-6.455662

TSB2

Thermal correction to Energy=	0.752329
Thermal correction to Enthalpy=	0.753273
Thermal correction to Gibbs Free Energy=	0.632526
Sum of electronic and zero-point Energies=	-1964.257741
Sum of electronic and thermal Energies=	-1964.215234
Sum of electronic and thermal Enthalpies=	-1964.214290
Sum of electronic and thermal Free Energies=	-1964.335037

Esol = -1965.6397985

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.381638	2.614239	-0.232366
2	6	0	1.296894	0.903234	1.172240
3	6	0	-0.877451	2.091716	0.012942
4	1	0	0.483592	3.495584	-0.855887
5	6	0	0.006344	0.442037	1.380448
6	1	0	2.134368	0.379880	1.622093
7	1	0	-1.784920	2.489896	-0.429088

8	1	0	-0.238411	-0.414046	2.001733
9	7	0	-1.047711	1.022388	0.798819
10	6	0	-3.950761	0.552450	-2.707206
11	6	0	-4.401079	-0.904876	-2.380591
12	5	0	-2.971988	-0.149927	-0.755481
13	8	0	-2.797815	0.715175	-1.867223
14	8	0	-4.027533	-1.032662	-1.003347
15	6	0	-5.898529	-1.148711	-2.501201
16	1	0	-6.247508	-0.945071	-3.519453
17	1	0	-6.118365	-2.193676	-2.266524
18	1	0	-6.453166	-0.519497	-1.803117
19	6	0	-4.976874	1.592094	-2.252728
20	1	0	-4.525483	2.584928	-2.331899
21	1	0	-5.882484	1.572626	-2.866174
22	1	0	-5.243836	1.424208	-1.204733
23	6	0	-3.557800	0.788814	-4.157122
24	1	0	-4.402010	0.588542	-4.825272
25	1	0	-3.257593	1.831763	-4.292053
26	1	0	-2.721424	0.150348	-4.449260
27	6	0	-3.635244	-1.952075	-3.190431
28	1	0	-3.807783	-2.933383	-2.740346
29	1	0	-3.973207	-1.979632	-4.230979
30	1	0	-2.561290	-1.753650	-3.171950
31	6	0	-3.728928	1.106698	2.726000
32	6	0	-3.528053	-0.437445	2.846655
33	5	0	-2.602637	0.316427	0.863912
34	8	0	-3.514462	1.332147	1.336022
35	8	0	-2.483524	-0.689588	1.906804
36	6	0	-3.084302	-0.914545	4.222639
37	1	0	-3.830184	-0.662508	4.984015
38	1	0	-2.963496	-2.001551	4.212192
39	1	0	-2.129219	-0.466779	4.506634
40	6	0	-2.685706	1.890288	3.530269
41	1	0	-2.699817	2.931462	3.196183
42	1	0	-2.897169	1.864804	4.603995
43	1	0	-1.679998	1.491476	3.368278
44	6	0	-5.126464	1.593330	3.084571
45	1	0	-5.387700	1.325848	4.114281
46	1	0	-5.170530	2.682335	2.992514
47	1	0	-5.866712	1.165139	2.406671
48	6	0	-4.765985	-1.213005	2.390086
49	1	0	-4.499113	-2.269780	2.299072
50	1	0	-5.591543	-1.122979	3.103078
51	1	0	-5.092274	-0.863996	1.406301

52	6	0	-0.186597	-0.811160	-1.694465
53	6	0	1.126938	-1.212213	-1.487261
54	6	0	0.296773	-2.804043	0.098343
55	6	0	-0.984088	-2.331228	-0.165051
56	1	0	-0.449450	-0.003599	-2.375770
57	1	0	1.939837	-0.709439	-2.002098
58	1	0	0.441043	-3.613161	0.806552
59	7	0	-1.215106	-1.352867	-1.041005
60	1	0	-1.858311	-2.704824	0.360800
61	6	0	1.504500	2.009433	0.343408
62	6	0	1.386652	-2.228908	-0.561967
63	6	0	2.775166	-2.653170	-0.263039
64	6	0	3.148316	-2.969007	1.049160
65	6	0	3.735531	-2.731510	-1.278453
66	6	0	4.447957	-3.352807	1.345361
67	1	0	2.415680	-2.892389	1.847021
68	6	0	5.037602	-3.116505	-0.994546
69	1	0	3.451655	-2.512463	-2.302956
70	6	0	5.396973	-3.426552	0.321039
71	1	0	4.737027	-3.590469	2.363134
72	1	0	5.778798	-3.186897	-1.782959
73	6	0	2.870432	2.515797	0.071926
74	6	0	3.211990	2.979535	-1.203776
75	6	0	3.837099	2.531961	1.083862
76	6	0	4.490136	3.449544	-1.467479
77	1	0	2.475706	2.949475	-2.001142
78	6	0	5.117015	3.003444	0.832272
79	1	0	3.574710	2.197926	2.082665
80	6	0	5.445743	3.463050	-0.446833
81	1	0	4.757692	3.801524	-2.457545
82	1	0	5.863075	3.026792	1.618888
83	6	0	6.748177	-3.819580	0.623252
84	7	0	7.834860	-4.131894	0.868998
85	6	0	6.771937	3.954643	-0.713988
86	7	0	7.837084	4.351283	-0.930086

IntB2

Thermal correction to Energy=	0.754238
Thermal correction to Enthalpy=	0.755183
Thermal correction to Gibbs Free Energy=	0.636225
Sum of electronic and zero-point Energies=	-1964.260722
Sum of electronic and thermal Energies=	-1964.218245
Sum of electronic and thermal Enthalpies=	-1964.217301

Sum of electronic and thermal Free Energies= -1964.336259

Esol = -1965.644001

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.876628	2.109216	-3.203908
2	6	0	-1.527705	3.451896	-1.329518
3	6	0	-0.857827	1.008741	-2.365679
4	1	0	-0.655966	1.982187	-4.257823
5	6	0	-1.497121	2.306217	-0.550062
6	1	0	-1.775774	4.404386	-0.873929
7	1	0	-0.603109	0.006513	-2.692500
8	1	0	-1.736536	2.290247	0.509358
9	7	0	-1.165244	1.116447	-1.065537
10	6	0	2.467364	-1.151699	-1.302580
11	6	0	2.652055	-1.675729	0.156996
12	5	0	0.871069	-0.204392	0.078581
13	8	0	1.676359	0.021892	-1.115464
14	8	0	1.391816	-1.373164	0.747891
15	6	0	2.891818	-3.174950	0.265548
16	1	0	3.785538	-3.474306	-0.293072
17	1	0	3.036293	-3.448910	1.314631
18	1	0	2.031041	-3.727659	-0.114962
19	6	0	1.654657	-2.128833	-2.156102
20	1	0	1.400819	-1.634043	-3.099395
21	1	0	2.216277	-3.038586	-2.390247
22	1	0	0.724301	-2.391794	-1.642065
23	6	0	3.762333	-0.776710	-2.009220
24	1	0	4.432137	-1.640488	-2.080403
25	1	0	3.542033	-0.432944	-3.024050
26	1	0	4.280126	0.027345	-1.482053
27	6	0	3.752724	-0.913314	0.902824
28	1	0	3.668423	-1.134336	1.970755
29	1	0	4.751601	-1.206551	0.564659
30	1	0	3.643122	0.166435	0.762961
31	6	0	-2.658996	-1.668183	-0.156275
32	6	0	-2.472759	-1.144626	1.303280
33	5	0	-0.873807	-0.201908	-0.077922
34	8	0	-1.397931	-1.369235	-0.747214
35	8	0	-1.678538	0.026773	1.116057
36	6	0	-3.766654	-0.766056	2.009979

37	1	0	-4.438767	-1.628025	2.081275
38	1	0	-3.545352	-0.422819	3.024769
39	1	0	-4.282360	0.039331	1.482802
40	6	0	-3.757518	-0.902656	-0.902087
41	1	0	-3.673726	-1.123769	-1.970040
42	1	0	-4.757234	-1.193208	-0.564065
43	1	0	-3.645025	0.176778	-0.762076
44	6	0	-2.903014	-3.166724	-0.264799
45	1	0	-3.797463	-3.463611	0.293969
46	1	0	-3.048444	-3.440253	-1.313863
47	1	0	-2.043710	-3.721841	0.115537
48	6	0	-1.662702	-2.123967	2.156773
49	1	0	-1.407360	-1.629821	3.099998
50	1	0	-2.226860	-3.032106	2.391063
51	1	0	-0.733150	-2.389583	1.642643
52	6	0	1.500549	2.302279	0.550067
53	6	0	1.533609	3.448143	1.329155
54	6	0	0.880101	2.107346	3.204054
55	6	0	0.858915	1.006655	2.366181
56	1	0	1.739604	2.285497	-0.509422
57	1	0	1.783518	4.399982	0.873214
58	1	0	0.659322	1.981123	4.258038
59	7	0	1.166226	1.113356	1.065935
60	1	0	0.602132	0.005073	2.693354
61	6	0	-1.212916	3.366973	-2.689440
62	6	0	1.218677	3.364306	2.689108
63	6	0	1.242729	4.564228	3.557418
64	6	0	0.283463	4.731089	4.563485
65	6	0	2.226514	5.545780	3.386897
66	6	0	0.301367	5.851681	5.380945
67	1	0	-0.497369	3.987841	4.689910
68	6	0	2.256009	6.668375	4.201071
69	1	0	2.991762	5.413709	2.628618
70	6	0	1.290275	6.823947	5.200650
71	1	0	-0.447765	5.984717	6.153349
72	1	0	3.024157	7.423075	4.074848
73	6	0	-1.235371	4.566611	-3.558180
74	6	0	-0.276277	4.731959	-4.564648
75	6	0	-2.217911	5.549400	-3.387653
76	6	0	-0.293151	5.852323	-5.382465
77	1	0	0.503623	3.987741	-4.691160
78	6	0	-2.246387	6.671759	-4.202177
79	1	0	-2.983078	5.418460	-2.629096
80	6	0	-1.280834	6.825839	-5.202148

81	1	0	0.455851	5.984213	-6.155194
82	1	0	-3.013634	7.427372	-4.075942
83	6	0	1.312273	7.990000	6.044058
84	7	0	1.328429	8.929079	6.719733
85	6	0	-1.301759	7.991624	-6.045953
86	7	0	-1.317060	8.930503	-6.721925

TSB3

Thermal correction to Energy= 0.752522
Thermal correction to Enthalpy= 0.753466
Thermal correction to Gibbs Free Energy= 0.635865
Sum of electronic and zero-point Energies= -1964.251169
Sum of electronic and thermal Energies= -1964.209117
Sum of electronic and thermal Enthalpies= -1964.208172
Sum of electronic and thermal Free Energies= -1964.325774

Esol = -1965.631134

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040027	3.156941	-0.595562
2	6	0	-1.462291	1.311052	-1.124746
3	6	0	1.048535	2.348355	-0.760684
4	1	0	0.124590	4.206112	-0.376825
5	6	0	-0.337123	0.516556	-1.259628
6	1	0	-2.433152	0.847190	-1.264902
7	1	0	2.070554	2.692544	-0.668588
8	1	0	-0.377192	-0.523982	-1.561218
9	7	0	0.917145	1.021200	-1.083073
10	6	0	3.216139	1.413901	2.353333
11	6	0	3.866314	-0.003747	2.490788
12	5	0	2.112878	-0.111910	1.052022
13	8	0	1.956766	1.121097	1.722172
14	8	0	3.369731	-0.693037	1.332431
15	6	0	5.385342	-0.012258	2.444231
16	1	0	5.804478	0.595273	3.253086
17	1	0	5.749428	-1.036441	2.561894
18	1	0	5.743141	0.372567	1.487538
19	6	0	4.013027	2.335264	1.431677
20	1	0	3.421352	3.237641	1.248156
21	1	0	4.957332	2.639820	1.892833

22	1	0	4.215770	1.845317	0.475006
23	6	0	2.939226	2.109704	3.678488
24	1	0	3.869950	2.269240	4.233071
25	1	0	2.484574	3.085704	3.489219
26	1	0	2.254020	1.528342	4.297435
27	6	0	3.360158	-0.757574	3.721718
28	1	0	3.677958	-1.800607	3.646554
29	1	0	3.757863	-0.337733	4.650128
30	1	0	2.266653	-0.734163	3.768090
31	6	0	3.866668	0.003439	-2.490535
32	6	0	3.216310	-1.414135	-2.353195
33	5	0	2.113018	0.111785	-1.052045
34	8	0	3.369973	0.692782	-1.332258
35	8	0	1.956867	-1.121190	-1.722241
36	6	0	2.939539	-2.109903	-3.678399
37	1	0	3.870339	-2.269552	-4.232821
38	1	0	2.484735	-3.085846	-3.489208
39	1	0	2.254513	-1.528456	-4.297465
40	6	0	3.360804	0.757327	-3.721548
41	1	0	3.678698	1.800327	-3.646321
42	1	0	3.758633	0.337451	-4.649889
43	1	0	2.267306	0.734027	-3.768114
44	6	0	5.385691	0.011772	-2.443728
45	1	0	5.804886	-0.595840	-3.252491
46	1	0	5.749922	1.035906	-2.561369
47	1	0	5.743282	-0.373060	-1.486960
48	6	0	4.012938	-2.335593	-1.431408
49	1	0	3.421127	-3.237903	-1.247994
50	1	0	4.957288	-2.640252	-1.892403
51	1	0	4.215572	-1.845677	-0.474698
52	6	0	-0.337333	-0.516430	1.259297
53	6	0	-1.462558	-1.310834	1.124346
54	6	0	-0.040407	-3.156884	0.595435
55	6	0	1.048209	-2.348383	0.760612
56	1	0	-0.377343	0.524128	1.560827
57	1	0	-2.433389	-0.846871	1.264373
58	1	0	0.124144	-4.206084	0.376785
59	7	0	0.916907	-1.021202	1.082921
60	1	0	2.070206	-2.692673	0.668645
61	6	0	-1.353184	2.656379	-0.771874
62	6	0	-1.353538	-2.656202	0.771600
63	6	0	-2.537446	3.511281	-0.589876
64	6	0	-3.714912	3.276630	-1.317694
65	6	0	-2.519291	4.580057	0.319730

66	6	0	-4.835370	4.071232	-1.141055
67	1	0	-3.741339	2.478701	-2.052794
68	6	0	-3.633426	5.383818	0.501190
69	1	0	-1.630051	4.763701	0.913982
70	6	0	-4.800286	5.131397	-0.228017
71	1	0	-5.738371	3.886171	-1.712515
72	1	0	-3.613191	6.202248	1.212563
73	6	0	-2.537851	-3.511047	0.589661
74	6	0	-2.519711	-4.579992	-0.319747
75	6	0	-3.715347	-3.276199	1.317372
76	6	0	-3.633878	-5.383729	-0.501115
77	1	0	-1.630448	-4.763805	-0.913912
78	6	0	-4.835839	-4.070773	1.140821
79	1	0	-3.741774	-2.478138	2.052328
80	6	0	-4.800765	-5.131111	0.227983
81	1	0	-3.613647	-6.202297	-1.212328
82	1	0	-5.738858	-3.885555	1.712201
83	6	0	-5.960352	5.959601	-0.039767
84	7	0	-6.894498	6.625976	0.113151
85	6	0	-5.960860	-5.959296	0.039841
86	7	0	-6.895034	-6.625654	-0.112984

IntB3

Thermal correction to Energy=	0.584419
Thermal correction to Enthalpy=	0.585364
Thermal correction to Gibbs Free Energy=	0.490141
Sum of electronic and zero-point Energies=	-1502.542337
Sum of electronic and thermal Energies=	-1502.509748
Sum of electronic and thermal Enthalpies=	-1502.508803
Sum of electronic and thermal Free Energies=	-1502.604026

Esol = -1503.6203191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192411	2.918531	-0.064897
2	6	0	-2.265922	0.855173	-0.809719
3	6	0	0.017750	2.368775	-0.277069
4	1	0	-1.294106	3.935734	0.285978
5	6	0	-0.963968	0.155567	-0.535331
6	1	0	-3.108999	0.298453	-1.202832

7	1	0	0.943598	2.920113	-0.155419
8	1	0	-0.825382	-0.704150	-1.197988
9	7	0	0.159565	1.068443	-0.739529
10	6	0	2.399557	1.473403	2.999795
11	6	0	3.261204	0.164621	3.064959
12	5	0	1.355574	-0.217096	1.924984
13	8	0	1.116824	0.979379	2.547387
14	8	0	2.653518	-0.658825	2.042750
15	6	0	4.730203	0.352394	2.728815
16	1	0	5.203630	1.030687	3.445580
17	1	0	5.241980	-0.611951	2.779209
18	1	0	4.855815	0.760237	1.724315
19	6	0	2.902889	2.461933	1.953014
20	1	0	2.161819	3.258607	1.847194
21	1	0	3.850140	2.914096	2.260405
22	1	0	3.037030	1.980959	0.978552
23	6	0	2.204511	2.169772	4.336803
24	1	0	3.168698	2.482964	4.749644
25	1	0	1.587649	3.060427	4.195053
26	1	0	1.705452	1.519598	5.056463
27	6	0	3.103367	-0.584015	4.386124
28	1	0	3.560946	-1.571143	4.287754
29	1	0	3.590226	-0.052629	5.208039
30	1	0	2.046465	-0.719593	4.633978
31	6	0	3.437111	0.737400	-2.235186
32	6	0	2.920858	-0.742810	-2.268869
33	5	0	1.387095	0.608614	-1.308586
34	8	0	2.540299	1.358174	-1.285844
35	8	0	1.515940	-0.590416	-1.958684
36	6	0	3.048389	-1.425081	-3.620960
37	1	0	4.098781	-1.477570	-3.924679
38	1	0	2.660603	-2.444120	-3.551800
39	1	0	2.484311	-0.896130	-4.390246
40	6	0	3.244598	1.463657	-3.564159
41	1	0	3.432844	2.529066	-3.413381
42	1	0	3.933457	1.090845	-4.326623
43	1	0	2.220376	1.345188	-3.929846
44	6	0	4.862980	0.902059	-1.738421
45	1	0	5.560985	0.379437	-2.400079
46	1	0	5.127288	1.962522	-1.729988
47	1	0	4.977590	0.508020	-0.726818
48	6	0	3.535918	-1.608327	-1.173878
49	1	0	3.005454	-2.564025	-1.150468
50	1	0	4.592618	-1.807509	-1.373236

51	1	0	3.442695	-1.134676	-0.190851
52	6	0	-0.955623	-0.376781	0.938995
53	6	0	-2.050984	-1.391630	1.116033
54	6	0	-0.422711	-3.103837	0.499804
55	6	0	0.582379	-2.261421	0.802488
56	1	0	-1.099686	0.484114	1.599023
57	1	0	-3.038408	-1.073711	1.430537
58	1	0	-0.228543	-4.112452	0.163155
59	7	0	0.345422	-0.969108	1.248629
60	1	0	1.625171	-2.557081	0.771565
61	6	0	-2.367400	2.159121	-0.486852
62	6	0	-1.785168	-2.675900	0.809525
63	6	0	-2.822166	-3.673264	0.881555
64	7	0	-3.644721	-4.486049	0.926494
65	6	0	-3.619896	2.853224	-0.643575
66	7	0	-4.621534	3.422403	-0.752386

TSB3

Thermal correction to Energy=	0.580769
Thermal correction to Enthalpy=	0.581713
Thermal correction to Gibbs Free Energy=	0.485500
Sum of electronic and zero-point Energies=	-1502.501972
Sum of electronic and thermal Energies=	-1502.469157
Sum of electronic and thermal Enthalpies=	-1502.468213
Sum of electronic and thermal Free Energies=	-1502.564426

Esol = -1503.5796455

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.813266	-0.721878	-3.081922
2	6	0	3.295701	0.440979	-1.557725
3	6	0	0.752098	-0.205929	-2.431409
4	1	0	1.657925	-1.363977	-3.939803
5	6	0	2.185340	0.850480	-0.820900
6	1	0	4.281445	0.718931	-1.199876
7	1	0	-0.269332	-0.373921	-2.743638
8	1	0	2.255235	1.600607	-0.042401
9	7	0	0.895381	0.642158	-1.326602
10	6	0	-1.468480	-2.858782	-0.354684
11	6	0	-2.248458	-2.351226	0.909340

12	5	0	-0.239303	-1.350731	0.795476
13	8	0	-0.128427	-2.359375	-0.120751
14	8	0	-1.513982	-1.157179	1.274434
15	6	0	-3.697073	-1.974706	0.652669
16	1	0	-4.266287	-2.848325	0.320038
17	1	0	-4.147312	-1.605991	1.578162
18	1	0	-3.773524	-1.195051	-0.106838
19	6	0	-1.977210	-2.236513	-1.649976
20	1	0	-1.272880	-2.479213	-2.449970
21	1	0	-2.957412	-2.640495	-1.918846
22	1	0	-2.054468	-1.148492	-1.561217
23	6	0	-1.398097	-4.371605	-0.487604
24	1	0	-2.404166	-4.794108	-0.573899
25	1	0	-0.839655	-4.630824	-1.390092
26	1	0	-0.895825	-4.825681	0.367551
27	6	0	-2.143244	-3.306615	2.095937
28	1	0	-2.537030	-2.808968	2.985026
29	1	0	-2.715573	-4.221966	1.924615
30	1	0	-1.100792	-3.577540	2.288463
31	6	0	-2.248562	2.351353	-0.909353
32	6	0	-1.468470	2.858989	0.354541
33	5	0	-0.239335	1.350993	-0.795679
34	8	0	-1.514081	1.157298	-1.274411
35	8	0	-0.128361	2.359854	0.120304
36	6	0	-1.398406	4.371808	0.487566
37	1	0	-2.404561	4.794080	0.573985
38	1	0	-0.839930	4.631101	1.390011
39	1	0	-0.896324	4.826038	-0.367620
40	6	0	-2.143488	3.306673	-2.096015
41	1	0	-2.537277	2.808932	-2.985051
42	1	0	-2.715899	4.221978	-1.924716
43	1	0	-1.101073	3.577692	-2.288609
44	6	0	-3.697145	1.974840	-0.652491
45	1	0	-4.266279	2.848462	-0.319727
46	1	0	-4.147546	1.606182	-1.577928
47	1	0	-3.773493	1.195158	0.106996
48	6	0	-1.976771	2.236381	1.649835
49	1	0	-1.272196	2.478927	2.449658
50	1	0	-2.956946	2.640158	1.919107
51	1	0	-2.053919	1.148372	1.560703
52	6	0	2.185402	-0.850334	0.820800
53	6	0	3.295764	-0.440941	1.557669
54	6	0	1.813352	0.721461	3.082233
55	6	0	0.752175	0.205697	2.431587

56	1	0	2.255266	-1.600335	0.042176
57	1	0	4.281503	-0.718761	1.199703
58	1	0	1.658020	1.363261	3.940340
59	7	0	0.895449	-0.642038	1.326499
60	1	0	-0.269244	0.373517	2.743953
61	6	0	3.152845	-0.376288	-2.666508
62	6	0	3.152924	0.376058	2.666655
63	6	0	4.284493	0.862746	3.380465
64	7	0	5.199866	1.266103	3.969703
65	6	0	4.284359	-0.863040	-3.380257
66	7	0	5.199719	-1.266481	-3.969456

IntB4

Thermal correction to Energy=	0.375207
Thermal correction to Enthalpy=	0.376151
Thermal correction to Gibbs Free Energy=	0.302653
Sum of electronic and zero-point Energies=	-982.134825
Sum of electronic and thermal Energies=	-982.113789
Sum of electronic and thermal Enthalpies=	-982.112845
Sum of electronic and thermal Free Energies=	-982.186344

Esol = -982.8317588

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.311745	1.189839	-0.083370
2	6	0	3.666733	1.202835	-0.091005
3	6	0	3.666792	-1.202611	0.090998
4	6	0	2.311803	-1.189680	0.083379
5	7	0	1.589371	0.000062	0.000006
6	1	0	1.709027	2.088024	-0.128736
7	1	0	4.155880	2.168878	-0.128625
8	1	0	4.155986	-2.168630	0.128615
9	1	0	1.709128	-2.087893	0.128753
10	5	0	0.150216	0.000027	0.000000
11	8	0	-0.588869	-1.139615	0.167576
12	8	0	-0.588925	1.139631	-0.167587
13	6	0	-1.954477	-0.769890	-0.142785
14	6	0	-1.954522	0.769834	0.142742
15	6	0	-2.894848	-1.577471	0.734766
16	1	0	-3.927244	-1.241977	0.594277

17	1	0	-2.837670	-2.633289	0.459543
18	1	0	-2.633021	-1.483251	1.789506
19	6	0	-2.177802	-1.096839	-1.617053
20	1	0	-1.949873	-2.152379	-1.781289
21	1	0	-3.213694	-0.913294	-1.914450
22	1	0	-1.519590	-0.499175	-2.254489
23	6	0	-2.894914	1.577364	-0.734833
24	1	0	-3.927293	1.241803	-0.594383
25	1	0	-2.837812	2.633184	-0.459597
26	1	0	-2.633045	1.483171	-1.789564
27	6	0	-2.177897	1.096774	1.617004
28	1	0	-1.950020	2.152324	1.781244
29	1	0	-3.213788	0.913182	1.914376
30	1	0	-1.519673	0.499140	2.254456
31	6	0	4.437335	0.000130	-0.000011
32	6	0	5.883453	0.000163	-0.000028
33	6	0	6.623107	1.116552	-0.456635
34	6	0	6.623168	-1.116194	0.456557
35	6	0	8.004104	1.119639	-0.457324
36	1	0	6.103800	1.983148	-0.850382
37	6	0	8.004165	-1.119223	0.457207
38	1	0	6.103909	-1.982813	0.850318
39	6	0	8.714086	0.000224	-0.000068
40	1	0	8.549220	1.984098	-0.821547
41	1	0	8.549329	-1.983659	0.821413
42	6	0	10.147850	0.000255	-0.000089
43	7	0	11.306634	0.000282	-0.000105

C

Thermal correction to Energy=	0.180372
Thermal correction to Enthalpy=	0.181316
Thermal correction to Gibbs Free Energy=	0.137163
Sum of electronic and zero-point Energies=	-478.973939
Sum of electronic and thermal Energies=	-478.965238
Sum of electronic and thermal Enthalpies=	-478.964293
Sum of electronic and thermal Free Energies=	-479.008447

Esol = -479.3061454

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.073196	-0.705476	-0.372490
2	6	0	1.125712	0.684082	-0.391043
3	6	0	-1.125758	0.683735	0.388877
4	6	0	-1.073340	-0.705784	0.368684
5	7	0	-0.000075	-1.406667	-0.002258
6	1	0	1.941023	-1.285918	-0.677772
7	1	0	2.023992	1.190585	-0.729071
8	1	0	-2.023773	1.189938	0.728036
9	1	0	-1.940975	-1.286505	0.673940
10	6	0	-0.000037	1.414365	-0.000829
11	6	0	0.000098	2.897056	0.000145
12	6	0	1.144076	3.608731	0.377213
13	6	0	-1.143800	3.609460	-0.375840
14	6	0	1.143722	4.999119	0.379534
15	1	0	2.029755	3.065984	0.694085
16	6	0	-1.143165	4.999831	-0.376190
17	1	0	-2.029501	3.067284	-0.693618
18	6	0	0.000329	5.698547	0.002252
19	1	0	2.035670	5.537948	0.682571
20	1	0	-2.035005	5.539273	-0.678420
21	1	0	0.000394	6.783647	0.003134

TSC1

Thermal correction to Energy=	0.568892
Thermal correction to Enthalpy=	0.569836
Thermal correction to Gibbs Free Energy=	0.480506
Sum of electronic and zero-point Energies=	-1300.838309
Sum of electronic and thermal Energies=	-1300.809340
Sum of electronic and thermal Enthalpies=	-1300.808396
Sum of electronic and thermal Free Energies=	-1300.897726

Esol = -1301.8270465

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893877	-0.787741	-1.212906
2	6	0	-1.837285	-1.094297	1.162674
3	6	0	-0.509403	-0.691980	-1.187302
4	1	0	-2.430784	-0.673917	-2.148607
5	6	0	-0.454204	-0.986266	1.097109
6	1	0	-2.325515	-1.272584	2.114733

7	1	0	0.079997	-0.504794	-2.081634
8	1	0	0.184449	-1.048289	1.975360
9	7	0	0.187826	-0.794459	-0.054730
10	6	0	0.749096	3.330617	-0.796442
11	6	0	0.330452	3.113116	0.691251
12	5	0	1.609529	1.367585	-0.014079
13	8	0	1.239081	2.028752	-1.168865
14	8	0	1.225809	2.067426	1.112787
15	6	0	0.515333	4.322681	1.593836
16	1	0	-0.093119	5.162752	1.242986
17	1	0	0.200474	4.071398	2.609808
18	1	0	1.560356	4.633715	1.628825
19	6	0	1.913658	4.307989	-0.947383
20	1	0	2.291044	4.247131	-1.970790
21	1	0	1.604711	5.337946	-0.746886
22	1	0	2.728141	4.045365	-0.266537
23	6	0	-0.388299	3.712355	-1.731557
24	1	0	-0.850911	4.653217	-1.415907
25	1	0	0.000715	3.844285	-2.744329
26	1	0	-1.153052	2.933728	-1.758398
27	6	0	-1.088796	2.560021	0.829422
28	1	0	-1.233061	2.222675	1.859283
29	1	0	-1.842784	3.317985	0.597782
30	1	0	-1.239348	1.702596	0.165029
31	6	0	3.275308	-2.111963	-0.703872
32	6	0	3.578520	-1.872621	0.811988
33	5	0	2.208014	-0.223790	0.009289
34	8	0	2.756824	-0.840365	-1.118418
35	8	0	2.609497	-0.882743	1.182375
36	6	0	3.404580	-3.098236	1.697571
37	1	0	4.082092	-3.901406	1.389070
38	1	0	3.635498	-2.834701	2.733097
39	1	0	2.378775	-3.469740	1.660791
40	6	0	2.198974	-3.175729	-0.932802
41	1	0	1.874029	-3.121369	-1.975643
42	1	0	2.586218	-4.180991	-0.740845
43	1	0	1.329888	-3.007371	-0.293833
44	6	0	4.497518	-2.435661	-1.552450
45	1	0	4.987037	-3.348663	-1.197297
46	1	0	4.189212	-2.593380	-2.589401
47	1	0	5.218030	-1.616817	-1.533467
48	6	0	4.957800	-1.252267	1.041731
49	1	0	5.021101	-0.920632	2.080900
50	1	0	5.764553	-1.965887	0.849938

51	1	0	5.096569	-0.380463	0.396245
52	6	0	-2.587886	-0.990242	-0.013358
53	6	0	-4.066980	-1.077769	0.010558
54	6	0	-4.794394	-0.492357	1.052387
55	6	0	-4.757626	-1.742156	-1.008546
56	6	0	-6.182481	-0.569725	1.074004
57	1	0	-4.267799	0.050058	1.832305
58	6	0	-6.145472	-1.823279	-0.983467
59	1	0	-4.200361	-2.219658	-1.809100
60	6	0	-6.861219	-1.236644	0.057136
61	1	0	-6.735422	-0.102548	1.882284
62	1	0	-6.668518	-2.350664	-1.774429
63	1	0	-7.944311	-1.298389	0.075202

IntC1

Thermal correction to Energy=	0.570174
Thermal correction to Enthalpy=	0.571118
Thermal correction to Gibbs Free Energy=	0.480374
Sum of electronic and zero-point Energies=	-1300.840996
Sum of electronic and thermal Energies=	-1300.811650
Sum of electronic and thermal Enthalpies=	-1300.810706
Sum of electronic and thermal Free Energies=	-1300.901451

Esol = -1301.8310155

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.110252	2.010370	-3.263446
2	6	0	-1.507762	3.276595	-1.271501
3	6	0	-1.002757	0.877938	-2.475657
4	1	0	-1.020831	1.925684	-4.340384
5	6	0	-1.396020	2.100868	-0.547850
6	1	0	-1.684548	4.211619	-0.752128
7	1	0	-0.809157	-0.110321	-2.878370
8	1	0	-1.509620	2.041103	0.529647
9	7	0	-1.147741	0.932575	-1.147789
10	6	0	2.725043	-1.280675	-1.406099
11	6	0	2.767658	-1.765294	0.076060
12	5	0	0.707180	-0.903044	-0.399363
13	8	0	1.537057	-0.465760	-1.423824
14	8	0	1.373917	-1.780006	0.432227

15	6	0	3.347655	-3.156695	0.277977
16	1	0	4.384758	-3.197886	-0.071266
17	1	0	3.333845	-3.405826	1.341950
18	1	0	2.764614	-3.909186	-0.254970
19	6	0	2.493708	-2.424493	-2.393377
20	1	0	2.267564	-2.000582	-3.375073
21	1	0	3.376031	-3.064373	-2.484589
22	1	0	1.643220	-3.036537	-2.080063
23	6	0	3.915712	-0.440211	-1.840152
24	1	0	4.844879	-1.012342	-1.748901
25	1	0	3.796039	-0.148148	-2.886760
26	1	0	4.000300	0.466974	-1.239966
27	6	0	3.455568	-0.765206	1.005037
28	1	0	3.256744	-1.056171	2.039015
29	1	0	4.537830	-0.744299	0.846941
30	1	0	3.056599	0.241443	0.851336
31	6	0	-3.007762	-1.573246	-0.116233
32	6	0	-2.513046	-1.182373	1.311909
33	5	0	-0.962926	-0.499270	-0.257005
34	8	0	-1.808727	-1.491736	-0.882903
35	8	0	-1.526554	-0.190550	1.038882
36	6	0	-3.584812	-0.585011	2.213265
37	1	0	-4.405513	-1.293753	2.367524
38	1	0	-3.151669	-0.346607	3.188538
39	1	0	-3.990650	0.334804	1.786573
40	6	0	-4.029917	-0.573284	-0.668788
41	1	0	-4.133100	-0.739472	-1.744892
42	1	0	-5.011757	-0.697478	-0.201181
43	1	0	-3.701511	0.457733	-0.509551
44	6	0	-3.561035	-2.987637	-0.229642
45	1	0	-4.408817	-3.133173	0.448646
46	1	0	-3.905883	-3.167573	-1.251883
47	1	0	-2.789295	-3.722766	0.003653
48	6	0	-1.818308	-2.350693	2.016228
49	1	0	-1.310283	-1.965627	2.903994
50	1	0	-2.527490	-3.125262	2.324476
51	1	0	-1.061877	-2.792416	1.361253
52	6	0	-1.367197	3.248627	-2.663276
53	6	0	-1.489151	4.483435	-3.472109
54	6	0	-2.424835	5.465725	-3.129537
55	6	0	-0.672455	4.684855	-4.590165
56	6	0	-2.542862	6.623089	-3.890520
57	1	0	-3.082041	5.306932	-2.279786
58	6	0	-0.787708	5.845332	-5.347129

59	1	0	0.074987	3.940781	-4.848898
60	6	0	-1.723803	6.816290	-5.000103
61	1	0	-3.279934	7.372110	-3.620603
62	1	0	-0.141099	5.994545	-6.205496
63	1	0	-1.814711	7.720659	-5.592634

TSC2

Thermal correction to Energy= 0.751937
Thermal correction to Enthalpy= 0.752881
Thermal correction to Gibbs Free Energy= 0.641510
Sum of electronic and zero-point Energies= -1779.829617
Sum of electronic and thermal Energies= -1779.790834
Sum of electronic and thermal Enthalpies= -1779.789889
Sum of electronic and thermal Free Energies= -1779.901260

Esol = -1781.1449941

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.927504	1.694301	2.017512
2	6	0	-1.844196	1.502168	-0.184846
3	6	0	0.329563	1.493316	1.473332
4	1	0	-1.028686	1.866639	3.083070
5	6	0	-0.555404	1.320685	-0.660734
6	1	0	-2.682204	1.453903	-0.872343
7	1	0	1.235653	1.447229	2.067985
8	1	0	-0.315201	1.160485	-1.707064
9	7	0	0.500356	1.303022	0.159545
10	6	0	3.324661	-1.589364	2.295775
11	6	0	3.779925	-2.372823	1.024845
12	5	0	2.398268	-0.645257	0.419242
13	8	0	2.204400	-0.835827	1.811938
14	8	0	3.441221	-1.462926	-0.027502
15	6	0	5.274046	-2.657730	0.957742
16	1	0	5.597170	-3.257609	1.815424
17	1	0	5.497597	-3.216655	0.045094
18	1	0	5.847816	-1.729795	0.936983
19	6	0	4.372068	-0.574292	2.758308
20	1	0	3.924534	0.064498	3.524595
21	1	0	5.256491	-1.059233	3.182085
22	1	0	4.673531	0.062455	1.921114

23	6	0	2.880611	-2.463175	3.459231
24	1	0	3.700766	-3.103965	3.799961
25	1	0	2.572613	-1.830479	4.296355
26	1	0	2.036009	-3.095568	3.178013
27	6	0	2.994102	-3.668670	0.817232
28	1	0	3.187571	-4.032064	-0.195564
29	1	0	3.298553	-4.440974	1.530578
30	1	0	1.920254	-3.496108	0.916075
31	6	0	3.196481	2.695009	-1.153859
32	6	0	2.979858	1.687689	-2.327197
33	5	0	2.043865	0.837332	-0.387607
34	8	0	2.973526	1.879479	-0.009412
35	8	0	1.923974	0.863935	-1.838361
36	6	0	2.547397	2.326706	-3.640009
37	1	0	3.301071	3.037071	-3.996484
38	1	0	2.423102	1.551805	-4.401866
39	1	0	1.595969	2.851737	-3.528672
40	6	0	2.168961	3.832661	-1.171595
41	1	0	2.196646	4.340320	-0.203424
42	1	0	2.385290	4.564527	-1.956478
43	1	0	1.157161	3.447979	-1.328255
44	6	0	4.602385	3.275337	-1.070852
45	1	0	4.867196	3.802689	-1.993933
46	1	0	4.657749	3.986810	-0.241967
47	1	0	5.333225	2.485392	-0.890288
48	6	0	4.204964	0.796668	-2.548670
49	1	0	3.926823	-0.011195	-3.231317
50	1	0	5.041796	1.350411	-2.985957
51	1	0	4.518390	0.342977	-1.604237
52	6	0	-0.417002	-1.741846	0.616043
53	6	0	-1.739156	-1.865051	0.209304
54	6	0	-0.951511	-1.863373	-2.049904
55	6	0	0.340058	-1.729310	-1.552367
56	1	0	-0.135808	-1.659801	1.664536
57	1	0	-2.538680	-1.867902	0.943581
58	1	0	-1.116639	-1.927011	-3.120340
59	7	0	0.598992	-1.668528	-0.245531
60	1	0	1.201707	-1.625502	-2.205701
61	6	0	-2.053590	1.686059	1.185550
62	6	0	-2.027945	-1.919966	-1.158979
63	6	0	-3.426150	-1.998358	-1.644515
64	6	0	-3.820108	-1.291108	-2.786104
65	6	0	-4.376977	-2.768676	-0.966456
66	6	0	-5.133602	-1.352861	-3.238803

67	1	0	-3.094606	-0.673235	-3.307858
68	6	0	-5.689161	-2.833355	-1.421640
69	1	0	-4.076590	-3.339420	-0.092783
70	6	0	-6.071409	-2.125117	-2.558267
71	1	0	-5.426141	-0.793451	-4.121447
72	1	0	-6.413406	-3.443258	-0.891612
73	6	0	-3.417828	1.847331	1.739084
74	6	0	-3.755014	1.272778	2.969610
75	6	0	-4.390485	2.569755	1.039449
76	6	0	-5.036931	1.417088	3.488327
77	1	0	-3.014287	0.689342	3.508744
78	6	0	-5.670401	2.717825	1.561440
79	1	0	-4.132190	3.039603	0.095170
80	6	0	-5.997154	2.141224	2.786295
81	1	0	-5.287860	0.958946	4.439342
82	1	0	-6.412288	3.289574	1.013793
83	1	0	-6.996724	2.255966	3.192284
84	1	0	-7.095733	-2.175404	-2.912461

IntC2

Thermal correction to Energy=	0.753034
Thermal correction to Enthalpy=	0.753978
Thermal correction to Gibbs Free Energy=	0.642694
Sum of electronic and zero-point Energies=	-1779.833112
Sum of electronic and thermal Energies=	-1779.794176
Sum of electronic and thermal Enthalpies=	-1779.793232
Sum of electronic and thermal Free Energies=	-1779.904516

Esol = -1781.1487271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.859761	2.128873	-3.158161
2	6	0	-1.527597	3.435717	-1.267187
3	6	0	-0.850197	1.012823	-2.341031
4	1	0	-0.626531	2.022473	-4.211484
5	6	0	-1.506927	2.275823	-0.509397
6	1	0	-1.776803	4.379856	-0.795495
7	1	0	-0.589258	0.018103	-2.684460
8	1	0	-1.754523	2.241694	0.547624
9	7	0	-1.169280	1.094851	-1.041813

10	6	0	2.459845	-1.189366	-1.315901
11	6	0	2.664223	-1.696640	0.146584
12	5	0	0.869223	-0.240706	0.073368
13	8	0	1.664314	-0.020868	-1.131930
14	8	0	1.407885	-1.401284	0.747053
15	6	0	2.921029	-3.192560	0.268360
16	1	0	3.809206	-3.489000	-0.300469
17	1	0	3.084059	-3.453221	1.318081
18	1	0	2.060525	-3.758391	-0.092662
19	6	0	1.646499	-2.182109	-2.151874
20	1	0	1.387180	-1.702886	-3.101525
21	1	0	2.210007	-3.093806	-2.374119
22	1	0	0.718366	-2.439779	-1.631502
23	6	0	3.744402	-0.812202	-2.041350
24	1	0	4.417141	-1.673053	-2.120052
25	1	0	3.507597	-0.472198	-3.053704
26	1	0	4.266073	-0.004030	-1.524508
27	6	0	3.765635	-0.916517	0.873665
28	1	0	3.686669	-1.120653	1.945297
29	1	0	4.764598	-1.210190	0.535613
30	1	0	3.650101	0.160141	0.717943
31	6	0	-2.671172	-1.690148	-0.145910
32	6	0	-2.465540	-1.183175	1.316495
33	5	0	-0.872610	-0.238602	-0.072928
34	8	0	-1.414107	-1.397986	-0.746416
35	8	0	-1.667167	-0.016645	1.132347
36	6	0	-3.749175	-0.802792	2.041898
37	1	0	-4.424023	-1.661985	2.120656
38	1	0	-3.511553	-0.463289	3.054229
39	1	0	-4.268854	0.006615	1.524983
40	6	0	-3.770664	-0.907413	-0.873093
41	1	0	-3.692159	-1.111835	-1.944705
42	1	0	-4.770345	-1.198640	-0.535047
43	1	0	-3.652542	0.168978	-0.717458
44	6	0	-2.931687	-3.185445	-0.267456
45	1	0	-3.820579	-3.479587	0.301450
46	1	0	-3.095398	-3.445866	-1.317129
47	1	0	-2.072579	-3.753354	0.093634
48	6	0	-1.654616	-2.177787	2.152598
49	1	0	-1.394089	-1.699053	3.102166
50	1	0	-2.220365	-3.088054	2.375005
51	1	0	-0.727136	-2.437828	1.632240
52	6	0	1.509762	2.272247	0.509451
53	6	0	1.532990	3.432269	1.266974

54	6	0	0.861519	2.127462	3.158069
55	6	0	0.849510	1.011248	2.341199
56	1	0	1.757562	2.237269	-0.547496
57	1	0	1.784568	4.375700	0.795123
58	1	0	0.627739	2.021866	4.211350
59	7	0	1.169095	1.092218	1.042035
60	1	0	0.586050	0.017243	2.684776
61	6	0	-1.196298	3.379807	-2.625270
62	6	0	1.201132	3.377477	2.624966
63	6	0	1.203601	4.595071	3.468484
64	6	0	0.236662	4.768380	4.465174
65	6	0	2.170128	5.589868	3.283350
66	6	0	0.235577	5.911077	5.257143
67	1	0	-0.533428	4.014775	4.600593
68	6	0	2.170781	6.730205	4.078803
69	1	0	2.941449	5.453570	2.531138
70	6	0	1.203107	6.894358	5.066913
71	1	0	-0.525623	6.036370	6.020153
72	1	0	2.932979	7.488378	3.931990
73	6	0	-1.196345	4.597177	-3.469113
74	6	0	-0.229416	4.768109	-4.466223
75	6	0	-2.160649	5.594112	-3.283897
76	6	0	-0.226184	5.910572	-5.258529
77	1	0	0.538986	4.012797	-4.601726
78	6	0	-2.159163	6.734213	-4.079685
79	1	0	-2.931977	5.459689	-2.531354
80	6	0	-1.191525	6.895988	-5.068221
81	1	0	0.534988	6.034004	-6.021870
82	1	0	-2.919670	7.494068	-3.932801
83	1	0	-1.190452	7.786317	-5.688320
84	1	0	1.203709	7.784877	5.686742

TSC3

Thermal correction to Energy= 0.751175
Thermal correction to Enthalpy= 0.752119
Thermal correction to Gibbs Free Energy= 0.642687
Sum of electronic and zero-point Energies= -1779.818835
Sum of electronic and thermal Energies= -1779.780303
Sum of electronic and thermal Enthalpies= -1779.779359
Sum of electronic and thermal Free Energies= -1779.888791

Esol = -1781.131222

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.561679	3.154615	-0.616302
2	6	0	-1.997237	1.308077	-1.092493
3	6	0	0.521458	2.344517	-0.783769
4	1	0	-0.393409	4.207469	-0.418167
5	6	0	-0.877192	0.499940	-1.221040
6	1	0	-2.971631	0.844914	-1.210897
7	1	0	1.544599	2.691303	-0.720337
8	1	0	-0.928106	-0.539763	-1.522482
9	7	0	0.386381	1.006568	-1.082824
10	6	0	2.695522	1.443787	2.337782
11	6	0	3.366345	0.034916	2.473687
12	5	0	1.572500	-0.110155	1.092917
13	8	0	1.425426	1.130448	1.741494
14	8	0	2.838602	-0.678599	1.344363
15	6	0	4.883060	0.042135	2.375911
16	1	0	5.322061	0.664311	3.162866
17	1	0	5.262356	-0.976576	2.493545
18	1	0	5.203939	0.419348	1.403252
19	6	0	3.458823	2.367225	1.390415
20	1	0	2.849941	3.258972	1.212306
21	1	0	4.409149	2.688040	1.827872
22	1	0	3.646785	1.871390	0.433927
23	6	0	2.441811	2.148931	3.662995
24	1	0	3.383367	2.324482	4.194124
25	1	0	1.971037	3.117379	3.474625
26	1	0	1.777693	1.565631	4.302652
27	6	0	2.910897	-0.707319	3.731155
28	1	0	3.243847	-1.746027	3.662296
29	1	0	3.328879	-0.265991	4.640589
30	1	0	1.819039	-0.701844	3.809019
31	6	0	3.365803	-0.034588	-2.474061
32	6	0	2.695134	-1.443529	-2.338016
33	5	0	1.572230	0.110312	-1.092900
34	8	0	2.838185	0.678924	-1.344678
35	8	0	1.425162	-1.130331	-1.741398
36	6	0	2.441137	-2.148652	-3.663190
37	1	0	3.382570	-2.324124	-4.194564
38	1	0	1.970478	-3.117137	-3.474725
39	1	0	1.776815	-1.565383	-4.302662
40	6	0	2.910089	0.707583	-3.731470

41	1	0	3.243036	1.746300	-3.662726
42	1	0	3.327885	0.266223	-4.640974
43	1	0	1.818214	0.702090	-3.809101
44	6	0	4.882536	-0.041668	-2.376524
45	1	0	5.321472	-0.663835	-3.163524
46	1	0	5.261722	0.977073	-2.494255
47	1	0	5.203593	-0.418817	-1.403899
48	6	0	3.458754	-2.366955	-1.390899
49	1	0	2.850077	-3.258852	-1.212832
50	1	0	4.409073	-2.687529	-1.828545
51	1	0	3.646770	-1.871234	-0.434364
52	6	0	-0.876841	-0.500131	1.221708
53	6	0	-1.996818	-1.308388	1.093280
54	6	0	-0.561128	-3.154660	0.616431
55	6	0	0.521944	-2.344465	0.783829
56	1	0	-0.927811	0.539518	1.523322
57	1	0	-2.971249	-0.845376	1.211975
58	1	0	-0.392783	-4.207457	0.418059
59	7	0	0.386767	-1.006572	1.083097
60	1	0	1.545113	-2.691115	0.720119
61	6	0	-1.883059	2.655727	-0.765982
62	6	0	-1.882538	-2.655949	0.766446
63	6	0	-3.061997	3.521806	-0.585126
64	6	0	-4.242150	3.294395	-1.307743
65	6	0	-3.034555	4.593736	0.317977
66	6	0	-5.355882	4.104718	-1.127680
67	1	0	-4.274731	2.491244	-2.038041
68	6	0	-4.147936	5.406888	0.494092
69	1	0	-2.140712	4.771585	0.908554
70	6	0	-5.315108	5.165897	-0.225935
71	1	0	-6.256838	3.913319	-1.702148
72	1	0	-4.106459	6.226680	1.204436
73	1	0	-6.184558	5.800118	-0.087224
74	6	0	-3.061399	-3.522108	0.585460
75	6	0	-3.033963	-4.593583	-0.318181
76	6	0	-4.241453	-3.295206	1.308393
77	6	0	-4.147271	-5.406782	-0.494533
78	1	0	-2.140195	-4.771001	-0.909001
79	6	0	-5.355110	-4.105589	1.128106
80	1	0	-4.274011	-2.492422	2.039099
81	6	0	-5.314352	-5.166299	0.225810
82	1	0	-4.105813	-6.226191	-1.205320
83	1	0	-6.255998	-3.914606	1.702821
84	1	0	-6.183751	-5.800548	0.086903

IntC3

Thermal correction to Energy= 0.756081
Thermal correction to Enthalpy= 0.757025
Thermal correction to Gibbs Free Energy= 0.647667
Sum of electronic and zero-point Energies= -1779.879422
Sum of electronic and thermal Energies= -1779.841057
Sum of electronic and thermal Enthalpies= -1779.840113
Sum of electronic and thermal Free Energies= -1779.949471

Esol =-1781.2016801

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.228466	2.915554	-0.111183
2	6	0	-2.261674	0.841584	-0.810796
3	6	0	-0.006214	2.382988	-0.291508
4	1	0	-1.325845	3.949541	0.194166
5	6	0	-0.954994	0.154608	-0.526199
6	1	0	-3.098499	0.241001	-1.152362
7	1	0	0.909361	2.952206	-0.170999
8	1	0	-0.805853	-0.707817	-1.183971
9	7	0	0.164300	1.075002	-0.730871
10	6	0	2.435193	1.438450	2.997349
11	6	0	3.282707	0.121212	3.064087
12	5	0	1.370200	-0.241733	1.922102
13	8	0	1.148950	0.958019	2.553543
14	8	0	2.668887	-0.694702	2.044526
15	6	0	4.754519	0.294476	2.730753
16	1	0	5.233876	0.968412	3.447941
17	1	0	5.256880	-0.674983	2.781107
18	1	0	4.885224	0.701038	1.726271
19	6	0	2.946042	2.417828	1.945174
20	1	0	2.209045	3.217482	1.833951
21	1	0	3.897348	2.865223	2.248022
22	1	0	3.072487	1.930777	0.972933
23	6	0	2.254601	2.142218	4.333102
24	1	0	3.223890	2.445279	4.742026
25	1	0	1.647681	3.039649	4.190298
26	1	0	1.749937	1.500262	5.056463
27	6	0	3.116623	-0.623140	4.387294
28	1	0	3.562098	-1.615974	4.289684

29	1	0	3.609313	-0.096779	5.209242
30	1	0	2.057759	-0.745805	4.633425
31	6	0	3.439183	0.784658	-2.233425
32	6	0	2.943259	-0.702168	-2.259635
33	5	0	1.391028	0.631196	-1.297691
34	8	0	2.540376	1.395385	-1.285128
35	8	0	1.539769	-0.567606	-1.952493
36	6	0	3.082711	-1.389131	-3.608761
37	1	0	4.134073	-1.428772	-3.911711
38	1	0	2.708386	-2.412986	-3.535101
39	1	0	2.511782	-0.871353	-4.380781
40	6	0	3.232567	1.502128	-3.565734
41	1	0	3.405840	2.570810	-3.419322
42	1	0	3.923375	1.136215	-4.330079
43	1	0	2.208148	1.367527	-3.925167
44	6	0	4.865421	0.970631	-1.744286
45	1	0	5.568740	0.457394	-2.407881
46	1	0	5.114022	2.035024	-1.737316
47	1	0	4.989271	0.579689	-0.732567
48	6	0	3.570407	-1.554206	-1.160417
49	1	0	3.051234	-2.515901	-1.131973
50	1	0	4.630306	-1.740343	-1.356951
51	1	0	3.466981	-1.078961	-0.179405
52	6	0	-0.944062	-0.376913	0.944935
53	6	0	-2.047488	-1.381008	1.134335
54	6	0	-0.461354	-3.111114	0.544510
55	6	0	0.563657	-2.283657	0.817504
56	1	0	-1.075525	0.489064	1.601747
57	1	0	-3.034917	-1.019874	1.403287
58	1	0	-0.264199	-4.133196	0.246818
59	7	0	0.355700	-0.978413	1.249516
60	1	0	1.601101	-2.598261	0.780436
61	6	0	-2.405090	2.151434	-0.533457
62	6	0	-1.825316	-2.680598	0.861975
63	6	0	-3.700599	2.851416	-0.721447
64	6	0	-4.541223	2.518098	-1.789811
65	6	0	-4.114959	3.849750	0.166769
66	6	0	-5.767467	3.151027	-1.956051
67	1	0	-4.212757	1.770716	-2.505636
68	6	0	-5.342347	4.484286	0.000810
69	1	0	-3.481468	4.113816	1.008744
70	6	0	-6.173793	4.136838	-1.060394
71	1	0	-6.402226	2.881647	-2.794424
72	1	0	-5.652175	5.249775	0.705550

73	6	0	-2.904820	-3.694864	0.956922
74	6	0	-2.985382	-4.748318	0.039639
75	6	0	-3.871683	-3.611821	1.965211
76	6	0	-4.014395	-5.681683	0.118390
77	1	0	-2.248793	-4.822523	-0.755470
78	6	0	-4.899425	-4.544139	2.044992
79	1	0	-3.796928	-2.819115	2.703329
80	6	0	-4.975406	-5.583144	1.120915
81	1	0	-4.067500	-6.486835	-0.607880
82	1	0	-5.636960	-4.465420	2.837600
83	1	0	-5.774866	-6.314280	1.185161
84	1	0	-7.129618	4.633847	-1.191471

TSC3

Thermal correction to Energy= 0.752108
Thermal correction to Enthalpy= 0.753053
Thermal correction to Gibbs Free Energy= 0.642661
Sum of electronic and zero-point Energies= -1779.833269
Sum of electronic and thermal Energies= -1779.794689
Sum of electronic and thermal Enthalpies= -1779.793745
Sum of electronic and thermal Free Energies= -1779.904137

Esol = -1781.1538146

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.078974	-3.110485	-0.593533
2	6	0	1.520165	-1.250398	-1.058492
3	6	0	-1.000141	-2.326733	-0.797705
4	1	0	-0.085868	-4.159553	-0.375669
5	6	0	0.405944	-0.420154	-1.131203
6	1	0	2.492587	-0.774594	-1.143651
7	1	0	-2.015058	-2.699824	-0.767888
8	1	0	0.463220	0.606840	-1.469677
9	7	0	-0.883379	-0.972905	-1.133643
10	6	0	-3.250781	-1.450445	2.479699
11	6	0	-4.038937	-0.093077	2.503681
12	5	0	-2.019105	0.208582	1.558551
13	8	0	-1.911716	-1.031407	2.134122
14	8	0	-3.302108	0.715420	1.558791
15	6	0	-5.482926	-0.189995	2.043640

16	1	0	-6.055056	-0.843307	2.709918
17	1	0	-5.939146	0.803577	2.064457
18	1	0	-5.546437	-0.581032	1.027041
19	6	0	-3.740301	-2.397940	1.390221
20	1	0	-3.023873	-3.218847	1.302640
21	1	0	-4.718522	-2.816788	1.644455
22	1	0	-3.812047	-1.886577	0.425592
23	6	0	-3.195613	-2.170726	3.818043
24	1	0	-4.204631	-2.423911	4.158996
25	1	0	-2.629026	-3.098437	3.706901
26	1	0	-2.706873	-1.561403	4.579563
27	6	0	-3.950857	0.619907	3.851478
28	1	0	-4.350491	1.630710	3.740936
29	1	0	-4.525315	0.098048	4.621460
30	1	0	-2.911125	0.697409	4.183316
31	6	0	-4.038878	0.093056	-2.503774
32	6	0	-3.250729	1.450427	-2.479778
33	5	0	-2.019066	-0.208592	-1.558600
34	8	0	-3.302068	-0.715432	-1.558862
35	8	0	-1.911669	1.031394	-2.134178
36	6	0	-3.195541	2.170709	-3.818121
37	1	0	-4.204554	2.423890	-4.159091
38	1	0	-2.628960	3.098423	-3.706968
39	1	0	-2.706785	1.561389	-4.579632
40	6	0	-3.950761	-0.619934	-3.851566
41	1	0	-4.350389	-1.630740	-3.741029
42	1	0	-4.525205	-0.098083	-4.621563
43	1	0	-2.911020	-0.697428	-4.183379
44	6	0	-5.482879	0.189970	-2.043770
45	1	0	-6.054994	0.843279	-2.710063
46	1	0	-5.939095	-0.803604	-2.064597
47	1	0	-5.546418	0.581008	-1.027173
48	6	0	-3.740272	2.397917	-1.390306
49	1	0	-3.023844	3.218822	-1.302704
50	1	0	-4.718487	2.816767	-1.644558
51	1	0	-3.812038	1.886545	-0.425683
52	6	0	0.405913	0.420156	1.131206
53	6	0	1.520132	1.250406	1.058523
54	6	0	0.078942	3.110490	0.593547
55	6	0	-1.000174	2.326732	0.797691
56	1	0	0.463187	-0.606839	1.469674
57	1	0	2.492554	0.774607	1.143699
58	1	0	-0.085900	4.159559	0.375688
59	7	0	-0.883412	0.972901	1.133621

60	1	0	-2.015092	2.699818	0.767856
61	6	0	1.420764	-2.601205	-0.755540
62	6	0	1.420731	2.601215	0.755578
63	6	0	2.597250	-3.463093	-0.602602
64	6	0	3.799043	-3.174076	-1.272326
65	6	0	2.565966	-4.604949	0.215886
66	6	0	4.918737	-3.979677	-1.119292
67	1	0	3.841354	-2.322923	-1.945083
68	6	0	3.685841	-5.414388	0.362034
69	1	0	1.662476	-4.842090	0.769372
70	6	0	4.870951	-5.107774	-0.301992
71	1	0	5.831190	-3.734351	-1.654198
72	1	0	3.635710	-6.286253	1.007338
73	6	0	2.597216	3.463109	0.602670
74	6	0	2.565943	4.604973	-0.215808
75	6	0	3.798997	3.174093	1.272416
76	6	0	3.685817	5.414418	-0.361927
77	1	0	1.662463	4.842114	-0.769310
78	6	0	4.918691	3.979701	1.119411
79	1	0	3.841299	2.322935	1.945167
80	6	0	4.870915	5.107805	0.302120
81	1	0	3.635695	6.286289	-1.007225
82	1	0	5.831134	3.734375	1.654334
83	1	0	5.744618	-5.741002	-0.188122
84	1	0	5.744581	5.741038	0.188273

IntC4

Thermal correction to Energy=	0.374767
Thermal correction to Enthalpy=	0.375711
Thermal correction to Gibbs Free Energy=	0.307495
Sum of electronic and zero-point Energies=	-889.914251
Sum of electronic and thermal Energies=	-889.895162
Sum of electronic and thermal Enthalpies=	-889.894218
Sum of electronic and thermal Free Energies=	-889.962434

Esol = -890.5771992

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.306263	1.193652	-0.070621
2	6	0	3.662088	1.202364	-0.077911

3	6	0	3.662143	-1.202166	0.077670
4	6	0	2.306318	-1.193519	0.070364
5	7	0	1.579449	0.000051	-0.000109
6	1	0	1.704415	2.092669	-0.105013
7	1	0	4.157772	2.166342	-0.104575
8	1	0	4.157875	-2.166120	0.104268
9	1	0	1.704511	-2.092566	0.104695
10	5	0	0.146532	0.000019	-0.000060
11	8	0	-0.598795	-1.142485	0.150412
12	8	0	-0.598854	1.142489	-0.150492
13	6	0	-1.960574	-0.766714	-0.156950
14	6	0	-1.960601	0.766657	0.156938
15	6	0	-2.905307	-1.590147	0.701492
16	1	0	-3.937049	-1.250476	0.565673
17	1	0	-2.848815	-2.640411	0.405300
18	1	0	-2.645187	-1.517734	1.758422
19	6	0	-2.181536	-1.064234	-1.638342
20	1	0	-1.951459	-2.115929	-1.823269
21	1	0	-3.217061	-0.875986	-1.934625
22	1	0	-1.522213	-0.453112	-2.261704
23	6	0	-2.905413	1.590046	-0.701458
24	1	0	-3.937134	1.250331	-0.565588
25	1	0	-2.848953	2.640314	-0.405272
26	1	0	-2.645343	1.517642	-1.758401
27	6	0	-2.181505	1.064167	1.638341
28	1	0	-1.951460	2.115871	1.823258
29	1	0	-3.217008	0.875876	1.934672
30	1	0	-1.522127	0.453071	2.261671
31	6	0	4.429598	0.000120	-0.000087
32	6	0	5.885834	0.000160	-0.000045
33	6	0	6.620080	1.074447	-0.540881
34	6	0	6.620113	-1.074087	0.540833
35	6	0	8.007723	1.073653	-0.537639
36	1	0	6.094676	1.904552	-1.002514
37	6	0	8.007755	-1.073212	0.537665
38	1	0	6.094733	-1.904219	1.002442
39	6	0	8.715455	0.000241	0.000032
40	1	0	8.541977	1.913763	-0.971364
41	1	0	8.542038	-1.913285	0.971428
42	1	0	9.800252	0.000272	0.000065

D

Thermal correction to Energy= 0.102955

Thermal correction to Enthalpy= 0.103899
Thermal correction to Gibbs Free Energy= 0.061367
Sum of electronic and zero-point Energies= -585.018512
Sum of electronic and thermal Energies= -585.010861
Sum of electronic and thermal Enthalpies= -585.009917
Sum of electronic and thermal Free Energies= -585.052448

Esol = -585.346213

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.529287	1.140149	0.000086
2	6	0	0.139733	1.192126	-0.000068
3	6	0	-0.555418	-0.012361	-0.000156
4	6	0	0.149068	-1.207049	-0.000111
5	6	0	1.541440	-1.139914	0.000024
6	7	0	2.227631	0.002026	0.000136
7	1	0	2.110671	2.058560	0.000160
8	1	0	-0.367847	-2.159167	-0.000231
9	1	0	2.130786	-2.053337	0.000035
10	1	0	-0.384793	2.141558	-0.000167
11	6	0	-2.059422	0.010626	-0.000000
12	9	0	-2.580221	-1.221750	-0.002208
13	9	0	-2.531879	0.654947	-1.075774
14	9	0	-2.531695	0.650911	1.078284

TSD1

Thermal correction to Energy= 0.491235
Thermal correction to Enthalpy= 0.492179
Thermal correction to Gibbs Free Energy= 0.404740
Sum of electronic and zero-point Energies= -1406.880992
Sum of electronic and thermal Energies= -1406.853206
Sum of electronic and thermal Enthalpies= -1406.852261
Sum of electronic and thermal Free Energies= -1406.939700

Esol =-1407.865000

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.029811	-1.253188	1.230885
2	6	0	1.921086	-1.608945	-1.152447
3	6	0	0.691342	-0.880104	1.186384
4	1	0	2.577227	-1.261283	2.165616
5	6	0	0.587731	-1.223655	-1.102227
6	1	0	2.384727	-1.895357	-2.089643
7	1	0	0.134038	-0.561961	2.063622
8	1	0	-0.056016	-1.179239	-1.977024
9	7	0	0.004685	-0.874299	0.044441
10	6	0	0.262636	3.312229	0.724607
11	6	0	0.596707	3.031318	-0.773017
12	5	0	-0.930270	1.517756	-0.027655
13	8	0	-0.416480	2.102584	1.114092
14	8	0	-0.472963	2.150231	-1.166390
15	6	0	0.595045	4.257027	-1.671898
16	1	0	1.345295	4.981134	-1.337257
17	1	0	0.836694	3.960786	-2.695752
18	1	0	-0.383183	4.740212	-1.679331
19	6	0	-0.727882	4.460481	0.904942
20	1	0	-1.084103	4.456646	1.937691
21	1	0	-0.264426	5.429061	0.696402
22	1	0	-1.590079	4.332113	0.244471
23	6	0	1.472692	3.507768	1.624286
24	1	0	2.070701	4.362111	1.290409
25	1	0	1.140244	3.701535	2.647364
26	1	0	2.104903	2.617710	1.634243
27	6	0	1.895343	2.243078	-0.948969
28	1	0	1.956368	1.896140	-1.983787
29	1	0	2.775907	2.853733	-0.730238
30	1	0	1.908507	1.364645	-0.293675
31	6	0	-3.198568	-1.571104	0.761281
32	6	0	-3.483352	-1.288732	-0.749959
33	5	0	-1.751995	0.022565	-0.012815
34	8	0	-2.410596	-0.435718	1.141843
35	8	0	-2.319901	-0.563336	-1.166879
36	6	0	-3.634505	-2.533555	-1.612071
37	1	0	-4.470661	-3.149451	-1.264130
38	1	0	-3.835244	-2.238935	-2.645662
39	1	0	-2.725203	-3.137814	-1.601100
40	6	0	-2.372939	-2.842115	0.977317
41	1	0	-2.006217	-2.848746	2.007801
42	1	0	-2.977234	-3.740478	0.818365
43	1	0	-1.512795	-2.882282	0.305023
44	6	0	-4.438800	-1.616799	1.643184

45	1	0	-5.125357	-2.402075	1.308977
46	1	0	-4.146294	-1.834056	2.674109
47	1	0	-4.962570	-0.659821	1.633514
48	6	0	-4.684466	-0.363653	-0.951376
49	1	0	-4.698962	-0.034741	-1.993264
50	1	0	-5.630396	-0.865788	-0.727535
51	1	0	-4.595115	0.521267	-0.314734
52	6	0	2.643426	-1.616833	0.036995
53	6	0	4.106080	-1.975773	0.003974
54	9	0	4.837270	-0.956675	-0.464496
55	9	0	4.568723	-2.281465	1.220812
56	9	0	4.327225	-3.024231	-0.798081

IntD1

Thermal correction to Energy=	0.492717
Thermal correction to Enthalpy=	0.493662
Thermal correction to Gibbs Free Energy=	0.405701
Sum of electronic and zero-point Energies=	-1406.882525
Sum of electronic and thermal Energies=	-1406.854430
Sum of electronic and thermal Enthalpies=	-1406.853485
Sum of electronic and thermal Free Energies=	-1406.941446

Esol = -1407.8676756

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.662676	-0.793338	1.012506
2	6	0	-2.977234	0.053269	-1.220743
3	6	0	-1.364583	-0.309007	0.966997
4	1	0	-3.029596	-1.310623	1.890736
5	6	0	-1.668845	0.514095	-1.184352
6	1	0	-3.592747	0.204428	-2.099505
7	1	0	-0.659923	-0.412409	1.784890
8	1	0	-1.194189	1.057236	-1.995254
9	7	0	-0.898890	0.330332	-0.109085
10	6	0	2.325644	-2.693071	0.460372
11	6	0	3.383545	-2.037129	-0.480021
12	5	0	1.660399	-0.585276	-0.119271
13	8	0	1.186485	-1.826290	0.284059
14	8	0	2.995363	-0.650806	-0.455682
15	6	0	4.823452	-2.158775	-0.006545

16	1	0	5.117184	-3.211096	0.069865
17	1	0	5.485523	-1.670033	-0.725727
18	1	0	4.963549	-1.681258	0.964320
19	6	0	2.717977	-2.612565	1.935121
20	1	0	1.854488	-2.891914	2.544169
21	1	0	3.544223	-3.289056	2.171369
22	1	0	3.009130	-1.591979	2.199705
23	6	0	1.934301	-4.115162	0.092095
24	1	0	2.806309	-4.776342	0.128811
25	1	0	1.193525	-4.488143	0.804227
26	1	0	1.499997	-4.161009	-0.907832
27	6	0	3.260276	-2.510448	-1.927608
28	1	0	3.869064	-1.860751	-2.560542
29	1	0	3.606677	-3.541333	-2.045831
30	1	0	2.223014	-2.445300	-2.268535
31	6	0	0.782827	2.977696	0.857530
32	6	0	1.293281	3.039364	-0.616962
33	5	0	0.733114	0.866647	-0.082196
34	8	0	0.895849	1.586326	1.156437
35	8	0	0.806025	1.814870	-1.166495
36	6	0	0.745369	4.203179	-1.430094
37	1	0	1.022424	5.160795	-0.976527
38	1	0	1.160343	4.171172	-2.441216
39	1	0	-0.343098	4.153136	-1.506217
40	6	0	-0.683471	3.404804	0.981128
41	1	0	-1.056203	3.094372	1.961499
42	1	0	-0.796048	4.489849	0.892459
43	1	0	-1.302145	2.933399	0.212164
44	6	0	1.629273	3.755944	1.855425
45	1	0	1.673371	4.817669	1.589380
46	1	0	1.190816	3.671083	2.853866
47	1	0	2.644004	3.356915	1.894473
48	6	0	2.820941	3.008367	-0.695218
49	1	0	3.110596	2.837035	-1.735054
50	1	0	3.267858	3.947652	-0.354939
51	1	0	3.214618	2.182820	-0.095212
52	6	0	-3.473715	-0.602610	-0.100534
53	6	0	-4.910644	-1.056463	-0.070928
54	9	0	-5.348588	-1.367893	-1.295743
55	9	0	-5.068515	-2.128377	0.712257
56	9	0	-5.703139	-0.088974	0.406354

TSD2

Thermal correction to Energy= 0.596695
Thermal correction to Enthalpy= 0.597639
Thermal correction to Gibbs Free Energy= 0.493533
Sum of electronic and zero-point Energies= -1991.918348
Sum of electronic and thermal Energies= -1991.882008
Sum of electronic and thermal Enthalpies= -1991.881064
Sum of electronic and thermal Free Energies= -1991.985170

Esol =-1993.2218255

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.480250	0.772049	2.420727
2	6	0	-2.302929	1.563441	0.299335
3	6	0	-0.196979	0.813946	1.894440
4	1	0	-1.648015	0.450162	3.441654
5	6	0	-0.990055	1.585191	-0.148995
6	1	0	-3.118617	1.848857	-0.353711
7	1	0	0.684428	0.498362	2.443473
8	1	0	-0.696383	1.890252	-1.148442
9	7	0	0.022976	1.194220	0.630431
10	6	0	2.824577	-2.348980	1.469726
11	6	0	3.223696	-2.622254	-0.014006
12	5	0	1.835822	-0.800016	0.093717
13	8	0	1.681584	-1.491781	1.327868
14	8	0	2.861122	-1.393308	-0.654138
15	6	0	4.709853	-2.863908	-0.235808
16	1	0	5.056035	-3.730027	0.338589
17	1	0	4.893900	-3.060039	-1.295504
18	1	0	5.293384	-1.988794	0.054804
19	6	0	3.889365	-1.545383	2.218141
20	1	0	3.472765	-1.222066	3.176053
21	1	0	4.789180	-2.136687	2.411924
22	1	0	4.156722	-0.650355	1.648093
23	6	0	2.433835	-3.586459	2.262729
24	1	0	3.269965	-4.291584	2.316083
25	1	0	2.164723	-3.300318	3.283305
26	1	0	1.578216	-4.092784	1.810869
27	6	0	2.410831	-3.754875	-0.643024
28	1	0	2.554783	-3.723930	-1.726334
29	1	0	2.733408	-4.733690	-0.274990
30	1	0	1.344162	-3.635442	-0.437825

31	6	0	2.844008	2.840507	0.007732
32	6	0	2.603123	2.413678	-1.475293
33	5	0	1.583009	0.903276	-0.051412
34	8	0	2.545549	1.642966	0.721535
35	8	0	1.496133	1.517034	-1.363618
36	6	0	2.227994	3.554381	-2.410565
37	1	0	3.023619	4.305994	-2.446848
38	1	0	2.080695	3.166129	-3.422320
39	1	0	1.302523	4.039622	-2.092083
40	6	0	1.881608	3.944977	0.456413
41	1	0	1.917964	4.016952	1.546950
42	1	0	2.153917	4.916881	0.032818
43	1	0	0.852686	3.718695	0.161367
44	6	0	4.276852	3.247538	0.323213
45	1	0	4.592589	4.093419	-0.297229
46	1	0	4.350605	3.546465	1.372693
47	1	0	4.958925	2.411734	0.158423
48	6	0	3.784462	1.625818	-2.045559
49	1	0	3.478260	1.184279	-2.998097
50	1	0	4.655792	2.264239	-2.222071
51	1	0	4.058615	0.808630	-1.372314
52	6	0	-0.912757	-1.818030	0.003398
53	6	0	-2.252466	-1.739635	-0.349879
54	6	0	-1.546982	-0.856749	-2.477402
55	6	0	-0.231269	-0.959635	-2.027793
56	1	0	-0.579769	-2.170701	0.976935
57	1	0	-3.033555	-2.031085	0.343981
58	1	0	-1.769695	-0.466830	-3.463490
59	7	0	0.066597	-1.421446	-0.814135
60	1	0	0.613313	-0.618296	-2.619810
61	6	0	-2.542796	1.128015	1.595978
62	6	0	-2.562557	-1.237400	-1.610853
63	6	0	-3.961157	0.942711	2.064434
64	6	0	-4.010297	-1.042615	-1.968395
65	9	0	-4.170518	-0.684980	-3.245847
66	9	0	-4.723413	-2.152471	-1.754748
67	9	0	-4.553983	-0.074941	-1.205909
68	9	0	-4.386978	-0.298417	1.777458
69	9	0	-4.070820	1.104867	3.387115
70	9	0	-4.794253	1.798051	1.466611

IntD2

Thermal correction to Energy= 0.597692

Thermal correction to Enthalpy= 0.598636
Thermal correction to Gibbs Free Energy= 0.491663
Sum of electronic and zero-point Energies= -1991.918383
Sum of electronic and thermal Energies= -1991.881631
Sum of electronic and thermal Enthalpies= -1991.880687
Sum of electronic and thermal Free Energies= -1991.987660

Esol =-1993.2235673

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.993060	-3.189131	-0.811203
2	6	0	-2.338442	-1.849533	0.671582
3	6	0	0.114596	-2.467192	-0.397998
4	1	0	-0.892427	-3.976804	-1.547968
5	6	0	-1.182944	-1.176879	1.041593
6	1	0	-3.295185	-1.583260	1.105142
7	1	0	1.117492	-2.631234	-0.776052
8	1	0	-1.157140	-0.374968	1.773975
9	7	0	0.005756	-1.485765	0.508542
10	6	0	2.248440	0.019446	-2.805441
11	6	0	2.777346	1.393187	-2.283126
12	5	0	1.329355	0.481527	-0.734274
13	8	0	1.086457	-0.191838	-2.001671
14	8	0	2.493885	1.315565	-0.887487
15	6	0	4.273808	1.605902	-2.460619
16	1	0	4.559666	1.542963	-3.516201
17	1	0	4.550347	2.596939	-2.089745
18	1	0	4.835043	0.861500	-1.893366
19	6	0	3.230648	-1.116862	-2.509837
20	1	0	2.737216	-2.068114	-2.734760
21	1	0	4.134334	-1.051605	-3.123590
22	1	0	3.505765	-1.110775	-1.450141
23	6	0	1.849742	0.009923	-4.274150
24	1	0	2.706357	0.250555	-4.912875
25	1	0	1.488938	-0.985029	-4.550231
26	1	0	1.051348	0.728273	-4.471119
27	6	0	2.005189	2.571728	-2.885258
28	1	0	2.231874	3.469725	-2.303395
29	1	0	2.285780	2.752952	-3.927600
30	1	0	0.925768	2.396884	-2.844880
31	6	0	2.777350	-1.393192	2.283135

32	6	0	2.248419	-0.019465	2.805460
33	5	0	1.329359	-0.481539	0.734280
34	8	0	2.493901	-1.315560	0.887494
35	8	0	1.086441	0.191811	2.001682
36	6	0	1.849707	-0.009966	4.274165
37	1	0	2.706319	-0.250594	4.912896
38	1	0	1.488887	0.984978	4.550255
39	1	0	1.051321	-0.728329	4.471118
40	6	0	2.005203	-2.571750	2.885247
41	1	0	2.231911	-3.469739	2.303381
42	1	0	2.285782	-2.752977	3.927592
43	1	0	0.925780	-2.396923	2.844854
44	6	0	4.273813	-1.605888	2.460641
45	1	0	4.559660	-1.542956	3.516226
46	1	0	4.550370	-2.596917	2.089758
47	1	0	4.835043	-0.861472	1.893401
48	6	0	3.230615	1.116860	2.509880
49	1	0	2.737171	2.068102	2.734819
50	1	0	4.134299	1.051603	3.123635
51	1	0	3.505736	1.110796	1.450185
52	6	0	-1.183021	1.176692	-1.041410
53	6	0	-2.338507	1.849361	-0.671386
54	6	0	-0.993007	3.189304	0.810982
55	6	0	0.114631	2.467337	0.397781
56	1	0	-1.157267	0.374645	-1.773644
57	1	0	-3.295289	1.582962	-1.104782
58	1	0	-0.892321	3.977124	1.547583
59	7	0	0.005729	1.485732	-0.508559
60	1	0	1.117565	2.631499	0.775684
61	6	0	-2.233888	-2.867788	-0.269209
62	6	0	-2.233887	2.867799	0.269199
63	6	0	-3.454985	-3.655659	-0.663928
64	6	0	-3.454970	3.655692	0.663917
65	9	0	-3.358855	4.107196	1.919704
66	9	0	-3.621020	4.717684	-0.133131
67	9	0	-4.563780	2.910594	0.575388
68	9	0	-4.563819	-2.910631	-0.575093
69	9	0	-3.359021	-4.106893	-1.919823
70	9	0	-3.620877	-4.717826	0.132920

TSD3

Thermal correction to Energy= 0.596759

Thermal correction to Enthalpy= 0.597703

Thermal correction to Gibbs Free Energy= 0.494519
Sum of electronic and zero-point Energies= -1991.909698
Sum of electronic and thermal Energies= -1991.873751
Sum of electronic and thermal Enthalpies= -1991.872807
Sum of electronic and thermal Free Energies= -1991.975991

Esol = -1993.2141484

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.970158	3.205963	-0.372294
2	6	0	-2.425208	1.397428	-1.000408
3	6	0	0.107269	2.396691	-0.591370
4	1	0	-0.815752	4.234170	-0.065365
5	6	0	-1.301563	0.602451	-1.194684
6	1	0	-3.408790	0.980870	-1.184591
7	1	0	1.134613	2.716329	-0.476413
8	1	0	-1.347461	-0.406050	-1.589395
9	7	0	-0.045675	1.093663	-1.000301
10	6	0	2.229678	1.253397	2.454304
11	6	0	2.877488	-0.170644	2.501654
12	5	0	1.147921	-0.175726	1.031008
13	8	0	0.979167	1.006468	1.786370
14	8	0	2.404423	-0.772277	1.286044
15	6	0	4.397326	-0.177964	2.484086
16	1	0	4.800936	0.371459	3.340982
17	1	0	4.758791	-1.208445	2.537635
18	1	0	4.773129	0.271025	1.562913
19	6	0	3.038750	2.233151	1.606472
20	1	0	2.452324	3.148720	1.480505
21	1	0	3.980203	2.501135	2.095220
22	1	0	3.248314	1.807899	0.620449
23	6	0	1.934756	1.855782	3.820218
24	1	0	2.857312	1.972553	4.398674
25	1	0	1.484546	2.843739	3.693030
26	1	0	1.239084	1.234485	4.386570
27	6	0	2.348320	-1.010921	3.665050
28	1	0	2.668917	-2.045919	3.521129
29	1	0	2.727455	-0.658170	4.628517
30	1	0	1.254157	-0.990654	3.692477
31	6	0	2.877510	0.170629	-2.501639
32	6	0	2.229692	-1.253408	-2.454294

33	5	0	1.147934	0.175722	-1.031004
34	8	0	2.404443	0.772263	-1.286030
35	8	0	0.979177	-1.006471	-1.786368
36	6	0	1.934776	-1.855791	-3.820210
37	1	0	2.857335	-1.972566	-4.398660
38	1	0	1.484561	-2.843746	-3.693025
39	1	0	1.239111	-1.234491	-4.386566
40	6	0	2.348353	1.010910	-3.665036
41	1	0	2.668954	2.045906	-3.521113
42	1	0	2.727491	0.658158	-4.628502
43	1	0	1.254190	0.990649	-3.692469
44	6	0	4.397348	0.177940	-2.484063
45	1	0	4.800959	-0.371484	-3.340958
46	1	0	4.758819	1.208419	-2.537610
47	1	0	4.773144	-0.271052	-1.562889
48	6	0	3.038751	-2.233166	-1.606455
49	1	0	2.452317	-3.148731	-1.480490
50	1	0	3.980205	-2.501158	-2.095196
51	1	0	3.248311	-1.807913	-0.620431
52	6	0	-1.301581	-0.602434	1.194656
53	6	0	-2.425231	-1.397402	1.000366
54	6	0	-0.970187	-3.205953	0.372282
55	6	0	0.107245	-2.396689	0.591367
56	1	0	-1.347477	0.406069	1.589361
57	1	0	-3.408811	-0.980833	1.184529
58	1	0	-0.815788	-4.234160	0.065350
59	7	0	-0.045695	-1.093658	1.000292
60	1	0	1.134587	-2.716334	0.476421
61	6	0	-2.271818	2.702768	-0.573799
62	6	0	-2.271845	-2.702745	0.573765
63	6	0	-3.446611	-3.592820	0.320901
64	6	0	-3.446585	3.592834	-0.320909
65	9	0	-4.602468	-3.003916	0.655269
66	9	0	-3.533009	-3.942667	-0.973333
67	9	0	-3.354104	-4.736302	1.018110
68	9	0	-3.353911	4.736474	-1.017833
69	9	0	-4.602415	3.004058	-0.655598
70	9	0	-3.533194	3.942375	0.973393

IntD3

Thermal correction to Energy= 0.601435
Thermal correction to Enthalpy= 0.602379
Thermal correction to Gibbs Free Energy= 0.497656

Sum of electronic and zero-point Energies= -1991.979359
Sum of electronic and thermal Energies= -1991.943251
Sum of electronic and thermal Enthalpies= -1991.942307
Sum of electronic and thermal Free Energies= -1992.047030

Esol =-1993.2940619

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.184406	2.920644	-0.054868
2	6	0	-2.260895	0.865913	-0.801220
3	6	0	0.026494	2.375406	-0.272145
4	1	0	-1.284083	3.937081	0.301578
5	6	0	-0.957637	0.161531	-0.537937
6	1	0	-3.109109	0.312436	-1.187142
7	1	0	0.953370	2.924935	-0.150210
8	1	0	-0.820927	-0.693844	-1.206522
9	7	0	0.167112	1.075577	-0.740423
10	6	0	2.406366	1.466615	2.998055
11	6	0	3.267644	0.157803	3.061731
12	5	0	1.362765	-0.221651	1.917285
13	8	0	1.125052	0.973924	2.544630
14	8	0	2.662657	-0.662381	2.037111
15	6	0	4.737595	0.346479	2.729626
16	1	0	5.209515	1.023327	3.448830
17	1	0	5.249329	-0.618010	2.778814
18	1	0	4.865167	0.756450	1.726215
19	6	0	2.911590	2.456892	1.953643
20	1	0	2.170485	3.253525	1.848015
21	1	0	3.858749	2.908279	2.262797
22	1	0	3.045980	1.977475	0.978485
23	6	0	2.210810	2.161430	4.336027
24	1	0	3.174702	2.473996	4.750211
25	1	0	1.594019	3.052240	4.194689
26	1	0	1.710802	1.510427	5.054322
27	6	0	3.107183	-0.593385	4.381366
28	1	0	3.564295	-1.580628	4.281624
29	1	0	3.592665	-0.063983	5.205472
30	1	0	2.049628	-0.728925	4.626387
31	6	0	3.445046	0.746000	-2.233932
32	6	0	2.927176	-0.733253	-2.272540
33	5	0	1.392831	0.616841	-1.309062

34	8	0	2.549224	1.364469	-1.284067
35	8	0	1.523094	-0.580085	-1.965441
36	6	0	3.057081	-1.412534	-3.626119
37	1	0	4.108041	-1.465872	-3.927950
38	1	0	2.667496	-2.431119	-3.559887
39	1	0	2.495065	-0.881073	-4.395230
40	6	0	3.254676	1.475879	-3.561451
41	1	0	3.443334	2.540801	-3.407540
42	1	0	3.943902	1.104591	-4.324439
43	1	0	2.230546	1.359018	-3.927891
44	6	0	4.871136	0.907412	-1.736203
45	1	0	5.568983	0.385624	-2.398783
46	1	0	5.136754	1.967575	-1.724551
47	1	0	4.984438	0.510528	-0.725538
48	6	0	3.540054	-1.602289	-1.178926
49	1	0	3.007439	-2.556817	-1.157922
50	1	0	4.596751	-1.802755	-1.377551
51	1	0	3.446095	-1.130800	-0.194955
52	6	0	-0.947666	-0.379510	0.930406
53	6	0	-2.042332	-1.398526	1.099097
54	6	0	-0.413652	-3.106183	0.493023
55	6	0	0.593052	-2.266067	0.794714
56	1	0	-1.092848	0.477296	1.595543
57	1	0	-3.033244	-1.083100	1.404236
58	1	0	-0.217755	-4.115264	0.155796
59	7	0	0.355104	-0.971944	1.239654
60	1	0	1.636358	-2.559894	0.764089
61	6	0	-2.354605	2.161336	-0.474458
62	6	0	-1.771139	-2.674608	0.797830
63	6	0	-3.641616	2.912985	-0.617297
64	6	0	-2.823091	-3.737263	0.877886
65	9	0	-2.903804	-4.418392	-0.278335
66	9	0	-4.038663	-3.242173	1.140523
67	9	0	-2.540039	-4.636589	1.833652
68	9	0	-4.649173	2.137256	-1.036169
69	9	0	-4.008578	3.454831	0.556838
70	9	0	-3.525083	3.928998	-1.487454

TSD4

Thermal correction to Energy= 0.597329
Thermal correction to Enthalpy= 0.598273
Thermal correction to Gibbs Free Energy= 0.492892
Sum of electronic and zero-point Energies= -1991.930028

Sum of electronic and thermal Energies= -1991.893642
Sum of electronic and thermal Enthalpies= -1991.892697
Sum of electronic and thermal Free Energies= -1991.998078

Esol =-1993.2433571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.814550	-0.702671	-3.101333
2	6	0	3.291491	0.452983	-1.575415
3	6	0	0.747838	-0.186073	-2.456980
4	1	0	1.659251	-1.340746	-3.963606
5	6	0	2.183126	0.884343	-0.853507
6	1	0	4.278316	0.725296	-1.216735
7	1	0	-0.273026	-0.350855	-2.772436
8	1	0	2.248228	1.615242	-0.057322
9	7	0	0.890181	0.659836	-1.348745
10	6	0	-1.460046	-2.860910	-0.366706
11	6	0	-2.259847	-2.346760	0.883271
12	5	0	-0.242155	-1.357245	0.803330
13	8	0	-0.123559	-2.368241	-0.111559
14	8	0	-1.525389	-1.158327	1.261396
15	6	0	-3.700793	-1.960477	0.599764
16	1	0	-4.270146	-2.829651	0.255848
17	1	0	-4.165133	-1.589372	1.517506
18	1	0	-3.757263	-1.178876	-0.159571
19	6	0	-1.944894	-2.242439	-1.672582
20	1	0	-1.224338	-2.486896	-2.457254
21	1	0	-2.920085	-2.646738	-1.959120
22	1	0	-2.023096	-1.154523	-1.588400
23	6	0	-1.393380	-4.374852	-0.494252
24	1	0	-2.398395	-4.794791	-0.602845
25	1	0	-0.814923	-4.637385	-1.383271
26	1	0	-0.911718	-4.828817	0.372884
27	6	0	-2.182491	-3.303450	2.070712
28	1	0	-2.590472	-2.803756	2.952402
29	1	0	-2.755428	-4.216470	1.888625
30	1	0	-1.144944	-3.578710	2.282529
31	6	0	-2.259675	2.346986	-0.883166
32	6	0	-1.459791	2.860961	0.366825
33	5	0	-0.242150	1.357135	-0.803281
34	8	0	-1.525432	1.158423	-1.261314

35	8	0	-0.123388	2.368071	0.111657
36	6	0	-1.392866	4.374887	0.494415
37	1	0	-2.397812	4.794998	0.602986
38	1	0	-0.814394	4.637294	1.383462
39	1	0	-0.911097	4.828793	-0.372692
40	6	0	-2.182121	3.303691	-2.070584
41	1	0	-2.590176	2.804096	-2.952295
42	1	0	-2.754889	4.216814	-1.888487
43	1	0	-1.144518	3.578763	-2.282374
44	6	0	-3.700703	1.960991	-0.599685
45	1	0	-4.269870	2.830279	-0.255751
46	1	0	-4.165116	1.590011	-1.517439
47	1	0	-3.757362	1.179384	0.159630
48	6	0	-1.944739	2.242523	1.672677
49	1	0	-1.224036	2.486669	2.457307
50	1	0	-2.919775	2.647117	1.959330
51	1	0	-2.023311	1.154644	1.588354
52	6	0	2.183168	-0.884686	0.853456
53	6	0	3.291590	-0.453408	1.575326
54	6	0	1.814788	0.702465	3.101221
55	6	0	0.748016	0.185943	2.456907
56	1	0	2.248176	-1.615617	0.057290
57	1	0	4.278383	-0.725827	1.216638
58	1	0	1.659568	1.340596	3.963466
59	7	0	0.890264	-0.660044	1.348723
60	1	0	-0.272837	0.350817	2.772342
61	6	0	3.143291	-0.363689	-2.676961
62	6	0	3.143487	0.363318	2.676848
63	6	0	4.305248	0.925407	3.410562
64	6	0	4.304982	-0.925833	-3.410745
65	9	0	4.213570	-0.709093	-4.737379
66	9	0	4.399897	-2.264246	-3.266569
67	9	0	5.468671	-0.402597	-2.995843
68	9	0	5.468846	0.401759	2.995923
69	9	0	4.213651	0.709086	4.737251
70	9	0	4.400514	2.263756	3.265996

IntD4

Thermal correction to Energy=	0.296011
Thermal correction to Enthalpy=	0.296955
Thermal correction to Gibbs Free Energy=	0.232812
Sum of electronic and zero-point Energies=	-995.961767
Sum of electronic and thermal Energies=	-995.944425

Sum of electronic and thermal Enthalpies= -995.943480
Sum of electronic and thermal Free Energies= -996.007624

Esol =-996.6203033

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.238434	1.222533	-0.177713
2	6	0	2.245924	-1.176718	0.192549
3	6	0	0.878620	1.205776	-0.172164
4	1	0	2.754818	2.163740	-0.323512
5	6	0	0.889695	-1.171403	0.193118
6	1	0	0.268081	2.088909	-0.306218
7	1	0	0.286726	-2.059504	0.331047
8	7	0	0.165255	0.013469	0.010654
9	6	0	-3.381464	0.770254	0.103051
10	6	0	-3.371605	-0.781677	-0.108198
11	5	0	-1.270989	0.005870	0.007438
12	8	0	-2.018399	1.131396	-0.222396
13	8	0	-2.008201	-1.127575	0.232014
14	6	0	-4.315410	-1.552929	0.797925
15	1	0	-5.350209	-1.242239	0.622084
16	1	0	-4.237356	-2.621349	0.582666
17	1	0	-4.073150	-1.396453	1.849926
18	6	0	-3.611390	1.164422	1.559628
19	1	0	-3.390611	2.227995	1.674976
20	1	0	-4.646929	0.987625	1.862466
21	1	0	-2.950632	0.601374	2.225337
22	6	0	-4.323965	1.530539	-0.813717
23	1	0	-5.356089	1.202236	-0.654973
24	1	0	-4.266638	2.599170	-0.593062
25	1	0	-4.063364	1.382382	-1.862571
26	6	0	-3.581616	-1.177401	-1.567357
27	1	0	-3.350055	-2.238880	-1.680880
28	1	0	-4.615260	-1.009466	-1.881410
29	1	0	-2.918765	-0.607904	-2.225448
30	6	0	2.971694	0.029050	0.004645
31	1	0	2.769518	-2.115373	0.337552
32	6	0	4.453374	0.000870	-0.004456
33	9	0	4.945438	-0.783659	-0.986518
34	9	0	4.978752	1.224974	-0.175708
35	9	0	4.964381	-0.496467	1.141054

E

Thermal correction to Energy=	0.102943
Thermal correction to Enthalpy=	0.103887
Thermal correction to Gibbs Free Energy=	0.061617
Sum of electronic and zero-point Energies=	-585.018931
Sum of electronic and thermal Energies=	-585.011280
Sum of electronic and thermal Enthalpies=	-585.010336
Sum of electronic and thermal Free Energies=	-585.052606

Esol =-585.3466388

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.516723	1.126428	0.146702
2	6	0	0.123038	1.163387	0.117839
3	6	0	-0.566312	-0.036399	0.022851
4	6	0	0.172294	-1.214155	-0.037782
5	6	0	1.561828	-1.145609	-0.005299
6	7	0	2.232201	0.003353	0.085246
7	1	0	2.085986	2.050008	0.221154
8	1	0	2.154144	-2.055014	-0.060841
9	1	0	-0.400720	2.111067	0.165773
10	6	0	-0.535285	-2.535327	-0.099864
11	9	0	-1.037738	-2.879467	1.095271
12	9	0	-1.567464	-2.493506	-0.956236
13	9	0	0.281176	-3.521728	-0.489342
14	1	0	-1.651032	-0.067181	-0.010723

TSE1

Thermal correction to Energy=	0.491497
Thermal correction to Enthalpy=	0.492442
Thermal correction to Gibbs Free Energy=	0.406087
Sum of electronic and zero-point Energies=	-1406.882094
Sum of electronic and thermal Energies=	-1406.854378
Sum of electronic and thermal Enthalpies=	-1406.853434
Sum of electronic and thermal Free Energies=	-1406.939789

Esol =-1407.8655805

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.146141	-1.443792	2.592865
2	6	0	1.712920	-2.168085	0.380460
3	6	0	0.063581	-0.769636	2.039556
4	1	0	1.324892	-1.408978	3.660797
5	6	0	0.603724	-1.478258	-0.095829
6	1	0	-0.634188	-0.176558	2.625919
7	1	0	0.329779	-1.443221	-1.147572
8	7	0	-0.191086	-0.803510	0.730572
9	6	0	1.198459	3.313402	0.339541
10	6	0	1.872080	2.295945	-0.631240
11	5	0	-0.246691	1.619172	-0.144676
12	8	0	0.051333	2.573251	0.804678
13	8	0	0.741854	1.542455	-1.110097
14	6	0	2.598273	2.917612	-1.812924
15	1	0	3.408464	3.568679	-1.468492
16	1	0	3.032034	2.128123	-2.431681
17	1	0	1.915799	3.500502	-2.432995
18	6	0	0.670920	4.554004	-0.379190
19	1	0	0.025042	5.107631	0.306201
20	1	0	1.485339	5.209225	-0.701219
21	1	0	0.079484	4.270751	-1.254330
22	6	0	2.045259	3.715367	1.536871
23	1	0	2.972743	4.196237	1.209262
24	1	0	1.490341	4.425855	2.154541
25	1	0	2.295098	2.850322	2.153457
26	6	0	2.784437	1.305577	0.094209
27	1	0	3.041230	0.491913	-0.589043
28	1	0	3.708559	1.780936	0.435468
29	1	0	2.273560	0.874948	0.963370
30	6	0	-3.513845	-0.433440	0.553378
31	6	0	-3.339028	-0.504122	-0.998334
32	5	0	-1.488737	0.452537	-0.037881
33	8	0	-2.506327	0.514153	0.932669
34	8	0	-1.939056	-0.257024	-1.174991
35	6	0	-3.694018	-1.847689	-1.619342
36	1	0	-4.742826	-2.099558	-1.429865
37	1	0	-3.544114	-1.799367	-2.701041
38	1	0	-3.063039	-2.646031	-1.224427
39	6	0	-3.220924	-1.771834	1.237293
40	1	0	-3.122586	-1.600929	2.313392

41	1	0	-4.032334	-2.487398	1.074232
42	1	0	-2.292424	-2.214509	0.869535
43	6	0	-4.866305	0.088988	1.018154
44	1	0	-5.677628	-0.546914	0.648415
45	1	0	-4.902268	0.089265	2.110949
46	1	0	-5.030755	1.110638	0.673113
47	6	0	-4.088229	0.619309	-1.717740
48	1	0	-3.756129	0.647111	-2.758266
49	1	0	-5.171494	0.467356	-1.697936
50	1	0	-3.858647	1.585239	-1.258972
51	6	0	1.988777	-2.154257	1.743970
52	1	0	2.848158	-2.693637	2.128043
53	6	0	2.632078	-2.860653	-0.584355
54	9	0	3.551143	-2.014710	-1.074811
55	9	0	1.960980	-3.363606	-1.625145
56	9	0	3.295035	-3.863343	0.007266

IntE1

Thermal correction to Energy=	0.492584
Thermal correction to Enthalpy=	0.493529
Thermal correction to Gibbs Free Energy=	0.404219
Sum of electronic and zero-point Energies=	-1406.882947
Sum of electronic and thermal Energies=	-1406.854579
Sum of electronic and thermal Enthalpies=	-1406.853635
Sum of electronic and thermal Free Energies=	-1406.942945

Esol = -1407.8679698

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.046711	2.949757	-0.757436
2	6	0	-0.116208	3.005101	0.801090
3	5	0	0.357546	0.852121	0.109341
4	8	0	-0.186835	1.554446	-1.025688
5	8	0	0.553126	1.800510	1.175344
6	6	0	0.619686	4.182086	1.426800
7	1	0	0.220643	5.133666	1.059439
8	1	0	0.498471	4.156985	2.513451
9	1	0	1.686157	4.133575	1.201904
10	6	0	1.321351	3.387431	-1.286093
11	1	0	1.381969	3.125881	-2.345409

12	1	0	1.476739	4.465502	-1.180599
13	1	0	2.119474	2.854517	-0.761128
14	6	0	-1.156665	3.709109	-1.470100
15	1	0	-1.129904	4.772820	-1.210882
16	1	0	-1.026416	3.617893	-2.551747
17	1	0	-2.139207	3.309192	-1.210615
18	6	0	-1.557695	2.962230	1.319608
19	1	0	-1.537107	2.731638	2.388601
20	1	0	-2.066228	3.921125	1.180223
21	1	0	-2.140977	2.189582	0.810699
22	6	0	3.656714	-1.119247	-0.812013
23	6	0	3.128774	-1.932140	0.410622
24	5	0	1.689132	-0.225306	-0.079564
25	8	0	2.851774	0.073250	-0.756496
26	8	0	1.762029	-1.482265	0.505618
27	6	0	3.147293	-3.442038	0.232550
28	1	0	4.169782	-3.797745	0.069016
29	1	0	2.759136	-3.922510	1.134444
30	1	0	2.528551	-3.749343	-0.611823
31	6	0	3.356111	-1.798070	-2.147922
32	1	0	3.549758	-1.085193	-2.952587
33	1	0	3.982262	-2.681562	-2.302336
34	1	0	2.305265	-2.096229	-2.202466
35	6	0	5.125293	-0.731756	-0.736279
36	1	0	5.758061	-1.624038	-0.686015
37	1	0	5.399180	-0.167279	-1.630976
38	1	0	5.325309	-0.106338	0.134948
39	6	0	3.815518	-1.542218	1.719184
40	1	0	3.264358	-1.987271	2.551537
41	1	0	4.848472	-1.899619	1.755168
42	1	0	3.812708	-0.456006	1.846890
43	6	0	-1.948058	-0.449925	-0.208062
44	6	0	-2.952094	-1.326022	0.177970
45	6	0	-1.827628	-1.618255	2.271745
46	6	0	-0.855613	-0.736843	1.819619
47	1	0	-1.925342	0.063702	-1.164566
48	1	0	-1.743494	-2.058971	3.257281
49	7	0	-0.930471	-0.176154	0.609699
50	1	0	0.010732	-0.450357	2.406207
51	6	0	-2.894247	-1.921098	1.434677
52	1	0	-3.670276	-2.614422	1.742108
53	6	0	-4.117720	-1.588286	-0.733857
54	9	0	-5.149547	-0.782995	-0.449304
55	9	0	-3.793115	-1.389057	-2.014743

56	9	0	-4.553731	-2.848684	-0.604885

TSE2

Thermal correction to Energy= 0.596917
Thermal correction to Enthalpy= 0.597861
Thermal correction to Gibbs Free Energy= 0.489033
Sum of electronic and zero-point Energies= -1991.915921
Sum of electronic and thermal Energies= -1991.879134
Sum of electronic and thermal Enthalpies= -1991.878190
Sum of electronic and thermal Free Energies= -1991.987018

Esol =-1993.2215842

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.169950	-1.446624	-1.157253
2	6	0	1.261868	-2.368321	-2.273385
3	6	0	2.331432	-0.994464	-0.152826
4	6	0	0.479181	-1.889975	-1.228205
5	1	0	0.800558	-2.905544	-3.093173
6	1	0	2.679399	-0.435070	0.708691
7	1	0	-0.597209	-2.025357	-1.164203
8	7	0	1.015625	-1.218916	-0.206609
9	6	0	1.635846	3.005577	0.340171
10	6	0	0.265090	3.483849	0.917019
11	5	0	0.201829	1.227458	0.530200
12	8	0	1.316626	1.710794	-0.191176
13	8	0	-0.348347	2.246236	1.306768
14	6	0	0.373673	4.378737	2.143457
15	1	0	0.940886	5.287139	1.914014
16	1	0	-0.627234	4.673506	2.469513
17	1	0	0.859308	3.855183	2.968313
18	6	0	2.684675	2.779171	1.431296
19	1	0	3.537164	2.255221	0.988595
20	1	0	3.040421	3.718365	1.864655
21	1	0	2.270621	2.152605	2.227899
22	6	0	2.203573	3.880038	-0.767245
23	1	0	2.385093	4.897066	-0.404306
24	1	0	3.155529	3.465298	-1.109837
25	1	0	1.523708	3.928547	-1.620088
26	6	0	-0.618407	4.150676	-0.138007

27	1	0	-1.631216	4.240135	0.263983
28	1	0	-0.253614	5.150878	-0.390804
29	1	0	-0.664794	3.549410	-1.048469
30	6	0	-0.147109	-1.813101	2.815215
31	6	0	-1.556369	-1.603682	2.176092
32	5	0	0.033977	-0.438270	0.964505
33	8	0	0.603066	-0.738061	2.252070
34	8	0	-1.235674	-1.132223	0.866935
35	6	0	-2.402090	-2.863115	2.052778
36	1	0	-2.623801	-3.284788	3.038761
37	1	0	-3.347734	-2.614689	1.563350
38	1	0	-1.896612	-3.622033	1.451800
39	6	0	0.485455	-3.143867	2.394304
40	1	0	1.549810	-3.117986	2.644480
41	1	0	0.026693	-3.992312	2.911422
42	1	0	0.387797	-3.305440	1.316838
43	6	0	-0.115027	-1.683338	4.331824
44	1	0	-0.790834	-2.405497	4.802642
45	1	0	0.898220	-1.874496	4.696144
46	1	0	-0.401324	-0.675581	4.636601
47	6	0	-2.349630	-0.500091	2.881410
48	1	0	-3.247538	-0.290144	2.292236
49	1	0	-2.663338	-0.795874	3.886954
50	1	0	-1.750800	0.414370	2.944074
51	6	0	-0.749870	0.831170	-2.366396
52	6	0	-1.526050	0.203903	-3.337025
53	6	0	-3.275884	0.071450	-1.710543
54	6	0	-2.435971	0.715211	-0.807387
55	1	0	0.278190	1.139754	-2.550189
56	1	0	-1.125646	0.020302	-4.327395
57	7	0	-1.199882	1.079295	-1.136277
58	1	0	-2.738034	0.920582	0.215484
59	6	0	2.630795	-2.140049	-2.239154
60	6	0	-2.816265	-0.190217	-2.996779
61	1	0	-3.456072	-0.701090	-3.708609
62	1	0	3.278339	-2.484240	-3.039231
63	6	0	-4.660077	-0.317064	-1.280349
64	6	0	4.651518	-1.212755	-1.071078
65	9	0	-4.670920	-0.766930	-0.017762
66	9	0	-5.505693	0.721627	-1.332855
67	9	0	-5.165215	-1.280754	-2.063830
68	9	0	5.293747	-2.304009	-0.633830
69	9	0	4.945066	-0.210222	-0.237277
70	9	0	5.159415	-0.915213	-2.275318

IntE2

Thermal correction to Energy= 0.598044
Thermal correction to Enthalpy= 0.598988
Thermal correction to Gibbs Free Energy= 0.492476
Sum of electronic and zero-point Energies= -1991.918498
Sum of electronic and thermal Energies= -1991.881774
Sum of electronic and thermal Enthalpies= -1991.880829
Sum of electronic and thermal Free Energies= -1991.987341

Esol = -1993.2241875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.290372	-0.735631	-1.524745
2	6	0	1.536176	-1.388514	-3.015340
3	6	0	2.391460	-0.820198	-0.472727
4	6	0	0.686910	-1.448577	-1.919597
5	1	0	1.162338	-1.629010	-4.003269
6	1	0	2.653925	-0.607553	0.558678
7	1	0	-0.361764	-1.726675	-1.977000
8	7	0	1.117325	-1.161624	-0.683409
9	6	0	1.476434	2.451400	1.344043
10	6	0	0.070118	2.713855	1.970436
11	5	0	-0.034809	0.878059	0.578138
12	8	0	1.165313	1.619364	0.224816
13	8	0	-0.586796	1.462992	1.770366
14	6	0	0.087181	3.019068	3.461495
15	1	0	0.703890	3.898407	3.676833
16	1	0	-0.930514	3.221861	3.806659
17	1	0	0.472220	2.166036	4.022429
18	6	0	2.377085	1.645905	2.285065
19	1	0	3.276630	1.351643	1.734895
20	1	0	2.689547	2.229655	3.156041
21	1	0	1.855669	0.743562	2.623675
22	6	0	2.205190	3.692376	0.849622
23	1	0	2.405860	4.384459	1.674177
24	1	0	3.161857	3.396771	0.408987
25	1	0	1.624796	4.213784	0.085659
26	6	0	-0.694683	3.809054	1.219851
27	1	0	-1.745673	3.768305	1.519447

28	1	0	-0.305434	4.805920	1.449126
29	1	0	-0.637244	3.657520	0.137848
30	6	0	-0.070180	-2.713571	1.970793
31	6	0	-1.476474	-2.451178	1.344327
32	5	0	0.034807	-0.877961	0.578257
33	8	0	0.586757	-1.462744	1.770570
34	8	0	-1.165314	-1.619292	0.224999
35	6	0	-2.205238	-3.692209	0.850057
36	1	0	-2.405928	-4.384181	1.674700
37	1	0	-3.161895	-3.396653	0.409368
38	1	0	-1.624838	-4.213727	0.086172
39	6	0	0.694632	-3.808884	1.220387
40	1	0	1.745614	-3.768099	1.520007
41	1	0	0.305369	-4.805715	1.449793
42	1	0	0.637226	-3.657505	0.138362
43	6	0	-0.087293	-3.018574	3.461895
44	1	0	-0.704022	-3.897874	3.677335
45	1	0	0.930388	-3.221335	3.807119
46	1	0	-0.472338	-2.165458	4.022697
47	6	0	-2.377136	-1.645535	2.285210
48	1	0	-3.276656	-1.351332	1.734966
49	1	0	-2.689634	-2.229154	3.156260
50	1	0	-1.855711	-0.743154	2.623705
51	6	0	-0.686855	1.448270	-1.919795
52	6	0	-1.536099	1.388026	-3.015544
53	6	0	-3.290327	0.735399	-1.524876
54	6	0	-2.391437	0.820141	-0.472852
55	1	0	0.361819	1.726360	-1.977225
56	1	0	-1.162240	1.628359	-4.003504
57	7	0	-1.117296	1.161528	-0.683566
58	1	0	-2.653926	0.607688	0.558588
59	6	0	2.862891	-1.016983	-2.817542
60	6	0	-2.862820	1.016533	-2.817710
61	1	0	-3.557708	0.942936	-3.646713
62	1	0	3.557794	-0.943517	-3.646544
63	6	0	-4.704492	0.326091	-1.223159
64	6	0	4.704531	-0.326276	-1.223069
65	9	0	-4.738948	-0.828939	-0.545869
66	9	0	-5.326541	1.241559	-0.470624
67	9	0	-5.418970	0.165513	-2.344492
68	9	0	5.326659	-1.241758	-0.470617
69	9	0	4.738966	0.828722	-0.545723
70	9	0	5.418949	-0.165610	-2.344428

TSE3

Thermal correction to Energy= 0.596889
Thermal correction to Enthalpy= 0.597833
Thermal correction to Gibbs Free Energy= 0.494095
Sum of electronic and zero-point Energies= -1991.908550
Sum of electronic and thermal Energies= -1991.872575
Sum of electronic and thermal Enthalpies= -1991.871631
Sum of electronic and thermal Free Energies= -1991.975369

Esol =-1993.2123281

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.150820	-1.619454	0.684384
2	6	0	1.338540	-3.117315	1.096734
3	6	0	2.309737	-0.556313	0.845077
4	6	0	0.497012	-2.013545	1.226356
5	1	0	0.912801	-4.106983	1.220512
6	1	0	2.628508	0.475970	0.786484
7	1	0	-0.541766	-2.085612	1.527560
8	7	0	0.977619	-0.742161	1.109221
9	6	0	1.574120	1.489548	-2.275953
10	6	0	0.180607	2.167649	-2.499994
11	5	0	-0.042906	0.436455	-1.048399
12	8	0	1.216846	0.240954	-1.654793
13	8	0	-0.583250	1.699918	-1.376065
14	6	0	0.203956	3.686820	-2.471581
15	1	0	0.870315	4.080783	-3.246019
16	1	0	-0.802216	4.072745	-2.656080
17	1	0	0.537978	4.047870	-1.497289
18	6	0	2.455973	2.272879	-1.305223
19	1	0	3.329540	1.661889	-1.058644
20	1	0	2.810686	3.205181	-1.754707
21	1	0	1.909496	2.501298	-0.384847
22	6	0	2.341164	1.188256	-3.555055
23	1	0	2.545721	2.111213	-4.107655
24	1	0	3.297306	0.721251	-3.304205
25	1	0	1.785621	0.505393	-4.199783
26	6	0	-0.512876	1.660941	-3.765846
27	1	0	-1.551343	2.001560	-3.755513
28	1	0	-0.031127	2.036200	-4.673448

29	1	0	-0.509813	0.566570	-3.796787
30	6	0	-0.180609	2.167617	2.500018
31	6	0	-1.574122	1.489518	2.275969
32	5	0	0.042905	0.436442	1.048402
33	8	0	0.583247	1.699902	1.376082
34	8	0	-1.216847	0.240932	1.654794
35	6	0	-2.341165	1.188213	3.555068
36	1	0	-2.545719	2.111163	4.107679
37	1	0	-3.297309	0.721214	3.304213
38	1	0	-1.785624	0.505340	4.199787
39	6	0	0.512875	1.660892	3.765863
40	1	0	1.551348	2.001492	3.755521
41	1	0	0.031141	2.036157	4.673470
42	1	0	0.509793	0.566521	3.796801
43	6	0	-0.203962	3.686789	2.471627
44	1	0	-0.870338	4.080738	3.246057
45	1	0	0.802204	4.072716	2.656150
46	1	0	-0.537968	4.047849	1.497333
47	6	0	-2.455975	2.272861	1.305248
48	1	0	-3.329541	1.661873	1.058662
49	1	0	-2.810688	3.205157	1.754743
50	1	0	-1.909497	2.501292	0.384875
51	6	0	-0.497011	-2.013530	-1.226385
52	6	0	-1.338537	-3.117302	-1.096772
53	6	0	-3.150818	-1.619448	-0.684403
54	6	0	-2.309737	-0.556305	-0.845087
55	1	0	0.541766	-2.085591	-1.527594
56	1	0	-0.912796	-4.106968	-1.220561
57	7	0	-0.977619	-0.742147	-1.109234
58	1	0	-2.628509	0.475978	-0.786483
59	6	0	2.675674	-2.943347	0.804410
60	6	0	-2.675671	-2.943339	-0.804443
61	6	0	-4.609672	-1.383136	-0.432291
62	6	0	4.609674	-1.383139	0.432279
63	9	0	5.054976	-2.154292	-0.570397
64	9	0	5.349206	-1.685215	1.509915
65	9	0	4.869527	-0.107632	0.113643
66	9	0	-5.349208	-1.685202	-1.509927
67	9	0	-5.054969	-2.154300	0.570379
68	9	0	-4.869525	-0.107633	-0.113640
69	1	0	-3.349017	-3.782308	-0.674444
70	1	0	3.349023	-3.782314	0.674403

IntE3

Thermal correction to Energy= 0.601770
Thermal correction to Enthalpy= 0.602714
Thermal correction to Gibbs Free Energy= 0.498745
Sum of electronic and zero-point Energies= -1991.985228
Sum of electronic and thermal Energies= -1991.949340
Sum of electronic and thermal Enthalpies= -1991.948395
Sum of electronic and thermal Free Energies= -1992.052364

Esol = -1993.2991471

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.118238	2.910999	0.017628
2	6	0	-2.268681	0.929472	-0.753909
3	6	0	0.079281	2.346846	-0.240472
4	6	0	-0.982838	0.176655	-0.525770
5	1	0	-3.127459	0.397746	-1.147755
6	1	0	1.014232	2.885145	-0.136696
7	1	0	-0.876854	-0.664746	-1.216900
8	7	0	0.170814	1.060780	-0.723811
9	6	0	2.330505	1.546613	3.000815
10	6	0	3.246139	0.273420	3.025858
11	5	0	1.338665	-0.167599	1.912315
12	8	0	1.062667	1.009192	2.552796
13	8	0	2.654581	-0.557747	1.999973
14	6	0	4.700064	0.525769	2.666465
15	1	0	5.161153	1.206941	3.388494
16	1	0	5.249193	-0.419006	2.686812
17	1	0	4.789368	0.958153	1.668642
18	6	0	2.779799	2.579921	1.972992
19	1	0	2.003707	3.345070	1.885545
20	1	0	3.708049	3.065959	2.286868
21	1	0	2.935722	2.121134	0.990707
22	6	0	2.121688	2.205238	4.354869
23	1	0	3.076519	2.552185	4.762478
24	1	0	1.464557	3.070111	4.237486
25	1	0	1.660633	1.519135	5.066398
26	6	0	3.144324	-0.506122	4.334992
27	1	0	3.641396	-1.470864	4.209678
28	1	0	3.622622	0.030421	5.158607
29	1	0	2.098787	-0.691720	4.598329
30	6	0	3.448062	0.627189	-2.198073

31	6	0	2.872849	-0.830566	-2.269721
32	5	0	1.388863	0.561849	-1.287800
33	8	0	2.570290	1.263874	-1.239907
34	8	0	1.474714	-0.629187	-1.955640
35	6	0	2.969901	-1.483318	-3.638898
36	1	0	4.016473	-1.570489	-3.947666
37	1	0	2.541596	-2.487280	-3.591134
38	1	0	2.424680	-0.913986	-4.392891
39	6	0	3.293034	1.391484	-3.510708
40	1	0	3.522699	2.444853	-3.334424
41	1	0	3.970514	1.008469	-4.278324
42	1	0	2.266923	1.322752	-3.883989
43	6	0	4.875962	0.723332	-1.689163
44	1	0	5.556742	0.187653	-2.358339
45	1	0	5.181985	1.772214	-1.656620
46	1	0	4.967394	0.303099	-0.685899
47	6	0	3.454588	-1.749702	-1.200546
48	1	0	2.878468	-2.678961	-1.185707
49	1	0	4.498026	-1.994603	-1.418892
50	1	0	3.401050	-1.286417	-0.209515
51	6	0	-0.974673	-0.399532	0.928022
52	6	0	-2.036634	-1.462829	1.046615
53	6	0	-0.345256	-3.075156	0.426208
54	6	0	0.634831	-2.220920	0.785591
55	1	0	-1.154974	0.433794	1.613767
56	1	0	-3.037248	-1.174356	1.347782
57	7	0	0.345747	-0.955844	1.245239
58	1	0	1.681516	-2.501233	0.788894
59	6	0	-2.332952	2.218260	-0.396553
60	6	0	-1.731693	-2.721880	0.708385
61	1	0	-3.251749	2.790628	-0.483481
62	1	0	-2.475285	-3.513255	0.720878
63	6	0	-0.020980	-4.430588	-0.086350
64	6	0	-1.209105	4.291408	0.557032
65	9	0	-0.522235	-4.640570	-1.317131
66	9	0	-0.537336	-5.398739	0.693704
67	9	0	1.305723	-4.644468	-0.160550
68	9	0	-1.910994	4.338603	1.703914
69	9	0	0.001227	4.820886	0.812209
70	9	0	-1.836366	5.124508	-0.294494

TSE4

Thermal correction to Energy= 0.596749

Thermal correction to Enthalpy= 0.597693
Thermal correction to Gibbs Free Energy= 0.493471
Sum of electronic and zero-point Energies= -1991.928243
Sum of electronic and thermal Energies= -1991.891912
Sum of electronic and thermal Enthalpies= -1991.890968
Sum of electronic and thermal Free Energies= -1991.995191

Esol =-1993.2390427

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.328785	2.117337	-3.147297
2	6	0	-0.647060	3.609766	-1.544716
3	6	0	-0.116654	1.051279	-2.446423
4	6	0	-1.005929	2.515044	-0.766169
5	1	0	-0.881091	4.596337	-1.157677
6	1	0	0.024204	0.031457	-2.775037
7	1	0	-1.622955	2.589675	0.119853
8	7	0	-0.834840	1.209105	-1.262680
9	6	0	2.788370	-1.129716	-0.744433
10	6	0	2.435483	-1.939875	0.554769
11	5	0	1.452432	0.080299	0.622156
12	8	0	2.331760	0.205476	-0.418191
13	8	0	1.309361	-1.205452	1.092219
14	6	0	2.009282	-3.376728	0.310309
15	1	0	2.825859	-3.945840	-0.144945
16	1	0	1.753825	-3.847302	1.263664
17	1	0	1.138559	-3.423865	-0.345675
18	6	0	2.011644	-1.607107	-1.965636
19	1	0	2.149510	-0.886155	-2.775076
20	1	0	2.378882	-2.580497	-2.303807
21	1	0	0.943902	-1.692973	-1.742515
22	6	0	4.274055	-1.059385	-1.061742
23	1	0	4.677083	-2.062662	-1.232354
24	1	0	4.419417	-0.472887	-1.972068
25	1	0	4.834466	-0.584678	-0.255084
26	6	0	3.537574	-1.878312	1.609827
27	1	0	3.153984	-2.292988	2.544900
28	1	0	4.415879	-2.453366	1.305348
29	1	0	3.843672	-0.844147	1.794225
30	6	0	-2.432818	-1.942232	-0.555059
31	6	0	-2.786654	-1.132869	0.744437

32	5	0	-1.451986	0.079092	-0.621733
33	8	0	-1.307745	-1.206258	-1.092497
34	8	0	-2.331133	0.202864	0.418923
35	6	0	-4.272489	-1.063888	1.061399
36	1	0	-4.674725	-2.067533	1.231707
37	1	0	-4.418549	-0.477698	1.971812
38	1	0	-4.833128	-0.589480	0.254727
39	6	0	-3.535062	-1.881895	-1.610030
40	1	0	-3.151041	-2.296037	-2.545164
41	1	0	-4.412682	-2.457993	-1.305556
42	1	0	-3.842371	-0.848072	-1.794346
43	6	0	-2.004650	-3.378574	-0.310996
44	1	0	-2.820462	-3.948975	0.144016
45	1	0	-1.748458	-3.848488	-1.264479
46	1	0	-1.133900	-3.424689	0.345040
47	6	0	-2.010002	-1.610186	1.965718
48	1	0	-2.149445	-0.890200	2.775752
49	1	0	-2.376166	-2.584359	2.302801
50	1	0	-0.941945	-1.694400	1.743470
51	6	0	1.004015	2.515734	0.767305
52	6	0	0.644071	3.609878	1.546166
53	6	0	-0.331170	2.116066	3.147799
54	6	0	0.115396	1.050618	2.446707
55	1	0	1.621130	2.591206	-0.118581
56	1	0	0.877461	4.596779	1.159586
57	7	0	0.833980	1.209462	1.263342
58	1	0	-0.024878	0.030583	2.774915
59	6	0	0.047547	3.460476	-2.728159
60	6	0	-0.050793	3.459584	2.729332
61	1	0	0.374759	4.303087	-3.322854
62	1	0	-0.378785	4.301706	3.324289
63	6	0	1.101293	1.903506	-4.407395
64	6	0	-1.104396	1.901180	4.407276
65	9	0	2.302577	2.500987	-4.351152
66	9	0	0.467839	2.421781	-5.471676
67	9	0	1.317083	0.601945	-4.669021
68	9	0	-2.306656	2.496593	4.349857
69	9	0	-0.472755	2.420760	5.471998
70	9	0	-1.318207	0.599306	4.668927

IntE4

Thermal correction to Energy= 0.296874

Thermal correction to Enthalpy= 0.297819

Thermal correction to Gibbs Free Energy= 0.232163
Sum of electronic and zero-point Energies= -995.957661
Sum of electronic and thermal Energies= -995.939692
Sum of electronic and thermal Enthalpies= -995.938748
Sum of electronic and thermal Free Energies= -996.004403

Esol =-996.6158257

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.293789	1.191396	-0.211213
2	6	0	3.655922	1.192909	-0.202659
3	6	0	3.637039	-1.178173	0.217817
4	6	0	2.279978	-1.176975	0.206878
5	7	0	1.566259	0.003993	-0.006640
6	1	0	1.688622	2.073798	-0.369378
7	1	0	1.683762	-2.066778	0.359129
8	5	0	0.131520	0.001105	-0.007750
9	8	0	-0.608671	-1.125038	0.245336
10	8	0	-0.614343	1.123851	-0.258646
11	6	0	-1.973665	-0.781813	-0.089329
12	6	0	-1.975580	0.774681	0.086855
13	6	0	-2.909841	-1.529591	0.844059
14	1	0	-3.945065	-1.215102	0.678292
15	1	0	-2.841917	-2.602197	0.647083
16	1	0	-2.650078	-1.356003	1.889158
17	6	0	-2.200523	-1.209876	-1.536782
18	1	0	-1.976683	-2.275218	-1.627628
19	1	0	-3.236253	-1.042202	-1.844082
20	1	0	-1.540450	-0.660405	-2.214405
21	6	0	-2.922615	1.519013	-0.838370
22	1	0	-3.956054	1.206398	-0.658050
23	1	0	-2.851588	2.592549	-0.647335
24	1	0	-2.676195	1.340311	-1.885856
25	6	0	-2.191411	1.202146	1.536499
26	1	0	-1.973969	2.268993	1.624810
27	1	0	-3.222664	1.027722	1.854966
28	1	0	-1.520984	0.657079	2.207528
29	6	0	4.390014	0.008780	0.012522
30	1	0	5.471249	-0.007912	0.023378
31	6	0	4.369987	-2.461270	0.456860
32	9	0	5.145208	-2.384066	1.550106

33	9	0	3.543805	-3.504685	0.625068
34	9	0	5.184770	-2.756986	-0.568654
35	1	0	4.167470	2.134946	-0.366040

F

Thermal correction to Energy=	0.093992
Thermal correction to Enthalpy=	0.094936
Thermal correction to Gibbs Free Energy=	0.062359
Sum of electronic and zero-point Energies=	-248.088268
Sum of electronic and thermal Energies=	-248.084021
Sum of electronic and thermal Enthalpies=	-248.083077
Sum of electronic and thermal Free Energies=	-248.115654

Esol = -248.2645764

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.138278	-0.720957	-0.000006
2	6	0	1.195272	0.670695	0.000014
3	6	0	-1.195272	0.670695	-0.000014
4	6	0	-1.138279	-0.720957	0.000006
5	7	0	0.000000	-1.416793	0.000000
6	1	0	2.055001	-1.306471	0.000028
7	1	0	2.153520	1.178537	0.000036
8	1	0	-2.153520	1.178538	-0.000035
9	1	0	-2.055002	-1.306471	-0.000027
10	6	0	0.000000	1.381087	0.000000
11	1	0	0.000000	2.466627	0.000000

TSF1

Thermal correction to Energy=	0.482550
Thermal correction to Enthalpy=	0.483495
Thermal correction to Gibbs Free Energy=	0.406244
Sum of electronic and zero-point Energies=	-1069.951982
Sum of electronic and thermal Energies=	-1069.927816
Sum of electronic and thermal Enthalpies=	-1069.926871
Sum of electronic and thermal Free Energies=	-1070.004121

Esol = -1070.7850194

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.715874	3.241968	-1.220328
2	6	0	0.470034	3.350368	1.167867
3	6	0	0.094058	1.999268	-1.180823
4	1	0	1.045733	3.658480	-2.165261
5	6	0	-0.140946	2.101589	1.114475
6	1	0	0.605707	3.851387	2.119543
7	1	0	-0.076941	1.396337	-2.069985
8	1	0	-0.495838	1.576742	1.998739
9	7	0	-0.324617	1.457271	-0.036718
10	6	0	2.885125	-1.256209	-0.711362
11	6	0	2.893164	-0.720317	0.754458
12	5	0	0.749973	-0.899644	0.007731
13	8	0	1.531419	-0.991328	-1.126586
14	8	0	1.521118	-0.897247	1.153636
15	6	0	3.792992	-1.483481	1.713282
16	1	0	4.837437	-1.430136	1.388587
17	1	0	3.720020	-1.041740	2.710387
18	1	0	3.497913	-2.531441	1.783172
19	6	0	3.090803	-2.767621	-0.789806
20	1	0	2.865382	-3.099547	-1.806062
21	1	0	4.120480	-3.046879	-0.548099
22	1	0	2.414714	-3.284833	-0.103148
23	6	0	3.836638	-0.542331	-1.658989
24	1	0	4.872094	-0.642717	-1.317348
25	1	0	3.758959	-0.984791	-2.655369
26	1	0	3.591508	0.518674	-1.736832
27	6	0	3.187060	0.777952	0.832474
28	1	0	2.969558	1.125239	1.846021
29	1	0	4.234181	0.996114	0.602820
30	1	0	2.552610	1.337125	0.136615
31	6	0	-3.068704	-0.449007	-0.753472
32	6	0	-3.052664	-0.878846	0.749548
33	5	0	-0.915436	-0.560270	-0.002364
34	8	0	-1.707225	-0.670140	-1.149527
35	8	0	-1.710345	-0.577425	1.154627
36	6	0	-4.025993	-0.120050	1.639706
37	1	0	-5.057105	-0.262662	1.299203
38	1	0	-3.949185	-0.492835	2.664583
39	1	0	-3.802133	0.948407	1.647303
40	6	0	-3.397493	1.033591	-0.938707
41	1	0	-3.163662	1.316039	-1.969286

42	1	0	-4.457962	1.230944	-0.755192
43	1	0	-2.803885	1.658122	-0.268158
44	6	0	-3.974106	-1.287036	-1.645510
45	1	0	-5.014314	-1.228910	-1.307674
46	1	0	-3.925219	-0.910137	-2.670672
47	1	0	-3.661631	-2.332269	-1.652770
48	6	0	-3.244424	-2.385704	0.927583
49	1	0	-3.009103	-2.646576	1.962284
50	1	0	-4.271223	-2.695734	0.711403
51	1	0	-2.563852	-2.937277	0.272704
52	6	0	0.904542	3.926704	-0.021859
53	1	0	1.389896	4.897641	-0.015741

IntF1

Thermal correction to Energy= 0.483754
Thermal correction to Enthalpy= 0.484698
Thermal correction to Gibbs Free Energy= 0.405650
Sum of electronic and zero-point Energies= -1069.954771
Sum of electronic and thermal Energies= -1069.930152
Sum of electronic and thermal Enthalpies= -1069.929208
Sum of electronic and thermal Free Energies= -1070.008256

Esol = -1070.789125

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.518944	-1.175916	-1.307266
2	6	0	3.019643	-1.568392	0.118901
3	5	0	0.964668	-0.515966	0.266407
4	8	0	1.523721	-0.193978	-1.027149
5	8	0	1.820517	-1.500781	0.887729
6	6	0	3.585442	-2.978113	0.224664
7	1	0	4.430071	-3.113990	-0.459712
8	1	0	3.938017	-3.159200	1.244179
9	1	0	2.818076	-3.718485	-0.007019
10	6	0	1.833748	-2.347837	-2.014523
11	1	0	1.314696	-1.963029	-2.896053
12	1	0	2.551036	-3.110707	-2.333113
13	1	0	1.088197	-2.803678	-1.356714
14	6	0	3.583428	-0.565468	-2.207892
15	1	0	4.408154	-1.268249	-2.368557

16	1	0	3.145613	-0.324944	-3.180701
17	1	0	3.984769	0.354730	-1.777753
18	6	0	4.033465	-0.561343	0.673690
19	1	0	4.141792	-0.731791	1.748716
20	1	0	5.014880	-0.674543	0.202387
21	1	0	3.695669	0.467729	0.520132
22	6	0	-2.753007	-1.805974	-0.093644
23	6	0	-2.743265	-1.279638	1.375210
24	5	0	-0.704299	-0.927589	0.401298
25	8	0	-1.351702	-1.829128	-0.419168
26	8	0	-1.554450	-0.465427	1.396845
27	6	0	-3.941766	-0.425435	1.757487
28	1	0	-4.869641	-0.999856	1.666423
29	1	0	-3.842666	-0.098525	2.795972
30	1	0	-4.012725	0.461102	1.125495
31	6	0	-3.419938	-0.833287	-1.065611
32	1	0	-3.201482	-1.155671	-2.086337
33	1	0	-4.505005	-0.804766	-0.929628
34	1	0	-3.020533	0.176485	-0.934494
35	6	0	-3.327649	-3.203018	-0.268333
36	1	0	-4.373558	-3.234193	0.054971
37	1	0	-3.286597	-3.484280	-1.323651
38	1	0	-2.758869	-3.938907	0.302090
39	6	0	-2.536143	-2.395030	2.399606
40	1	0	-2.335022	-1.943866	3.374683
41	1	0	-3.420350	-3.033084	2.486033
42	1	0	-1.677983	-3.014665	2.124207
43	6	0	1.371643	2.089019	0.570885
44	6	0	1.466872	3.263872	1.303567
45	6	0	1.077241	1.974817	3.291940
46	6	0	0.987141	0.845108	2.493668
47	1	0	1.494583	2.030203	-0.505883
48	1	0	1.658849	4.201879	0.796470
49	1	0	0.958557	1.887944	4.365246
50	7	0	1.136208	0.916850	1.167637
51	1	0	0.797543	-0.149306	2.883655
52	6	0	1.318654	3.204137	2.685619
53	1	0	1.389528	4.106350	3.284520

TSF2

Thermal correction to Energy= 0.577961

Thermal correction to Enthalpy= 0.578905

Thermal correction to Gibbs Free Energy= 0.492107

Sum of electronic and zero-point Energies= -1318.057248
Sum of electronic and thermal Energies= -1318.028435
Sum of electronic and thermal Enthalpies= -1318.027490
Sum of electronic and thermal Free Energies= -1318.114288

Esol = -1319.0609519

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.900002	2.178595	3.025801
2	6	0	1.887354	3.209703	1.095347
3	6	0	0.767329	1.011946	2.287640
4	1	0	0.561913	2.206222	4.054738
5	6	0	1.730553	2.006005	0.422630
6	1	0	2.331880	4.056902	0.586419
7	1	0	0.318181	0.103671	2.674916
8	1	0	2.035569	1.841497	-0.606602
9	7	0	1.178316	0.943509	1.016681
10	6	0	-2.858886	-1.078186	1.051959
11	6	0	-2.904214	-1.501047	-0.449846
12	5	0	-0.885423	-0.521565	0.025223
13	8	0	-1.752628	-0.165673	1.086466
14	8	0	-1.524001	-1.426562	-0.826027
15	6	0	-3.398051	-2.920407	-0.692856
16	1	0	-4.414724	-3.052647	-0.306829
17	1	0	-3.410417	-3.123268	-1.767102
18	1	0	-2.739928	-3.649306	-0.216970
19	6	0	-2.495800	-2.244253	1.973670
20	1	0	-2.296538	-1.848399	2.973434
21	1	0	-3.302635	-2.979570	2.045445
22	1	0	-1.586976	-2.738066	1.616134
23	6	0	-4.110353	-0.375104	1.554915
24	1	0	-4.984712	-1.029067	1.468503
25	1	0	-3.984750	-0.111843	2.608993
26	1	0	-4.302842	0.541646	0.993684
27	6	0	-3.695088	-0.520372	-1.316742
28	1	0	-3.479914	-0.736159	-2.366730
29	1	0	-4.772794	-0.618718	-1.152354
30	1	0	-3.397080	0.510705	-1.114757
31	6	0	2.608522	-1.948774	0.344067
32	6	0	2.423862	-1.545454	-1.153235
33	5	0	0.829910	-0.477800	0.143159

34	8	0	1.354316	-1.585721	0.911607
35	8	0	1.639879	-0.358416	-1.060299
36	6	0	3.718523	-1.231881	-1.890376
37	1	0	4.383989	-2.101946	-1.901893
38	1	0	3.494727	-0.961710	-2.926446
39	1	0	4.242780	-0.394463	-1.424627
40	6	0	3.722561	-1.146748	1.025747
41	1	0	3.632345	-1.278765	2.107812
42	1	0	4.715975	-1.484759	0.713958
43	1	0	3.634707	-0.079775	0.801447
44	6	0	2.833406	-3.437457	0.573763
45	1	0	3.720355	-3.789827	0.035665
46	1	0	2.982409	-3.626868	1.640672
47	1	0	1.965793	-4.011232	0.243999
48	6	0	1.607912	-2.584657	-1.925983
49	1	0	1.336683	-2.160934	-2.897318
50	1	0	2.171218	-3.507907	-2.094549
51	1	0	0.683031	-2.813036	-1.388488
52	6	0	-1.422107	2.480015	-0.408452
53	6	0	-1.190943	3.771983	-0.870333
54	6	0	-0.093925	2.799450	-2.770122
55	6	0	-0.368918	1.545896	-2.229342
56	1	0	-1.929218	2.276409	0.533664
57	1	0	-1.528843	4.627791	-0.296339
58	1	0	0.438236	2.881635	-3.711275
59	7	0	-1.019929	1.398025	-1.075116
60	1	0	-0.034341	0.624419	-2.697364
61	6	0	1.464851	3.296387	2.417930
62	6	0	-0.512791	3.930530	-2.075786
63	1	0	1.573935	4.224641	2.969657
64	1	0	-0.312498	4.922752	-2.468706

IntF2

Thermal correction to Energy= 0.579896
Thermal correction to Enthalpy= 0.580840
Thermal correction to Gibbs Free Energy= 0.491088
Sum of electronic and zero-point Energies= -1318.061105
Sum of electronic and thermal Energies= -1318.031295
Sum of electronic and thermal Enthalpies= -1318.030351
Sum of electronic and thermal Free Energies= -1318.120103

Esol = -1319.0648664

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.887217	2.144557	-3.172690
2	6	0	-1.587497	3.442627	-1.277785
3	6	0	-0.848443	1.029551	-2.349749
4	1	0	-0.627222	2.048864	-4.220094
5	6	0	-1.535816	2.283241	-0.516131
6	1	0	-1.886514	4.377074	-0.817368
7	1	0	-0.554719	0.040482	-2.683774
8	1	0	-1.787209	2.238054	0.539711
9	7	0	-1.170695	1.112682	-1.052094
10	6	0	2.476680	-1.185918	-1.282854
11	6	0	2.659317	-1.689321	0.184293
12	5	0	0.868789	-0.227345	0.080186
13	8	0	1.680744	-0.014639	-1.114159
14	8	0	1.397330	-1.384114	0.767444
15	6	0	2.904745	-3.186307	0.313924
16	1	0	3.799802	-3.490416	-0.240194
17	1	0	3.049579	-3.444966	1.366907
18	1	0	2.046018	-3.747291	-0.059152
19	6	0	1.671507	-2.178676	-2.125714
20	1	0	1.421588	-1.699455	-3.077984
21	1	0	2.236533	-3.090914	-2.341819
22	1	0	0.738277	-2.434549	-1.613492
23	6	0	3.772343	-0.815042	-1.990927
24	1	0	4.445721	-1.677116	-2.050116
25	1	0	3.552909	-0.484127	-3.010224
26	1	0	4.285685	-0.002513	-1.472392
27	6	0	3.756159	-0.913977	0.922763
28	1	0	3.667455	-1.119624	1.993440
29	1	0	4.757008	-1.210126	0.592639
30	1	0	3.644803	0.163317	0.767485
31	6	0	-2.659311	-1.689329	-0.184293
32	6	0	-2.476676	-1.185926	1.282855
33	5	0	-0.868788	-0.227348	-0.080186
34	8	0	-1.397325	-1.384119	-0.767444
35	8	0	-1.680743	-0.014644	1.114158
36	6	0	-3.772339	-0.815053	1.990928
37	1	0	-4.445715	-1.677128	2.050117
38	1	0	-3.552906	-0.484137	3.010224
39	1	0	-4.285683	-0.002525	1.472393
40	6	0	-3.756155	-0.913988	-0.922763

41	1	0	-3.667452	-1.119636	-1.993440
42	1	0	-4.757003	-1.210140	-0.592638
43	1	0	-3.644803	0.163306	-0.767486
44	6	0	-2.904735	-3.186316	-0.313924
45	1	0	-3.799791	-3.490427	0.240196
46	1	0	-3.049568	-3.444976	-1.366906
47	1	0	-2.046006	-3.747297	0.059153
48	6	0	-1.671499	-2.178681	2.125715
49	1	0	-1.421582	-1.699459	3.077984
50	1	0	-2.236523	-3.090921	2.341819
51	1	0	-0.738268	-2.434551	1.613492
52	6	0	1.535808	2.283247	0.516131
53	6	0	1.587485	3.442632	1.277785
54	6	0	0.887207	2.144560	3.172690
55	6	0	0.848439	1.029554	2.349749
56	1	0	1.787203	2.238060	-0.539710
57	1	0	1.886498	4.377081	0.817368
58	1	0	0.627212	2.048866	4.220093
59	7	0	1.170692	1.112686	1.052094
60	1	0	0.554719	0.040484	2.683774
61	6	0	-1.258672	3.371128	-2.627903
62	6	0	1.258658	3.371132	2.627903
63	1	0	1.290676	4.260283	3.249247
64	1	0	-1.290694	4.260278	-3.249248

TSF3

Thermal correction to Energy=	0.578993
Thermal correction to Enthalpy=	0.579937
Thermal correction to Gibbs Free Energy=	0.494157
Sum of electronic and zero-point Energies=	-1318.042261
Sum of electronic and thermal Energies=	-1318.013335
Sum of electronic and thermal Enthalpies=	-1318.012391
Sum of electronic and thermal Free Energies=	-1318.098171

Esol = -1319.0445187

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.243134	2.083676	-3.217024
2	6	0	-0.666698	3.542559	-1.551108
3	6	0	-0.129289	1.007659	-2.468227

4	1	0	0.720551	1.912737	-4.174934
5	6	0	-0.994304	2.422918	-0.781329
6	1	0	-0.911518	4.522079	-1.153571
7	1	0	0.015528	-0.019767	-2.775297
8	1	0	-1.591320	2.475500	0.121693
9	7	0	-0.760672	1.157275	-1.250043
10	6	0	2.642050	-1.146976	-0.763585
11	6	0	2.389043	-1.819926	0.628978
12	5	0	1.018582	-0.026861	0.391614
13	8	0	1.981863	0.121502	-0.625326
14	8	0	1.107816	-1.294327	1.006481
15	6	0	2.299666	-3.336805	0.593768
16	1	0	3.227616	-3.774508	0.211006
17	1	0	2.133324	-3.717406	1.605291
18	1	0	1.467534	-3.657734	-0.035461
19	6	0	1.981918	-1.910108	-1.910785
20	1	0	2.049696	-1.297692	-2.815189
21	1	0	2.491871	-2.858810	-2.104446
22	1	0	0.927212	-2.100644	-1.692138
23	6	0	4.109448	-0.892799	-1.079589
24	1	0	4.671404	-1.832634	-1.092087
25	1	0	4.194375	-0.430999	-2.066845
26	1	0	4.560921	-0.219531	-0.349113
27	6	0	3.395308	-1.362737	1.686544
28	1	0	3.049762	-1.703026	2.666019
29	1	0	4.393610	-1.772397	1.506953
30	1	0	3.462421	-0.270303	1.707355
31	6	0	-2.388940	-1.820059	-0.628981
32	6	0	-2.641980	-1.147129	0.763586
33	5	0	-1.018576	-0.026922	-0.391614
34	8	0	-1.107738	-1.294393	-1.006479
35	8	0	-1.981863	0.121386	0.625329
36	6	0	-4.109391	-0.893033	1.079596
37	1	0	-4.671297	-1.832898	1.092089
38	1	0	-4.194340	-0.431245	2.066855
39	1	0	-4.560902	-0.219785	0.349126
40	6	0	-3.395228	-1.362912	-1.686544
41	1	0	-3.049667	-1.703179	-2.666021
42	1	0	-4.393510	-1.772621	-1.506953
43	1	0	-3.462393	-0.270481	-1.707348
44	6	0	-2.299487	-3.336933	-0.593781
45	1	0	-3.227421	-3.774685	-0.211034
46	1	0	-2.133115	-3.717519	-1.605305
47	1	0	-1.467348	-3.657827	0.035455

48	6	0	-1.981801	-1.910229	1.910779
49	1	0	-2.049607	-1.297820	2.815186
50	1	0	-2.491703	-2.858959	2.104441
51	1	0	-0.927086	-2.100707	1.692126
52	6	0	0.994164	2.422976	0.781332
53	6	0	0.666491	3.542597	1.551113
54	6	0	-0.243259	2.083658	3.217024
55	6	0	0.129228	1.007663	2.468226
56	1	0	1.591179	2.475595	-0.121688
57	1	0	0.911255	4.522131	1.153579
58	1	0	-0.720666	1.912689	4.174934
59	7	0	0.760605	1.157318	1.250043
60	1	0	-0.015528	-0.019772	2.775294
61	6	0	-0.025415	3.397059	-2.761530
62	6	0	0.025214	3.397057	2.761533
63	1	0	-0.255695	4.258277	3.355693
64	1	0	0.255442	4.258297	-3.355688

IntF3

Thermal correction to Energy= 0.583238
Thermal correction to Enthalpy= 0.584183
Thermal correction to Gibbs Free Energy= 0.497992
Sum of electronic and zero-point Energies= -1318.108111
Sum of electronic and thermal Energies= -1318.079247
Sum of electronic and thermal Enthalpies= -1318.078303
Sum of electronic and thermal Free Energies= -1318.164493

Esol = -1319.1190384

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204210	2.920602	-0.092224
2	6	0	-2.268959	0.859536	-0.805835
3	6	0	0.012130	2.377799	-0.287496
4	1	0	-1.293721	3.941858	0.254495
5	6	0	-0.964433	0.156171	-0.531717
6	1	0	-3.105745	0.282299	-1.183809
7	1	0	0.937286	2.930534	-0.164600
8	1	0	-0.823088	-0.704878	-1.192591
9	7	0	0.160646	1.070895	-0.741936
10	6	0	2.408251	1.463781	2.997105

11	6	0	3.265486	0.153014	3.062959
12	5	0	1.353601	-0.224908	1.923829
13	8	0	1.125211	0.973713	2.555499
14	8	0	2.657115	-0.666869	2.044069
15	6	0	4.735906	0.336702	2.728700
16	1	0	5.211158	1.014393	3.445110
17	1	0	5.245053	-0.629221	2.779244
18	1	0	4.862690	0.743412	1.723839
19	6	0	2.912062	2.446923	1.944895
20	1	0	2.170284	3.242312	1.835314
21	1	0	3.860941	2.899607	2.247597
22	1	0	3.041324	1.960955	0.972355
23	6	0	2.223999	2.166979	4.332741
24	1	0	3.191376	2.478005	4.740243
25	1	0	1.609704	3.059385	4.189889
26	1	0	1.725128	1.521673	5.057118
27	6	0	3.105801	-0.592151	4.386611
28	1	0	3.558320	-1.581816	4.288963
29	1	0	3.595242	-0.061961	5.208086
30	1	0	2.047970	-0.722238	4.633373
31	6	0	3.437716	0.749429	-2.233935
32	6	0	2.927638	-0.732235	-2.263393
33	5	0	1.383792	0.615199	-1.306712
34	8	0	2.541882	1.367448	-1.288122
35	8	0	1.524514	-0.584137	-1.962981
36	6	0	3.066729	-1.420574	-3.611927
37	1	0	4.118968	-1.469872	-3.910469
38	1	0	2.682685	-2.440936	-3.539557
39	1	0	2.503652	-0.897831	-4.386358
40	6	0	3.242345	1.469509	-3.566631
41	1	0	3.424208	2.536605	-3.419025
42	1	0	3.932854	1.098011	-4.328585
43	1	0	2.218153	1.343802	-3.929937
44	6	0	4.864360	0.921046	-1.740488
45	1	0	5.564213	0.399719	-2.401502
46	1	0	5.124142	1.982808	-1.733922
47	1	0	4.981009	0.529821	-0.728014
48	6	0	3.543061	-1.590205	-1.162063
49	1	0	3.013115	-2.545994	-1.133694
50	1	0	4.601247	-1.787898	-1.356741
51	1	0	3.443487	-1.112087	-0.181961
52	6	0	-0.956091	-0.376842	0.936920
53	6	0	-2.053555	-1.395584	1.112065
54	6	0	-0.437785	-3.107976	0.523977

55	6	0	0.576913	-2.271629	0.811902
56	1	0	-1.097146	0.485621	1.596041
57	1	0	-3.039045	-1.056279	1.411763
58	1	0	-0.231461	-4.116819	0.190764
59	7	0	0.346052	-0.971697	1.252304
60	1	0	1.619459	-2.568945	0.778563
61	6	0	-2.378218	2.161150	-0.503941
62	6	0	-1.798369	-2.679338	0.823246
63	1	0	-3.322163	2.683070	-0.631815
64	1	0	-2.582720	-3.428507	0.882138

TSF4

Thermal correction to Energy= 0.578342
Thermal correction to Enthalpy= 0.579286
Thermal correction to Gibbs Free Energy= 0.489733
Sum of electronic and zero-point Energies= -1318.054556
Sum of electronic and thermal Energies= -1318.024990
Sum of electronic and thermal Enthalpies= -1318.024045
Sum of electronic and thermal Free Energies= -1318.113599

Esol = -1319.0627074

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.068578	3.095505	-0.127042
2	6	0	-2.262175	1.116032	-0.787804
3	6	0	0.106867	2.464744	-0.348731
4	1	0	-1.044931	4.127420	0.205245
5	6	0	-1.053940	0.437495	-0.915136
6	1	0	-3.171293	0.551507	-0.972043
7	1	0	1.069370	2.946813	-0.246679
8	1	0	-0.971582	-0.555801	-1.337120
9	7	0	0.160423	1.135407	-0.796804
10	6	0	2.303360	1.559236	2.965462
11	6	0	3.283356	0.336784	2.874189
12	5	0	1.343145	-0.157523	1.843638
13	8	0	1.047922	0.990930	2.535692
14	8	0	2.689386	-0.468809	1.833707
15	6	0	4.703063	0.693178	2.468752
16	1	0	5.161563	1.351674	3.213427
17	1	0	5.303249	-0.218657	2.402403

18	1	0	4.720062	1.191350	1.498086
19	6	0	2.665902	2.681278	1.998086
20	1	0	1.832350	3.387702	1.965883
21	1	0	3.561551	3.213896	2.331922
22	1	0	2.837551	2.292279	0.990038
23	6	0	2.118888	2.115633	4.369313
24	1	0	3.072633	2.473406	4.770267
25	1	0	1.424181	2.958464	4.335744
26	1	0	1.709818	1.363288	5.045196
27	6	0	3.285797	-0.517537	4.140868
28	1	0	3.831866	-1.442228	3.939663
29	1	0	3.767258	-0.001011	4.975525
30	1	0	2.265108	-0.781246	4.434017
31	6	0	3.487366	0.573277	-2.051323
32	6	0	2.862421	-0.856515	-2.219656
33	5	0	1.397292	0.546604	-1.213463
34	8	0	2.613383	1.189199	-1.081194
35	8	0	1.469307	-0.630532	-1.916444
36	6	0	2.957660	-1.424125	-3.627900
37	1	0	4.004232	-1.523412	-3.933224
38	1	0	2.499393	-2.415905	-3.649682
39	1	0	2.436489	-0.791807	-4.348135
40	6	0	3.392398	1.415745	-3.322356
41	1	0	3.664797	2.446121	-3.081825
42	1	0	4.065399	1.048380	-4.101697
43	1	0	2.370474	1.415689	-3.713443
44	6	0	4.906325	0.583500	-1.509628
45	1	0	5.584861	0.071920	-2.199741
46	1	0	5.246699	1.616829	-1.398052
47	1	0	4.957455	0.094074	-0.535709
48	6	0	3.405212	-1.861840	-1.209240
49	1	0	2.778788	-2.756852	-1.247014
50	1	0	4.433879	-2.145796	-1.451162
51	1	0	3.377263	-1.454518	-0.194231
52	6	0	-1.016536	-0.670801	1.316422
53	6	0	-1.995562	-1.632308	1.085194
54	6	0	-0.282230	-3.235992	0.563410
55	6	0	0.668554	-2.330132	0.886062
56	1	0	-1.228840	0.305760	1.732055
57	1	0	-3.031310	-1.319300	1.176744
58	1	0	0.033541	-4.224146	0.247711
59	7	0	0.340794	-1.036069	1.320554
60	1	0	1.727069	-2.550878	0.880511
61	6	0	-2.313828	2.430700	-0.365951

62	6	0	-1.672140	-2.911945	0.676650
63	1	0	-3.255603	2.944382	-0.222532
64	1	0	-2.435005	-3.646155	0.452261

IntF4

Thermal correction to Energy=	0.287664
Thermal correction to Enthalpy=	0.288608
Thermal correction to Gibbs Free Energy=	0.231466
Sum of electronic and zero-point Energies=	-659.023644
Sum of electronic and thermal Energies=	-659.008995
Sum of electronic and thermal Enthalpies=	-659.008051
Sum of electronic and thermal Free Energies=	-659.065194

Esol = -659.529766

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.297045	1.188996	-0.185256
2	6	0	3.657955	1.192042	-0.186190
3	6	0	3.657954	-1.192045	0.186184
4	6	0	2.297044	-1.188998	0.185251
5	7	0	1.571394	-0.000001	-0.000002
6	1	0	1.692093	2.075593	-0.323328
7	1	0	4.165231	2.139438	-0.334370
8	1	0	4.165230	-2.139442	0.334363
9	1	0	1.692092	-2.075595	0.323324
10	5	0	0.142364	0.000000	0.000000
11	8	0	-0.607617	-1.129466	0.231025
12	8	0	-0.607617	1.129467	-0.231022
13	6	0	-1.966338	-0.775649	-0.105873
14	6	0	-1.966337	0.775651	0.105881
15	6	0	-2.914735	-1.541287	0.800885
16	1	0	-3.947574	-1.220834	0.630399
17	1	0	-2.847036	-2.609882	0.582472
18	1	0	-2.666566	-1.390208	1.852369
19	6	0	-2.183995	-1.167917	-1.565393
20	1	0	-1.956080	-2.230009	-1.681136
21	1	0	-3.218019	-0.995880	-1.876525
22	1	0	-1.520369	-0.599708	-2.223785
23	6	0	-2.914736	1.541291	-0.800873
24	1	0	-3.947575	1.220843	-0.630381

25	1	0	-2.847031	2.609886	-0.582463
26	1	0	-2.666573	1.390210	-1.852359
27	6	0	-2.183988	1.167920	1.565403
28	1	0	-1.956071	2.230012	1.681144
29	1	0	-3.218011	0.995884	1.876538
30	1	0	-1.520359	0.599710	2.223792
31	6	0	4.395838	-0.000002	-0.000003
32	1	0	5.477238	-0.000002	-0.000003

1,1-Diphenylethylene

Thermal correction to Energy= 0.227641
Thermal correction to Enthalpy= 0.228586
Thermal correction to Gibbs Free Energy= 0.178866
Sum of electronic and zero-point Energies= -540.260003
Sum of electronic and thermal Energies= -540.249035
Sum of electronic and thermal Enthalpies= -540.248090
Sum of electronic and thermal Free Energies= -540.297810

Esol=-540.6552872

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.554406	-1.139197	0.168162
2	6	0	-2.185340	-1.197498	0.403551
3	6	0	-1.336638	-0.185882	-0.062927
4	6	0	-1.892677	0.870940	-0.792145
5	6	0	-3.261853	0.928267	-1.030019
6	6	0	-4.097659	-0.075393	-0.548023
7	1	0	-4.199668	-1.926282	0.545316
8	1	0	-1.763666	-2.028193	0.961938
9	1	0	-1.237335	1.639819	-1.190098
10	1	0	-3.675408	1.753057	-1.601914
11	1	0	-5.165592	-0.033341	-0.736580
12	6	0	0.121691	-0.223074	0.233844
13	6	0	0.794928	0.898856	0.520254
14	1	0	1.866689	0.884517	0.687911
15	1	0	0.290046	1.856197	0.595505
16	6	0	0.812922	-1.541578	0.211634
17	6	0	1.799269	-1.844172	1.156731
18	6	0	0.505292	-2.496584	-0.765182
19	6	0	2.475292	-3.059034	1.116173

20	1	0	2.016793	-1.124424	1.940194
21	6	0	1.183431	-3.709768	-0.808233
22	1	0	-0.265489	-2.277430	-1.498383
23	6	0	2.171581	-3.994739	0.131350
24	1	0	3.233170	-3.278536	1.861653
25	1	0	0.940808	-4.434791	-1.578848
26	1	0	2.696135	-4.944361	0.100127

G

Thermal correction to Energy= 0.123490
Thermal correction to Enthalpy= 0.124434
Thermal correction to Gibbs Free Energy= 0.087078
Sum of electronic and zero-point Energies= -287.360713
Sum of electronic and thermal Energies= -287.354669
Sum of electronic and thermal Enthalpies= -287.353724
Sum of electronic and thermal Free Energies= -287.391080

Esol =-287.5766511

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.162473	1.135018	0.005887
2	6	0	0.227920	1.188783	-0.009559
3	6	0	0.957957	0.000477	-0.015123
4	6	0	0.228207	-1.188285	-0.009646
5	6	0	-1.161975	-1.135035	0.005797
6	7	0	-1.863655	-0.000030	0.013767
7	1	0	-1.743005	2.054995	0.008633
8	1	0	0.735334	2.148867	-0.019695
9	1	0	0.736049	-2.148166	-0.019883
10	1	0	-1.742308	-2.055123	0.008481
11	6	0	2.462991	0.000052	-0.001162
12	1	0	2.863410	0.894819	-0.483071
13	1	0	2.834956	-0.017667	1.028332
14	1	0	2.862817	-0.878425	-0.512785

TSG1

Thermal correction to Energy= 0.512074
Thermal correction to Enthalpy= 0.513018
Thermal correction to Gibbs Free Energy= 0.430195

Sum of electronic and zero-point Energies= -1109.225108
Sum of electronic and thermal Energies= -1109.198854
Sum of electronic and thermal Enthalpies= -1109.197910
Sum of electronic and thermal Free Energies= -1109.280733

Esol =-1110.0977339

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.133993	2.852447	-1.203564
2	6	0	0.767036	3.051315	1.150007
3	6	0	0.343989	1.710808	-1.186518
4	1	0	1.576870	3.193426	-2.134155
5	6	0	-0.010721	1.901323	1.080719
6	1	0	0.917780	3.549032	2.102710
7	1	0	0.154720	1.117029	-2.077556
8	1	0	-0.486837	1.457207	1.952187
9	7	0	-0.217989	1.255532	-0.065672
10	6	0	2.590073	-1.823013	-0.714028
11	6	0	2.652500	-1.372081	0.778882
12	5	0	0.512159	-1.229558	0.019337
13	8	0	1.286543	-1.363659	-1.117191
14	8	0	1.265752	-1.392679	1.164601
15	6	0	3.439783	-2.294770	1.695776
16	1	0	4.483285	-2.363265	1.371033
17	1	0	3.422447	-1.898797	2.714280
18	1	0	3.008798	-3.296786	1.712936
19	6	0	2.600149	-3.342239	-0.875441
20	1	0	2.338274	-3.586062	-1.907679
21	1	0	3.583914	-3.765414	-0.652631
22	1	0	1.859946	-3.804909	-0.216735
23	6	0	3.635002	-1.186933	-1.618192
24	1	0	4.645676	-1.435890	-1.278440
25	1	0	3.513273	-1.562939	-2.637161
26	1	0	3.526287	-0.100796	-1.639890
27	6	0	3.131867	0.071244	0.939851
28	1	0	2.937732	0.390755	1.966962
29	1	0	4.202762	0.166706	0.737627
30	1	0	2.586720	0.740565	0.265933
31	6	0	-3.204121	-0.270260	-0.769025
32	6	0	-3.253033	-0.632507	0.752082
33	5	0	-1.091104	-0.666883	0.000059
34	8	0	-1.889136	-0.701682	-1.145959

35	8	0	-1.880231	-0.528856	1.152708
36	6	0	-4.094501	0.307447	1.603557
37	1	0	-5.137831	0.305950	1.270796
38	1	0	-4.067019	-0.022444	2.645433
39	1	0	-3.712429	1.329097	1.558959
40	6	0	-3.315296	1.234578	-1.025130
41	1	0	-3.038354	1.430615	-2.064764
42	1	0	-4.337243	1.590955	-0.863872
43	1	0	-2.641067	1.799735	-0.378739
44	6	0	-4.220559	-1.007822	-1.630308
45	1	0	-5.241814	-0.786729	-1.302398
46	1	0	-4.117581	-0.686687	-2.670243
47	1	0	-4.061367	-2.086288	-1.590808
48	6	0	-3.678553	-2.081585	0.995240
49	1	0	-3.490850	-2.327727	2.043110
50	1	0	-4.739960	-2.237950	0.781217
51	1	0	-3.088970	-2.761697	0.374143
52	6	0	1.357226	3.550402	-0.012544
53	6	0	2.187544	4.804725	0.008117
54	1	0	2.996022	4.754514	-0.724486
55	1	0	1.568417	5.672574	-0.240476
56	1	0	2.621335	4.976229	0.995252

IntG1

Thermal correction to Energy= 0.513299
Thermal correction to Enthalpy= 0.514243
Thermal correction to Gibbs Free Energy= 0.429350
Sum of electronic and zero-point Energies= -1109.228145
Sum of electronic and thermal Energies= -1109.201510
Sum of electronic and thermal Enthalpies= -1109.200565
Sum of electronic and thermal Free Energies= -1109.285459

Esol = -1110.1021694

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.521525	-1.179351	-1.300385
2	6	0	3.008776	-1.566198	0.131402
3	5	0	0.956412	-0.504170	0.257243
4	8	0	1.527826	-0.192893	-1.034887
5	8	0	1.804318	-1.490994	0.889836

6	6	0	3.569559	-2.977255	0.249725
7	1	0	4.422689	-3.118497	-0.422748
8	1	0	3.908561	-3.154368	1.274426
9	1	0	2.803642	-3.717028	0.011953
10	6	0	1.838258	-2.352322	-2.008255
11	1	0	1.334011	-1.970998	-2.899789
12	1	0	2.553916	-3.123104	-2.311029
13	1	0	1.080002	-2.797767	-1.357936
14	6	0	3.595999	-0.576828	-2.195095
15	1	0	4.421680	-1.281099	-2.343184
16	1	0	3.168093	-0.341767	-3.173494
17	1	0	3.993780	0.345677	-1.766611
18	6	0	4.021476	-0.559855	0.689876
19	1	0	4.118203	-0.724736	1.766802
20	1	0	5.007168	-0.678767	0.229019
21	1	0	3.688010	0.469038	0.527565
22	6	0	-2.762617	-1.798086	-0.102506
23	6	0	-2.736457	-1.305518	1.377393
24	5	0	-0.711962	-0.919642	0.386668
25	8	0	-1.365739	-1.805401	-0.446131
26	8	0	-1.554214	-0.482693	1.401331
27	6	0	-3.936455	-0.470791	1.796621
28	1	0	-4.860970	-1.049642	1.700610
29	1	0	-3.827646	-0.172153	2.842558
30	1	0	-4.021975	0.432510	1.190725
31	6	0	-3.448790	-0.807371	-1.042759
32	1	0	-3.238989	-1.102412	-2.073411
33	1	0	-4.532520	-0.792647	-0.894247
34	1	0	-3.057610	0.202601	-0.890832
35	6	0	-3.331764	-3.194272	-0.302277
36	1	0	-4.371669	-3.240393	0.037920
37	1	0	-3.306820	-3.448876	-1.364751
38	1	0	-2.748657	-3.940152	0.239812
39	6	0	-2.506399	-2.442623	2.372736
40	1	0	-2.291810	-2.012014	3.354121
41	1	0	-3.385255	-3.087862	2.459579
42	1	0	-1.649139	-3.050626	2.070184
43	6	0	1.372910	2.098240	0.551092
44	6	0	1.467995	3.274971	1.277712
45	6	0	1.054767	2.009614	3.261170
46	6	0	0.965061	0.874364	2.474750
47	1	0	1.503246	2.038217	-0.524573
48	1	0	1.667597	4.208593	0.762660
49	1	0	0.921626	1.930531	4.334793

50	7	0	1.125338	0.929148	1.148473
51	1	0	0.762865	-0.113233	2.874847
52	6	0	1.311715	3.246898	2.664553
53	6	0	1.440662	4.495626	3.491884
54	1	0	0.765549	4.470891	4.349883
55	1	0	2.461655	4.589215	3.875324
56	1	0	1.222471	5.386878	2.900608

TSG2

Thermal correction to Energy=	0.638162
Thermal correction to Enthalpy=	0.639107
Thermal correction to Gibbs Free Energy=	0.540485
Sum of electronic and zero-point Energies=	-1396.602639
Sum of electronic and thermal Energies=	-1396.569318
Sum of electronic and thermal Enthalpies=	-1396.568374
Sum of electronic and thermal Free Energies=	-1396.666996

Esol = -1397.6860312

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.217361	0.448212	2.704546
2	6	0	-3.222207	1.320186	0.721715
3	6	0	-0.981913	0.560341	2.085411
4	1	0	-2.275572	0.062716	3.716796
5	6	0	-1.956691	1.416693	0.166862
6	1	0	-4.086371	1.630832	0.142795
7	1	0	-0.051937	0.250346	2.549980
8	1	0	-1.760251	1.795129	-0.831299
9	7	0	-0.866702	1.031022	0.839412
10	6	0	2.027901	-2.482435	1.167004
11	6	0	2.439825	-2.521768	-0.338064
12	5	0	1.046808	-0.738840	0.040597
13	8	0	0.896742	-1.601038	1.157211
14	8	0	2.069358	-1.213573	-0.786445
15	6	0	3.930373	-2.714445	-0.582152
16	1	0	4.279762	-3.657194	-0.147336
17	1	0	4.122533	-2.741426	-1.658097
18	1	0	4.505599	-1.891480	-0.154920
19	6	0	3.093990	-1.821467	2.043442
20	1	0	2.673586	-1.655554	3.039071
21	1	0	3.989110	-2.442704	2.142164

22	1	0	3.372142	-0.848508	1.627188
23	6	0	1.616781	-3.825386	1.751713
24	1	0	2.444485	-4.540878	1.703107
25	1	0	1.337570	-3.698387	2.801403
26	1	0	0.761233	-4.243371	1.217201
27	6	0	1.645203	-3.552990	-1.141201
28	1	0	1.804953	-3.360219	-2.205408
29	1	0	1.971302	-4.573518	-0.917144
30	1	0	0.575469	-3.468667	-0.938316
31	6	0	1.760270	2.964092	0.294974
32	6	0	1.504453	2.657153	-1.214553
33	5	0	0.656451	0.937838	0.083836
34	8	0	1.591478	1.685993	0.896579
35	8	0	0.475705	1.672194	-1.160950
36	6	0	1.014988	3.846848	-2.029292
37	1	0	1.747758	4.660773	-2.012467
38	1	0	0.867350	3.543470	-3.069718
39	1	0	0.064122	4.223303	-1.645369
40	6	0	0.722898	3.935004	0.871013
41	1	0	0.784710	3.900998	1.962318
42	1	0	0.901292	4.964000	0.542549
43	1	0	-0.290886	3.649710	0.575819
44	6	0	3.163344	3.467792	0.608092
45	1	0	3.385847	4.386561	0.054306
46	1	0	3.246498	3.683568	1.677145
47	1	0	3.907615	2.710915	0.355165
48	6	0	2.726578	2.022005	-1.883029
49	1	0	2.427119	1.644481	-2.864751
50	1	0	3.540706	2.740977	-2.018734
51	1	0	3.081582	1.172581	-1.292680
52	6	0	-1.759548	-1.885465	-0.257620
53	6	0	-3.089206	-1.892466	-0.655336
54	6	0	-2.420521	-0.732712	-2.631001
55	6	0	-1.112373	-0.762899	-2.152685
56	1	0	-1.429963	-2.312642	0.688014
57	1	0	-3.845735	-2.346641	-0.021470
58	1	0	-2.638461	-0.257425	-3.582365
59	7	0	-0.791848	-1.331169	-0.991495
60	1	0	-0.292461	-0.286167	-2.682912
61	6	0	-3.373918	0.820215	2.017094
62	6	0	-3.442320	-1.302914	-1.873334
63	6	0	-4.875827	-1.281724	-2.331380
64	1	0	-5.513168	-0.798200	-1.584712
65	1	0	-4.985022	-0.744321	-3.275136

66	1	0	-5.252586	-2.298986	-2.471793
67	6	0	-4.738141	0.661712	2.629451
68	1	0	-4.678179	0.550882	3.713565
69	1	0	-5.373655	1.520526	2.400919
70	1	0	-5.230273	-0.229540	2.226373

IntG2

Thermal correction to Energy= 0.639307
Thermal correction to Enthalpy= 0.640251
Thermal correction to Gibbs Free Energy= 0.542079
Sum of electronic and zero-point Energies= -1396.606383
Sum of electronic and thermal Energies= -1396.572976
Sum of electronic and thermal Enthalpies= -1396.572031
Sum of electronic and thermal Free Energies= -1396.670203

Esol =-1397.690204

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.880638	2.141912	-3.161895
2	6	0	-1.573777	3.433260	-1.275695
3	6	0	-0.845083	1.026103	-2.345711
4	1	0	-0.619941	2.046437	-4.210859
5	6	0	-1.527076	2.273881	-0.513955
6	1	0	-1.869642	4.368293	-0.811658
7	1	0	-0.554833	0.038465	-2.686165
8	1	0	-1.780699	2.233180	0.541532
9	7	0	-1.167487	1.101894	-1.046210
10	6	0	2.475557	-1.186190	-1.293636
11	6	0	2.670592	-1.686867	0.172426
12	5	0	0.867845	-0.239388	0.078532
13	8	0	1.673869	-0.020701	-1.120980
14	8	0	1.409094	-1.393891	0.762022
15	6	0	2.931907	-3.181486	0.302087
16	1	0	3.825390	-3.477154	-0.258830
17	1	0	3.087856	-3.437392	1.354082
18	1	0	2.076138	-3.751842	-0.063036
19	6	0	1.672718	-2.185767	-2.131787
20	1	0	1.418955	-1.711535	-3.085416
21	1	0	2.241146	-3.096455	-2.345583
22	1	0	0.741340	-2.444233	-1.617670

23	6	0	3.764260	-0.807000	-2.010748
24	1	0	4.440896	-1.665541	-2.081193
25	1	0	3.533913	-0.471446	-3.026071
26	1	0	4.278985	0.005030	-1.492913
27	6	0	3.764612	-0.900878	0.904698
28	1	0	3.676988	-1.100157	1.976622
29	1	0	4.766937	-1.194302	0.576409
30	1	0	3.648451	0.174779	0.742978
31	6	0	-2.670582	-1.686861	-0.172506
32	6	0	-2.475596	-1.186250	1.293585
33	5	0	-0.867849	-0.239375	-0.078496
34	8	0	-1.409071	-1.393855	-0.762055
35	8	0	-1.673904	-0.020751	1.121006
36	6	0	-3.764325	-0.807083	2.010662
37	1	0	-4.440969	-1.665624	2.081043
38	1	0	-3.534016	-0.471574	3.026009
39	1	0	-4.279025	0.004972	1.492841
40	6	0	-3.764574	-0.900829	-0.904772
41	1	0	-3.676922	-1.100061	-1.976703
42	1	0	-4.766911	-1.194257	-0.576523
43	1	0	-3.648401	0.174819	-0.743000
44	6	0	-2.931896	-3.181473	-0.302241
45	1	0	-3.825396	-3.477166	0.258637
46	1	0	-3.087814	-3.437332	-1.354252
47	1	0	-2.076138	-3.751847	0.062882
48	6	0	-1.672808	-2.185883	2.131721
49	1	0	-1.419068	-1.711696	3.085379
50	1	0	-2.241267	-3.096565	2.345463
51	1	0	-0.741420	-2.444357	1.617627
52	6	0	1.527483	2.273753	0.514163
53	6	0	1.574214	3.433126	1.275913
54	6	0	0.880276	2.141926	3.161921
55	6	0	0.844711	1.026125	2.345728
56	1	0	1.781403	2.232995	-0.541251
57	1	0	1.870408	4.368095	0.811957
58	1	0	0.619272	2.046510	4.210814
59	7	0	1.167498	1.101846	1.046318
60	1	0	0.554170	0.038544	2.686103
61	6	0	-1.247607	3.383302	-2.630611
62	6	0	1.247653	3.383238	2.630736
63	6	0	1.287755	4.609687	3.500356
64	1	0	0.311407	4.790929	3.958546
65	1	0	2.010503	4.481851	4.311299
66	1	0	1.569172	5.495290	2.927966

67	6	0	-1.287707	4.609755	-3.500224
68	1	0	-0.311496	4.790715	-3.958815
69	1	0	-2.010822	4.482113	-4.310872
70	1	0	-1.568645	5.495441	-2.927727

TSG3

Thermal correction to Energy= 0.638401
Thermal correction to Enthalpy= 0.639345
Thermal correction to Gibbs Free Energy= 0.546715
Sum of electronic and zero-point Energies= -1396.585376
Sum of electronic and thermal Energies= -1396.553207
Sum of electronic and thermal Enthalpies= -1396.552263
Sum of electronic and thermal Free Energies= -1396.644893

Esol =-1397.6669464

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.752664	0.871802	-3.106584
2	6	0	-3.219623	-0.326835	-1.661363
3	6	0	-0.682566	0.361280	-2.440345
4	1	0	-1.575893	1.527902	-3.953096
5	6	0	-2.104839	-0.801143	-0.957562
6	1	0	-4.203448	-0.638148	-1.321675
7	1	0	0.346286	0.567167	-2.705717
8	1	0	-2.170497	-1.573349	-0.199827
9	7	0	-0.836080	-0.497859	-1.371133
10	6	0	1.460832	2.741525	-0.239390
11	6	0	2.134666	2.229619	1.078924
12	5	0	0.347240	0.920123	0.579985
13	8	0	0.193461	2.066008	-0.228338
14	8	0	1.614969	0.898544	1.204306
15	6	0	3.651930	2.154395	1.026746
16	1	0	4.085452	3.140011	0.827087
17	1	0	4.034177	1.800050	1.988020
18	1	0	3.975322	1.458505	0.250399
19	6	0	2.224783	2.311962	-1.491102
20	1	0	1.616292	2.556913	-2.367151
21	1	0	3.176758	2.844345	-1.579788
22	1	0	2.410134	1.233894	-1.479706
23	6	0	1.206267	4.242021	-0.271484

24	1	0	2.147215	4.795699	-0.184360
25	1	0	0.738104	4.510690	-1.222219
26	1	0	0.539103	4.548519	0.535660
27	6	0	1.676271	3.015849	2.308629
28	1	0	2.011597	2.487659	3.204921
29	1	0	2.089512	4.028734	2.324196
30	1	0	0.584091	3.082387	2.338507
31	6	0	2.134413	-2.229781	-1.079027
32	6	0	1.460562	-2.741629	0.239304
33	5	0	0.347110	-0.920122	-0.580034
34	8	0	1.614804	-0.898672	-1.204424
35	8	0	0.193252	-2.066003	0.228278
36	6	0	1.205876	-4.242104	0.271384
37	1	0	2.146775	-4.795845	0.184124
38	1	0	0.737804	-4.510773	1.222163
39	1	0	0.538600	-4.548519	-0.535699
40	6	0	1.675957	-3.016008	-2.308708
41	1	0	2.011337	-2.487886	-3.205019
42	1	0	2.089106	-4.028931	-2.324230
43	1	0	0.583771	-3.082450	-2.338593
44	6	0	3.651682	-2.154655	-1.026868
45	1	0	4.085142	-3.140310	-0.827260
46	1	0	4.033933	-1.800292	-1.988134
47	1	0	3.975130	-1.458822	-0.250495
48	6	0	2.224571	-2.312149	1.491007
49	1	0	1.616074	-2.557066	2.367062
50	1	0	3.176506	-2.844609	1.579667
51	1	0	2.410010	-1.234097	1.479624
52	6	0	-2.104703	0.801391	0.957715
53	6	0	-3.219481	0.327089	1.661544
54	6	0	-1.752485	-0.871653	3.106670
55	6	0	-0.682398	-0.361160	2.440384
56	1	0	-2.170356	1.573658	0.200039
57	1	0	-4.203314	0.638452	1.321929
58	1	0	-1.575715	-1.527784	3.953160
59	7	0	-0.835937	0.498010	1.371201
60	1	0	0.346463	-0.567108	2.705681
61	6	0	-3.082384	0.532618	-2.728741
62	6	0	-3.082212	-0.532400	2.728893
63	6	0	-4.256356	-1.091948	3.480216
64	1	0	-4.299456	-2.182986	3.392754
65	1	0	-4.189769	-0.856784	4.547685
66	1	0	-5.197143	-0.686030	3.101821
67	6	0	-4.256640	1.092090	-3.480026

68	1	0	-4.300022	2.183098	-3.392421
69	1	0	-4.190024	0.857101	-4.547526
70	1	0	-5.197327	0.685877	-3.101694

IntG3

Thermal correction to Energy= 0.642284
Thermal correction to Enthalpy= 0.643228
Thermal correction to Gibbs Free Energy= 0.549517
Sum of electronic and zero-point Energies= -1396.653347
Sum of electronic and thermal Energies= -1396.621031
Sum of electronic and thermal Enthalpies= -1396.620087
Sum of electronic and thermal Free Energies= -1396.713798

Esol = -1397.7433476

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.197350	2.918542	-0.085683
2	6	0	-2.261105	0.868169	-0.794990
3	6	0	0.019120	2.379633	-0.282859
4	1	0	-1.288689	3.941691	0.259986
5	6	0	-0.957502	0.162226	-0.527270
6	1	0	-3.100570	0.288741	-1.167136
7	1	0	0.942543	2.934918	-0.157331
8	1	0	-0.821117	-0.695105	-1.194092
9	7	0	0.171094	1.073271	-0.735055
10	6	0	2.419552	1.462890	2.996608
11	6	0	3.276722	0.152043	3.061392
12	5	0	1.364825	-0.224905	1.921168
13	8	0	1.136898	0.973555	2.554057
14	8	0	2.668887	-0.666698	2.041662
15	6	0	4.747323	0.336091	2.727956
16	1	0	5.222389	1.013028	3.445218
17	1	0	5.256447	-0.629906	2.777597
18	1	0	4.874399	0.743852	1.723555
19	6	0	2.924216	2.447397	1.946038
20	1	0	2.182718	3.243194	1.837339
21	1	0	3.873087	2.899414	2.249827
22	1	0	3.053624	1.962842	0.972842
23	6	0	2.234873	2.164655	4.333017
24	1	0	3.202087	2.475178	4.741335
25	1	0	1.620723	3.057280	4.190842

26	1	0	1.735549	1.518640	5.056453
27	6	0	3.116635	-0.594313	4.384381
28	1	0	3.569195	-1.583892	4.285935
29	1	0	3.605744	-0.064932	5.206593
30	1	0	2.058681	-0.724621	4.630515
31	6	0	3.446151	0.753238	-2.230542
32	6	0	2.936310	-0.728495	-2.260529
33	5	0	1.393403	0.617853	-1.299965
34	8	0	2.551978	1.370236	-1.282882
35	8	0	1.533979	-0.581099	-1.957696
36	6	0	3.073268	-1.415450	-3.610056
37	1	0	4.124975	-1.464332	-3.910579
38	1	0	2.689467	-2.435938	-3.537991
39	1	0	2.508673	-0.892069	-4.382961
40	6	0	3.248510	1.474332	-3.562405
41	1	0	3.430471	2.541339	-3.414207
42	1	0	3.937736	1.103576	-4.325904
43	1	0	2.223676	1.348730	-3.923948
44	6	0	4.873673	0.924624	-1.739465
45	1	0	5.572507	0.403942	-2.402084
46	1	0	5.133343	1.986422	-1.732375
47	1	0	4.992030	0.532532	-0.727525
48	6	0	3.554102	-1.587587	-1.161359
49	1	0	3.024597	-2.543652	-1.133434
50	1	0	4.612061	-1.784606	-1.358031
51	1	0	3.455754	-1.110913	-0.180449
52	6	0	-0.947431	-0.382123	0.937512
53	6	0	-2.042127	-1.403978	1.105561
54	6	0	-0.429233	-3.104388	0.519558
55	6	0	0.585769	-2.271593	0.811244
56	1	0	-1.093386	0.475417	1.602076
57	1	0	-3.030673	-1.064044	1.398874
58	1	0	-0.223343	-4.115039	0.186289
59	7	0	0.357652	-0.971855	1.250802
60	1	0	1.627676	-2.571328	0.775879
61	6	0	-2.386904	2.171031	-0.496857
62	6	0	-1.802085	-2.692630	0.817044
63	6	0	-2.861643	-3.757428	0.869973
64	1	0	-2.949342	-4.260240	-0.099422
65	1	0	-2.607983	-4.525841	1.607975
66	1	0	-3.836239	-3.337531	1.128076
67	6	0	-3.677578	2.926501	-0.648514
68	1	0	-3.968300	3.385525	0.302794
69	1	0	-3.572646	3.737250	-1.377156

70	1	0	-4.487529	2.270573	-0.974715

TSG4

Thermal correction to Energy= 0.637062
Thermal correction to Enthalpy= 0.638006
Thermal correction to Gibbs Free Energy= 0.540465
Sum of electronic and zero-point Energies= -1396.597276
Sum of electronic and thermal Energies= -1396.564020
Sum of electronic and thermal Enthalpies= -1396.563076
Sum of electronic and thermal Free Energies= -1396.660617

Esol = -1397.6830655

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.054416	3.109596	-0.126863
2	6	0	-2.262126	1.151359	-0.787741
3	6	0	0.114857	2.474162	-0.357753
4	1	0	-1.023256	4.140787	0.212359
5	6	0	-1.061230	0.463822	-0.929949
6	1	0	-3.178440	0.595762	-0.971152
7	1	0	1.079773	2.951585	-0.255489
8	1	0	-0.992852	-0.530122	-1.351862
9	7	0	0.161294	1.148374	-0.811711
10	6	0	2.296576	1.557276	2.966282
11	6	0	3.271800	0.329923	2.897747
12	5	0	1.337555	-0.167232	1.856467
13	8	0	1.041628	0.988004	2.537944
14	8	0	2.683563	-0.483299	1.859350
15	6	0	4.697266	0.674566	2.502182
16	1	0	5.153101	1.334968	3.246790
17	1	0	5.291666	-0.241672	2.447485
18	1	0	4.726081	1.166836	1.528807
19	6	0	2.671018	2.661492	1.983759
20	1	0	1.844920	3.376047	1.937739
21	1	0	3.571465	3.190109	2.310849
22	1	0	2.841221	2.254091	0.982763
23	6	0	2.107574	2.136052	4.360182
24	1	0	3.060279	2.500438	4.757716
25	1	0	1.413287	2.978371	4.309482
26	1	0	1.695978	1.395819	5.047783

27	6	0	3.258360	-0.510030	4.173835
28	1	0	3.807428	-1.436767	3.990426
29	1	0	3.729185	0.017286	5.007818
30	1	0	2.234046	-0.770139	4.457378
31	6	0	3.482056	0.576897	-2.076693
32	6	0	2.859229	-0.855867	-2.223153
33	5	0	1.394547	0.557027	-1.231291
34	8	0	2.611128	1.202553	-1.109401
35	8	0	1.466246	-0.627000	-1.923744
36	6	0	2.956510	-1.446331	-3.621565
37	1	0	4.003821	-1.553641	-3.921700
38	1	0	2.495628	-2.437119	-3.627192
39	1	0	2.439160	-0.825442	-4.354366
40	6	0	3.379291	1.401950	-3.358421
41	1	0	3.656655	2.434895	-3.134703
42	1	0	4.045470	1.020789	-4.137001
43	1	0	2.354469	1.398713	-3.741829
44	6	0	4.903749	0.598195	-1.542330
45	1	0	5.580550	0.083363	-2.231710
46	1	0	5.239711	1.634012	-1.442278
47	1	0	4.962520	0.117190	-0.564679
48	6	0	3.404482	-1.841957	-1.195934
49	1	0	2.784941	-2.742354	-1.220415
50	1	0	4.436190	-2.122159	-1.428941
51	1	0	3.369861	-1.417242	-0.188288
52	6	0	-1.021868	-0.693147	1.320843
53	6	0	-1.991121	-1.659728	1.073134
54	6	0	-0.270894	-3.241581	0.554906
55	6	0	0.672588	-2.334478	0.888506
56	1	0	-1.247165	0.280659	1.735035
57	1	0	-3.031177	-1.355650	1.161327
58	1	0	0.051751	-4.227325	0.233026
59	7	0	0.339363	-1.045507	1.328351
60	1	0	1.731961	-2.551656	0.884789
61	6	0	-2.319007	2.465136	-0.358305
62	6	0	-1.673322	-2.940002	0.656532
63	6	0	-2.703730	-3.978298	0.326112
64	1	0	-2.626382	-4.309277	-0.716900
65	1	0	-2.592426	-4.872547	0.951393
66	1	0	-3.714144	-3.590366	0.478072
67	6	0	-3.604794	3.205599	-0.140486
68	1	0	-3.713432	3.532450	0.901037
69	1	0	-3.663615	4.106660	-0.763123
70	1	0	-4.465309	2.577132	-0.383516

IntG4

Thermal correction to Energy=	0.317707
Thermal correction to Enthalpy=	0.318651
Thermal correction to Gibbs Free Energy=	0.256882
Sum of electronic and zero-point Energies=	-698.293749
Sum of electronic and thermal Energies=	-698.277365
Sum of electronic and thermal Enthalpies=	-698.276421
Sum of electronic and thermal Free Energies=	-698.338190

Esol =-698.8393335

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.910254	1.190175	-0.160808
2	6	0	3.269951	1.190770	-0.159360
3	6	0	4.024669	0.002818	0.019351
4	6	0	3.269786	-1.184840	0.199598
5	6	0	1.910114	-1.184613	0.197504
6	7	0	1.180744	0.001702	0.010955
7	1	0	1.308777	2.080596	-0.287764
8	1	0	3.779853	2.140130	-0.296253
9	1	0	3.779539	-2.132452	0.348596
10	1	0	1.308564	-2.072947	0.337994
11	5	0	-0.246954	0.000804	0.004845
12	8	0	-0.997824	-1.129284	0.232858
13	8	0	-0.997402	1.130191	-0.227979
14	6	0	-2.355598	-0.775659	-0.107589
15	6	0	-2.357003	0.775270	0.103818
16	6	0	-3.305262	-1.542346	0.797463
17	1	0	-4.337932	-1.220980	0.628855
18	1	0	-3.238511	-2.610342	0.576246
19	1	0	-3.055604	-1.394519	1.849017
20	6	0	-2.569693	-1.168561	-1.567866
21	1	0	-2.342556	-2.230908	-1.682223
22	1	0	-3.602434	-0.995293	-1.882238
23	1	0	-1.903293	-0.601611	-2.224422
24	6	0	-3.301626	1.541077	-0.807223
25	1	0	-4.335029	1.218674	-0.645215
26	1	0	-3.237342	2.609127	-0.585541
27	1	0	-3.045112	1.393546	-1.857166

28	6	0	-2.580698	1.167951	1.562721
29	1	0	-2.355201	2.230491	1.678545
30	1	0	-3.615261	0.993816	1.870554
31	1	0	-1.918001	0.601551	2.223490
32	6	0	5.523175	-0.004633	-0.028499
33	1	0	5.906862	-0.160629	-1.045860
34	1	0	5.935989	0.943989	0.327942
35	1	0	5.935830	-0.803062	0.595689

H

Thermal correction to Energy= 0.130016
Thermal correction to Enthalpy= 0.130960
Thermal correction to Gibbs Free Energy= 0.092764
Sum of electronic and zero-point Energies= -362.537641
Sum of electronic and thermal Energies= -362.531096
Sum of electronic and thermal Enthalpies= -362.530152
Sum of electronic and thermal Free Energies= -362.568348

Esol =-362.793021

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.153891	-0.700247	0.000031
2	6	0	1.142158	0.684428	0.000216
3	6	0	-1.253309	0.565070	-0.000351
4	6	0	-1.109616	-0.821888	-0.000515
5	7	0	0.054471	-1.465284	-0.000308
6	1	0	2.103577	-1.230378	0.000200
7	1	0	2.056484	1.265960	0.000509
8	1	0	-2.243235	1.003040	-0.000550
9	1	0	-2.001282	-1.445401	-0.000789
10	6	0	-0.092944	1.339291	0.000043
11	8	0	-0.063181	2.689130	0.000228
12	6	0	-1.303491	3.367678	0.000291
13	1	0	-1.888736	3.123779	0.894081
14	1	0	-1.066654	4.430671	0.000460
15	1	0	-1.888670	3.124037	-0.893620

TSH1

Thermal correction to Energy= 0.518384

Thermal correction to Enthalpy= 0.519328
Thermal correction to Gibbs Free Energy= 0.435552
Sum of electronic and zero-point Energies= -1184.402718
Sum of electronic and thermal Energies= -1184.375863
Sum of electronic and thermal Enthalpies= -1184.374919
Sum of electronic and thermal Free Energies= -1184.458694

Esol =-1185.3143975

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.721355	2.349383	-0.977091
2	6	0	1.304514	2.527388	1.392327
3	6	0	0.667249	1.443163	-1.028596
4	1	0	2.260355	2.600111	-1.881320
5	6	0	0.276029	1.618245	1.230867
6	1	0	1.552658	2.947738	2.359353
7	1	0	0.377630	0.959570	-1.958685
8	1	0	-0.334289	1.273452	2.062366
9	7	0	-0.039498	1.092687	0.041980
10	6	0	1.908618	-2.548087	-0.747855
11	6	0	2.025098	-2.225794	0.774849
12	5	0	0.019876	-1.496474	-0.015977
13	8	0	0.778746	-1.748923	-1.143759
14	8	0	0.664001	-1.920008	1.129207
15	6	0	2.519915	-3.375514	1.638154
16	1	0	3.524146	-3.685068	1.330298
17	1	0	2.564422	-3.055029	2.682033
18	1	0	1.850432	-4.234449	1.574214
19	6	0	1.543762	-4.006738	-1.019022
20	1	0	1.268656	-4.108757	-2.071392
21	1	0	2.380624	-4.678567	-0.807259
22	1	0	0.686543	-4.308875	-0.410986
23	6	0	3.113747	-2.139484	-1.581517
24	1	0	4.015963	-2.657403	-1.239955
25	1	0	2.940835	-2.405004	-2.627546
26	1	0	3.281717	-1.062068	-1.525716
27	6	0	2.845273	-0.964793	1.050569
28	1	0	2.698731	-0.673831	2.093806
29	1	0	3.912706	-1.130824	0.877821
30	1	0	2.511599	-0.136562	0.416576
31	6	0	-3.299152	0.429300	-0.808278

32	6	0	-3.489526	0.011136	0.687211
33	5	0	-1.388352	-0.547325	-0.028579
34	8	0	-2.129383	-0.308896	-1.187935
35	8	0	-2.150718	-0.270925	1.116273
36	6	0	-4.082887	1.091838	1.579750
37	1	0	-5.079442	1.382097	1.230579
38	1	0	-4.175240	0.710911	2.600257
39	1	0	-3.446212	1.978321	1.602761
40	6	0	-3.008023	1.922461	-0.975192
41	1	0	-2.657740	2.095035	-1.996730
42	1	0	-3.906946	2.523779	-0.808727
43	1	0	-2.229864	2.255628	-0.285920
44	6	0	-4.443738	0.029364	-1.729681
45	1	0	-5.382641	0.491543	-1.406843
46	1	0	-4.227383	0.367551	-2.746550
47	1	0	-4.571325	-1.053804	-1.752069
48	6	0	-4.286135	-1.286289	0.835622
49	1	0	-4.204024	-1.628240	1.870123
50	1	0	-5.343884	-1.147078	0.593364
51	1	0	-3.874215	-2.063473	0.185829
52	6	0	2.045695	2.904965	0.265047
53	6	0	3.813904	4.183918	-0.645487
54	1	0	4.550275	4.890273	-0.266086
55	1	0	4.326454	3.324476	-1.091182
56	1	0	3.194309	4.673567	-1.404566
57	8	0	3.037330	3.791051	0.471339

IntH1

Thermal correction to Energy= 0.519620
Thermal correction to Enthalpy= 0.520565
Thermal correction to Gibbs Free Energy= 0.435349
Sum of electronic and zero-point Energies= -1184.406057
Sum of electronic and thermal Energies= -1184.378846
Sum of electronic and thermal Enthalpies= -1184.377902
Sum of electronic and thermal Free Energies= -1184.463118

Esol =-1185.3191647

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.518064	-1.193152	-1.308833

2	6	0	3.009760	-1.561510	0.126391
3	5	0	0.960369	-0.490179	0.245475
4	8	0	1.529920	-0.198794	-1.053766
5	8	0	1.809539	-1.470305	0.888597
6	6	0	3.565156	-2.973269	0.262220
7	1	0	4.414738	-3.127940	-0.411839
8	1	0	3.907843	-3.137129	1.287899
9	1	0	2.794995	-3.713024	0.038521
10	6	0	1.827444	-2.373524	-1.997131
11	1	0	1.320451	-2.002921	-2.891661
12	1	0	2.539039	-3.151029	-2.292277
13	1	0	1.070525	-2.807121	-1.337370
14	6	0	3.591452	-0.608309	-2.216604
15	1	0	4.413324	-1.318348	-2.358242
16	1	0	3.160474	-0.384976	-3.196443
17	1	0	3.995563	0.318165	-1.802670
18	6	0	4.030085	-0.552471	0.666163
19	1	0	4.129694	-0.702064	1.745003
20	1	0	5.013499	-0.683202	0.203510
21	1	0	3.701222	0.475694	0.490603
22	6	0	-2.755679	-1.800033	-0.094760
23	6	0	-2.730854	-1.284749	1.377355
24	5	0	-0.706828	-0.908605	0.380704
25	8	0	-1.358984	-1.808846	-0.438361
26	8	0	-1.551097	-0.458360	1.388316
27	6	0	-3.933186	-0.447188	1.784101
28	1	0	-4.856046	-1.030150	1.697375
29	1	0	-3.824822	-0.132000	2.825198
30	1	0	-4.021522	0.446406	1.164371
31	6	0	-3.444725	-0.825800	-1.050068
32	1	0	-3.234061	-1.136072	-2.076076
33	1	0	-4.528503	-0.811788	-0.901761
34	1	0	-3.056286	0.187428	-0.913607
35	6	0	-3.321097	-3.200682	-0.272993
36	1	0	-4.360794	-3.244499	0.068163
37	1	0	-3.295651	-3.471524	-1.331447
38	1	0	-2.735769	-3.936483	0.280364
39	6	0	-2.497424	-2.405836	2.389979
40	1	0	-2.284069	-1.959619	3.364631
41	1	0	-3.374390	-3.052248	2.486804
42	1	0	-1.638376	-3.015849	2.096656
43	6	0	1.415064	2.105741	0.504290
44	6	0	1.530089	3.301263	1.198367
45	6	0	1.054844	2.062065	3.212229

46	6	0	0.952086	0.926449	2.441487
47	1	0	1.562543	2.027004	-0.568189
48	1	0	1.762007	4.209265	0.658323
49	1	0	0.913243	2.033901	4.285169
50	7	0	1.132784	0.953253	1.111477
51	1	0	0.722664	-0.048750	2.856241
52	6	0	1.347853	3.280874	2.584196
53	6	0	1.726472	5.606380	2.782213
54	1	0	1.746184	6.330998	3.594109
55	1	0	2.702672	5.584257	2.286452
56	1	0	0.953124	5.886258	2.059160
57	8	0	1.432704	4.356300	3.382450

TSH2

Thermal correction to Energy= 0.650917
Thermal correction to Enthalpy= 0.651861
Thermal correction to Gibbs Free Energy= 0.550936
Sum of electronic and zero-point Energies= -1546.958107
Sum of electronic and thermal Energies= -1546.923509
Sum of electronic and thermal Enthalpies= -1546.922565
Sum of electronic and thermal Free Energies= -1547.023490

Esol = -1548.1197899

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.875863	0.743710	2.710540
2	6	0	-2.918648	1.414486	0.643140
3	6	0	-0.660748	0.773228	2.042837
4	1	0	-1.899759	0.468069	3.756144
5	6	0	-1.667640	1.427285	0.064637
6	1	0	-3.807979	1.662221	0.076832
7	1	0	0.273752	0.501194	2.522081
8	1	0	-1.489442	1.689786	-0.973275
9	7	0	-0.562591	1.105169	0.754427
10	6	0	2.286932	-2.383700	1.396237
11	6	0	2.725631	-2.550748	-0.092624
12	5	0	1.347635	-0.727294	0.111937
13	8	0	1.169833	-1.490906	1.294502
14	8	0	2.377551	-1.280914	-0.654264
15	6	0	4.218334	-2.776897	-0.291348

16	1	0	4.549133	-3.684180	0.225757
17	1	0	4.429733	-2.894018	-1.357602
18	1	0	4.795114	-1.927346	0.077787
19	6	0	3.347039	-1.669193	2.237376
20	1	0	2.911327	-1.418161	3.208371
21	1	0	4.230716	-2.292583	2.403006
22	1	0	3.647962	-0.737087	1.749698
23	6	0	1.845710	-3.669515	2.079473
24	1	0	2.663454	-4.397626	2.104470
25	1	0	1.549925	-3.454255	3.110124
26	1	0	0.993615	-4.117881	1.564480
27	6	0	1.935328	-3.637506	-0.823517
28	1	0	2.118229	-3.534914	-1.896495
29	1	0	2.245768	-4.639036	-0.509400
30	1	0	0.862933	-3.525654	-0.650905
31	6	0	2.041286	2.987613	-0.009875
32	6	0	1.773744	2.527510	-1.477735
33	5	0	0.949204	0.942045	-0.003954
34	8	0	1.887519	1.776359	0.719143
35	8	0	0.750157	1.550114	-1.314618
36	6	0	1.272106	3.625902	-2.405486
37	1	0	2.001753	4.439402	-2.480104
38	1	0	1.115460	3.216706	-3.407746
39	1	0	0.323518	4.036902	-2.052655
40	6	0	1.002378	4.006153	0.474187
41	1	0	1.074118	4.083506	1.562711
42	1	0	1.171029	4.997640	0.041574
43	1	0	-0.011999	3.686246	0.219295
44	6	0	3.443557	3.529371	0.236557
45	1	0	3.654778	4.388384	-0.409878
46	1	0	3.534735	3.853474	1.277288
47	1	0	4.190806	2.755134	0.055127
48	6	0	2.993398	1.831672	-2.088378
49	1	0	2.688189	1.356271	-3.024914
50	1	0	3.804169	2.535191	-2.302723
51	1	0	3.355578	1.047196	-1.417837
52	6	0	-1.481778	-1.888139	-0.147185
53	6	0	-2.798560	-1.935246	-0.566306
54	6	0	-2.077891	-0.948009	-2.641164
55	6	0	-0.786451	-0.943269	-2.116389
56	1	0	-1.178222	-2.229778	0.840893
57	1	0	-3.590089	-2.323561	0.063688
58	1	0	-2.253883	-0.557758	-3.635211
59	7	0	-0.490640	-1.403266	-0.904401

60	1	0	0.044856	-0.517773	-2.671659
61	6	0	-3.033240	1.064971	1.994825
62	6	0	-3.107118	-1.453678	-1.844820
63	6	0	-4.425469	0.718037	3.874144
64	1	0	-5.491943	0.779529	4.083363
65	1	0	-4.072655	-0.301320	4.063975
66	1	0	-3.884375	1.418713	4.518858
67	6	0	-4.744122	-1.036703	-3.498345
68	1	0	-5.819711	-1.174418	-3.597530
69	1	0	-4.499889	0.025981	-3.607401
70	1	0	-4.228584	-1.608426	-4.277775
71	8	0	-4.275029	1.062830	2.508189
72	8	0	-4.405181	-1.509589	-2.208851

IntH2

Thermal correction to Energy= 0.651876
Thermal correction to Enthalpy= 0.652821
Thermal correction to Gibbs Free Energy= 0.551729
Sum of electronic and zero-point Energies= -1546.962122
Sum of electronic and thermal Energies= -1546.927325
Sum of electronic and thermal Enthalpies= -1546.926381
Sum of electronic and thermal Free Energies= -1547.027472

Esol =-1548.1238507

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858393	2.111077	-3.177429
2	6	0	-1.594151	3.399905	-1.276849
3	6	0	-0.827112	1.002420	-2.345747
4	1	0	-0.579797	2.002126	-4.216828
5	6	0	-1.543094	2.243939	-0.526556
6	1	0	-1.899744	4.344409	-0.844123
7	1	0	-0.520723	0.019597	-2.686916
8	1	0	-1.808098	2.200298	0.525780
9	7	0	-1.163763	1.070058	-1.055165
10	6	0	2.488504	-1.214915	-1.275574
11	6	0	2.678694	-1.711123	0.192624
12	5	0	0.862717	-0.278276	0.084049
13	8	0	1.679148	-0.054586	-1.110303
14	8	0	1.412112	-1.426447	0.773736

15	6	0	2.950369	-3.203709	0.326553
16	1	0	3.848787	-3.494194	-0.229261
17	1	0	3.102923	-3.456422	1.379853
18	1	0	2.100536	-3.781047	-0.041479
19	6	0	1.695982	-2.221805	-2.115226
20	1	0	1.444844	-1.751980	-3.071811
21	1	0	2.270081	-3.130336	-2.323099
22	1	0	0.763032	-2.483289	-1.605469
23	6	0	3.778907	-0.830417	-1.986942
24	1	0	4.461003	-1.685118	-2.051628
25	1	0	3.552147	-0.498791	-3.004442
26	1	0	4.286109	-0.014015	-1.468511
27	6	0	3.764119	-0.916596	0.928778
28	1	0	3.670848	-1.112860	2.000829
29	1	0	4.770058	-1.205955	0.607815
30	1	0	3.643124	0.157825	0.763032
31	6	0	-2.680610	-1.712959	-0.192277
32	6	0	-2.490748	-1.215882	1.275672
33	5	0	-0.865562	-0.278879	-0.084421
34	8	0	-1.414211	-1.427754	-0.773529
35	8	0	-1.682135	-0.055119	1.109818
36	6	0	-3.781399	-0.831851	1.986839
37	1	0	-4.462939	-1.686961	2.051974
38	1	0	-3.554855	-0.499544	3.004165
39	1	0	-4.289134	-0.016052	1.467981
40	6	0	-3.766544	-0.919514	-0.928846
41	1	0	-3.673133	-1.116264	-2.000796
42	1	0	-4.772299	-1.209361	-0.607745
43	1	0	-3.646248	0.155070	-0.763652
44	6	0	-2.951313	-3.205788	-0.325453
45	1	0	-3.849550	-3.496576	0.230495
46	1	0	-3.103686	-3.459133	-1.378626
47	1	0	-2.101110	-3.782387	0.042883
48	6	0	-1.697578	-2.221831	2.115842
49	1	0	-1.446734	-1.751348	3.072180
50	1	0	-2.271094	-3.130622	2.324190
51	1	0	-0.764465	-2.482982	1.606214
52	6	0	1.538419	2.245237	0.524920
53	6	0	1.588682	3.401599	1.274656
54	6	0	0.854083	2.113121	3.175923
55	6	0	0.823543	1.004049	2.344769
56	1	0	1.803348	2.201302	-0.527423
57	1	0	1.893514	4.346125	0.841443
58	1	0	0.575654	2.004458	4.215397

59	7	0	1.160029	1.071324	1.054124
60	1	0	0.517930	0.021155	2.686430
61	6	0	-1.245591	3.339280	-2.632345
62	6	0	1.240320	3.341355	2.630221
63	6	0	-0.968232	4.466250	-4.692522
64	1	0	-1.086458	5.486898	-5.052178
65	1	0	0.069391	4.145392	-4.834023
66	1	0	-1.636034	3.801453	-5.250697
67	6	0	0.962248	4.469135	4.689879
68	1	0	1.079812	5.490032	5.049043
69	1	0	-0.075151	4.147647	4.831588
70	1	0	1.630523	3.805051	5.248338
71	8	0	-1.309916	4.494530	-3.317959
72	8	0	1.303845	4.496988	3.315283

TSH3

Thermal correction to Energy=	0.651016
Thermal correction to Enthalpy=	0.651960
Thermal correction to Gibbs Free Energy=	0.554932
Sum of electronic and zero-point Energies=	-1546.929055
Sum of electronic and thermal Energies=	-1546.895240
Sum of electronic and thermal Enthalpies=	-1546.894295
Sum of electronic and thermal Free Energies=	-1546.991323

Esol =-1548.088159

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.506402	-3.080084	0.990322
2	6	0	-2.991720	-1.200520	1.166886
3	6	0	-0.447679	-2.228617	1.048643
4	1	0	-1.310562	-4.142392	0.926321
5	6	0	-1.878171	-0.345935	1.137105
6	1	0	-3.987531	-0.775948	1.225115
7	1	0	0.580644	-2.566373	1.046206
8	1	0	-1.949370	0.702622	1.402830
9	7	0	-0.600931	-0.862905	1.157763
10	6	0	1.704661	-1.712921	-2.155517
11	6	0	2.374793	-0.329901	-2.461804
12	5	0	0.580349	-0.022221	-1.108226
13	8	0	0.434086	-1.331799	-1.605036

14	8	0	1.847162	0.512939	-1.426849
15	6	0	3.891660	-0.325583	-2.365393
16	1	0	4.329896	-1.034802	-3.075376
17	1	0	4.270487	0.672995	-2.600214
18	1	0	4.213681	-0.587681	-1.355843
19	6	0	2.468159	-2.510410	-1.099464
20	1	0	1.856988	-3.370694	-0.809362
21	1	0	3.417606	-2.886394	-1.492947
22	1	0	2.657230	-1.897670	-0.213380
23	6	0	1.457319	-2.575375	-3.385219
24	1	0	2.399463	-2.798591	-3.897048
25	1	0	1.001563	-3.521219	-3.080214
26	1	0	0.781694	-2.082128	-4.085796
27	6	0	1.916963	0.252555	-3.799936
28	1	0	2.251985	1.291164	-3.861534
29	1	0	2.331148	-0.299133	-4.648913
30	1	0	0.824796	0.239147	-3.871607
31	6	0	2.375072	0.329392	2.461631
32	6	0	1.704956	1.712536	2.155633
33	5	0	0.580182	0.022045	1.108437
34	8	0	1.846757	-0.513554	1.427137
35	8	0	0.434293	1.331658	1.605217
36	6	0	1.457765	2.574747	3.385553
37	1	0	2.399995	2.798093	3.897168
38	1	0	1.001726	3.520533	3.080795
39	1	0	0.782426	2.081271	4.086238
40	6	0	1.918005	-0.252928	3.800080
41	1	0	2.253225	-1.291474	3.861661
42	1	0	2.332501	0.298938	4.648787
43	1	0	0.825869	-0.239704	3.872255
44	6	0	3.891880	0.324839	2.364253
45	1	0	4.330713	1.033940	3.073984
46	1	0	4.270672	-0.673824	2.598769
47	1	0	4.213254	0.586923	1.354491
48	6	0	2.468340	2.510382	1.099762
49	1	0	1.857496	3.371234	0.810636
50	1	0	3.418173	2.885592	1.493044
51	1	0	2.656664	1.898345	0.213032
52	6	0	-1.877876	0.346356	-1.137648
53	6	0	-2.991237	1.201174	-1.167596
54	6	0	-1.505580	3.080389	-0.990055
55	6	0	-0.447017	2.228714	-1.048338
56	1	0	-1.949201	-0.702127	-1.403632
57	1	0	-3.987114	0.776829	-1.226325

58	1	0	-1.309556	4.142651	-0.925829
59	7	0	-0.600515	0.863064	-1.157814
60	1	0	0.581369	2.566278	-1.045608
61	6	0	-2.832174	-2.559874	1.054042
62	6	0	-2.831438	2.560459	-1.054251
63	8	0	-3.952337	3.331265	-1.020923
64	6	0	-3.780490	4.729269	-0.955156
65	1	0	-4.782256	5.158156	-0.949506
66	1	0	-3.255878	5.028272	-0.039527
67	1	0	-3.231089	5.109214	-1.825202
68	8	0	-3.953238	-3.330432	1.020448
69	6	0	-3.781745	-4.728551	0.956092
70	1	0	-4.783620	-5.157184	0.950570
71	1	0	-3.256946	-5.028586	0.040902
72	1	0	-3.232712	-5.107794	1.826661

IntH3

Thermal correction to Energy= 0.654745
Thermal correction to Enthalpy= 0.655689
Thermal correction to Gibbs Free Energy= 0.556269
Sum of electronic and zero-point Energies= -1546.995513
Sum of electronic and thermal Energies= -1546.961186
Sum of electronic and thermal Enthalpies= -1546.960241
Sum of electronic and thermal Free Energies= -1547.059662

Esol = -1548.1627143

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.173278	2.940352	0.002975
2	6	0	-2.248650	0.901916	-0.775161
3	6	0	0.037850	2.393711	-0.216192
4	1	0	-1.244569	3.944208	0.397612
5	6	0	-0.949478	0.188675	-0.521262
6	1	0	-3.105109	0.361274	-1.158066
7	1	0	0.962440	2.941157	-0.066963
8	1	0	-0.815233	-0.645959	-1.216460
9	7	0	0.183766	1.104510	-0.705498
10	6	0	2.443255	1.390898	3.023530
11	6	0	3.298927	0.078149	3.053418
12	5	0	1.385485	-0.267019	1.906065
13	8	0	1.159518	0.915021	2.568593

14	8	0	2.688784	-0.713413	2.013223
15	6	0	4.769370	0.268434	2.722827
16	1	0	5.246238	0.927324	3.455491
17	1	0	5.277319	-0.699085	2.748813
18	1	0	4.895886	0.699712	1.728230
19	6	0	2.948377	2.401733	1.998126
20	1	0	2.209764	3.203245	1.913190
21	1	0	3.899483	2.842479	2.311178
22	1	0	3.073471	1.943039	1.011822
23	6	0	2.259859	2.058372	4.377538
24	1	0	3.227432	2.358567	4.792725
25	1	0	1.645624	2.954305	4.258876
26	1	0	1.760919	1.394384	5.084660
27	6	0	3.139581	-0.702713	4.356478
28	1	0	3.590838	-1.689856	4.231464
29	1	0	3.630829	-0.195842	5.191419
30	1	0	2.081922	-0.838147	4.601061
31	6	0	3.453247	0.829230	-2.223156
32	6	0	2.948363	-0.653078	-2.285740
33	5	0	1.406211	0.664683	-1.285150
34	8	0	2.561768	1.420601	-1.255984
35	8	0	1.547584	-0.519035	-1.968257
36	6	0	3.076592	-1.306563	-3.652646
37	1	0	4.125947	-1.345512	-3.962656
38	1	0	2.695849	-2.329459	-3.602186
39	1	0	2.504204	-0.766510	-4.408108
40	6	0	3.245765	1.581120	-3.536265
41	1	0	3.425643	2.644857	-3.364184
42	1	0	3.931753	1.230411	-4.312060
43	1	0	2.219405	1.460861	-3.895312
44	6	0	4.882688	0.994408	-1.735454
45	1	0	5.580080	0.491998	-2.413466
46	1	0	5.138451	2.056733	-1.705486
47	1	0	5.008061	0.579882	-0.733293
48	6	0	3.577967	-1.536407	-1.212865
49	1	0	3.055670	-2.496861	-1.207749
50	1	0	4.636108	-1.721021	-1.420016
51	1	0	3.481535	-1.086158	-0.219374
52	6	0	-0.934849	-0.403046	0.923484
53	6	0	-2.022995	-1.430689	1.074181
54	6	0	-0.394198	-3.115879	0.423923
55	6	0	0.611164	-2.277507	0.739526
56	1	0	-1.080662	0.430579	1.617639
57	1	0	-3.019409	-1.132698	1.375183

58	1	0	-0.169963	-4.102089	0.042068
59	7	0	0.376798	-0.996813	1.217031
60	1	0	1.654446	-2.569343	0.683956
61	6	0	-2.356186	2.193464	-0.421140
62	6	0	-1.762046	-2.703272	0.732734
63	6	0	-3.612867	4.210904	-0.564726
64	1	0	-4.634698	4.478096	-0.836511
65	1	0	-3.380475	4.662581	0.407459
66	1	0	-2.922693	4.608011	-1.317930
67	6	0	-2.456931	-4.977945	0.834346
68	1	0	-3.394058	-5.500537	1.029904
69	1	0	-2.027004	-5.368341	-0.096046
70	1	0	-1.759093	-5.166991	1.658163
71	8	0	-3.576846	2.801424	-0.512272
72	8	0	-2.785532	-3.609500	0.729670

TSH4

Thermal correction to Energy= 0.649475
Thermal correction to Enthalpy= 0.650419
Thermal correction to Gibbs Free Energy= 0.548783
Sum of electronic and zero-point Energies= -1546.935882
Sum of electronic and thermal Energies= -1546.900957
Sum of electronic and thermal Enthalpies= -1546.900013
Sum of electronic and thermal Free Energies= -1547.001648

Esol = -1548.0988307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.785982	-0.715603	-3.162563
2	6	0	3.256995	0.457412	-1.654194
3	6	0	0.717373	-0.218348	-2.495031
4	1	0	1.600627	-1.357547	-4.014717
5	6	0	2.159160	0.867853	-0.911073
6	1	0	4.252254	0.723628	-1.314662
7	1	0	-0.301506	-0.406202	-2.803984
8	1	0	2.229121	1.594089	-0.112356
9	7	0	0.851613	0.635416	-1.392788
10	6	0	-1.490407	-2.854167	-0.287583
11	6	0	-2.296039	-2.295391	0.938903
12	5	0	-0.267410	-1.320568	0.845236

13	8	0	-0.156082	-2.366334	-0.040597
14	8	0	-1.561138	-1.102972	1.285647
15	6	0	-3.733701	-1.914454	0.629961
16	1	0	-4.304877	-2.794183	0.316497
17	1	0	-4.202950	-1.503127	1.528079
18	1	0	-3.780140	-1.163848	-0.160752
19	6	0	-1.963174	-2.273859	-1.616501
20	1	0	-1.236506	-2.545620	-2.386748
21	1	0	-2.939018	-2.680452	-1.898824
22	1	0	-2.032600	-1.183235	-1.565356
23	6	0	-1.438644	-4.372667	-0.368349
24	1	0	-2.447209	-4.787437	-0.464611
25	1	0	-0.861848	-4.667323	-1.248474
26	1	0	-0.960096	-4.803278	0.512226
27	6	0	-2.235917	-3.216397	2.156629
28	1	0	-2.648064	-2.686463	3.018669
29	1	0	-2.813350	-4.131329	1.999357
30	1	0	-1.201477	-3.489272	2.386457
31	6	0	-2.306774	2.290332	-0.924919
32	6	0	-1.494709	2.850756	0.296542
33	5	0	-0.275582	1.319759	-0.843920
34	8	0	-1.571598	1.099390	-1.276169
35	8	0	-0.160906	2.365824	0.041138
36	6	0	-1.445733	4.369352	0.377147
37	1	0	-2.454581	4.781923	0.479687
38	1	0	-0.864146	4.665183	1.253718
39	1	0	-0.973577	4.801076	-0.506330
40	6	0	-2.256025	3.211442	-2.142993
41	1	0	-2.672356	2.680648	-3.002490
42	1	0	-2.834375	4.125179	-1.982180
43	1	0	-1.223580	3.486457	-2.379156
44	6	0	-3.741728	1.906505	-0.607105
45	1	0	-4.312720	2.785091	-0.290117
46	1	0	-4.215694	1.494231	-1.502307
47	1	0	-3.781785	1.155818	0.183877
48	6	0	-1.957883	2.269241	1.628307
49	1	0	-1.226934	2.542359	2.394009
50	1	0	-2.932777	2.673733	1.916860
51	1	0	-2.025347	1.178487	1.577299
52	6	0	2.166731	-0.863417	0.897122
53	6	0	3.268323	-0.450638	1.633359
54	6	0	1.804268	0.719053	3.151061
55	6	0	0.732568	0.219526	2.490217
56	1	0	2.233246	-1.589448	0.097925

57	1	0	4.262005	-0.714664	1.287559
58	1	0	1.622896	1.360521	4.004432
59	7	0	0.861740	-0.633851	1.387069
60	1	0	-0.284761	0.405112	2.805589
61	6	0	3.113258	-0.361347	-2.759983
62	6	0	3.129752	0.367725	2.740095
63	6	0	4.086236	-1.524710	-4.577180
64	1	0	5.088568	-1.728284	-4.954830
65	1	0	3.571767	-2.478409	-4.400099
66	1	0	3.527087	-0.954206	-5.330309
67	6	0	4.111532	1.532965	4.551320
68	1	0	5.115753	1.738655	4.922757
69	1	0	3.593904	2.485571	4.377606
70	1	0	3.558316	0.961130	5.307814
71	8	0	4.250645	-0.792572	-3.388273
72	8	0	4.270116	0.801368	3.361279

IntH4

Thermal correction to Energy= 0.323229
Thermal correction to Enthalpy= 0.324174
Thermal correction to Gibbs Free Energy= 0.260953
Sum of electronic and zero-point Energies= -773.465189
Sum of electronic and thermal Energies= -773.447954
Sum of electronic and thermal Enthalpies= -773.447010
Sum of electronic and thermal Free Energies= -773.510230

Esol =-774.0487549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.254250	1.264608	-0.199728
2	6	0	3.622906	1.292650	-0.206076
3	6	0	3.646304	-1.099329	0.175458
4	6	0	2.293582	-1.112592	0.178309
5	7	0	1.542684	0.062913	-0.007725
6	1	0	1.641497	2.144307	-0.339220
7	1	0	4.107001	2.249853	-0.359582
8	1	0	4.197732	-2.020801	0.322262
9	1	0	1.707268	-2.010850	0.321971
10	5	0	0.118076	0.034686	-0.001081
11	8	0	-0.610103	-1.110735	0.234421

12	8	0	-0.658114	1.148889	-0.230484
13	6	0	-1.974558	-0.785076	-0.103008
14	6	0	-2.007146	0.765666	0.110240
15	6	0	-2.907506	-1.571679	0.802013
16	1	0	-3.947512	-1.277982	0.626822
17	1	0	-2.811892	-2.638758	0.586402
18	1	0	-2.667134	-1.412264	1.854093
19	6	0	-2.184629	-1.178678	-1.563456
20	1	0	-1.936496	-2.236016	-1.681516
21	1	0	-3.221633	-1.025430	-1.874601
22	1	0	-1.531733	-0.596237	-2.220149
23	6	0	-2.975058	1.511353	-0.792693
24	1	0	-3.999489	1.163920	-0.624087
25	1	0	-2.934640	2.580390	-0.569529
26	1	0	-2.722886	1.371279	-1.844800
27	6	0	-2.229203	1.151603	1.570933
28	1	0	-2.020832	2.217666	1.687376
29	1	0	-3.259062	0.960117	1.884790
30	1	0	-1.553034	0.595210	2.226681
31	6	0	4.364740	0.114083	-0.018803
32	8	0	5.727264	0.016235	-0.004451
33	6	0	6.447037	1.208763	-0.195212
34	1	0	6.226510	1.941646	0.592162
35	1	0	7.503604	0.943974	-0.154078
36	1	0	6.225556	1.660489	-1.171331

I

Thermal correction to Energy=	0.172139
Thermal correction to Enthalpy=	0.173083
Thermal correction to Gibbs Free Energy=	0.129456
Sum of electronic and zero-point Energies=	-381.930511
Sum of electronic and thermal Energies=	-381.921879
Sum of electronic and thermal Enthalpies=	-381.920935
Sum of electronic and thermal Free Energies=	-381.964562

Esol = -382.2270175

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609210	1.126724	-0.100503
2	6	0	0.241072	1.194431	0.116422

3	6	0	-0.497773	-0.000532	0.222870
4	6	0	0.239718	-1.196126	0.114243
5	6	0	1.607935	-1.129570	-0.102578
6	7	0	2.313314	-0.001716	-0.215079
7	1	0	2.175712	2.052535	-0.183386
8	1	0	-0.234574	-2.165309	0.199475
9	1	0	2.173392	-2.055873	-0.187104
10	1	0	-0.232140	2.163996	0.203317
11	7	0	-1.856601	0.000078	0.419359
12	6	0	-2.529628	-1.250469	0.703983
13	1	0	-3.595888	-1.061530	0.827375
14	1	0	-2.409142	-1.955719	-0.124959
15	1	0	-2.152323	-1.728307	1.618841
16	6	0	-2.528035	1.250776	0.707089
17	1	0	-2.407283	1.957721	-0.120373
18	1	0	-3.594424	1.062776	0.830785
19	1	0	-2.149585	1.726148	1.622748

TSI1

Thermal correction to Energy=	0.560968
Thermal correction to Enthalpy=	0.561912
Thermal correction to Gibbs Free Energy=	0.473158
Sum of electronic and zero-point Energies=	-1203.796618
Sum of electronic and thermal Energies=	-1203.767759
Sum of electronic and thermal Enthalpies=	-1203.766815
Sum of electronic and thermal Free Energies=	-1203.855568

Esol = -1204.7499636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.513350	0.936490	-0.747179
2	6	0	3.317957	1.155879	0.789761
3	5	0	1.726229	-0.277390	0.004671
4	8	0	2.291544	0.296807	-1.139974
5	8	0	2.440726	0.078195	1.146086
6	6	0	4.592501	1.036406	1.614595
7	1	0	5.330656	1.781705	1.299744
8	1	0	4.360340	1.208323	2.668937
9	1	0	5.031385	0.042045	1.521344
10	6	0	4.646454	-0.041838	-1.061673

11	1	0	4.593998	-0.305886	-2.120668
12	1	0	5.629785	0.390734	-0.854569
13	1	0	4.533241	-0.958368	-0.475977
14	6	0	3.688799	2.214336	-1.555244
15	1	0	4.577965	2.763731	-1.228300
16	1	0	3.811091	1.962433	-2.612022
17	1	0	2.817435	2.864568	-1.457485
18	6	0	2.617819	2.475832	1.119304
19	1	0	2.316468	2.453816	2.170264
20	1	0	3.284964	3.329516	0.965275
21	1	0	1.721622	2.611002	0.511106
22	6	0	-1.154126	-2.759033	-0.816572
23	6	0	-0.886699	-3.122861	0.678320
24	5	0	0.612375	-1.555752	-0.034289
25	8	0	0.053659	-2.070777	-1.187176
26	8	0	0.006901	-2.075345	1.094801
27	6	0	-2.118303	-3.097866	1.571323
28	1	0	-2.866245	-3.817725	1.222827
29	1	0	-1.833816	-3.365475	2.592175
30	1	0	-2.566041	-2.102145	1.591294
31	6	0	-2.300791	-1.761518	-0.986358
32	1	0	-2.283719	-1.382410	-2.011423
33	1	0	-3.272408	-2.228481	-0.798688
34	1	0	-2.182054	-0.910517	-0.308105
35	6	0	-1.352179	-3.950382	-1.740940
36	1	0	-2.219995	-4.541108	-1.429284
37	1	0	-1.526248	-3.595671	-2.759965
38	1	0	-0.471714	-4.594478	-1.750834
39	6	0	-0.136415	-4.443676	0.842690
40	1	0	0.200506	-4.527921	1.878550
41	1	0	-0.772437	-5.302274	0.608332
42	1	0	0.743839	-4.469329	0.194365
43	6	0	-0.592045	1.425871	-1.011740
44	6	0	-1.850072	1.994025	-1.105645
45	6	0	-2.118791	1.536127	1.241165
46	6	0	-0.847151	0.991829	1.220619
47	1	0	0.060023	1.338396	-1.878561
48	1	0	-2.193341	2.363356	-2.062927
49	1	0	-2.676397	1.541760	2.168443
50	7	0	-0.087617	0.938875	0.123699
51	1	0	-0.407273	0.555515	2.114505
52	6	0	-2.661670	2.067492	0.048449
53	7	0	-3.910370	2.619340	0.013537
54	6	0	-4.740688	2.594487	1.201078

55	1	0	-4.267928	3.138965	2.026016
56	1	0	-5.691952	3.077138	0.980712
57	1	0	-4.942979	1.569157	1.536125
58	6	0	-4.459797	3.072003	-1.248870
59	1	0	-4.541135	2.253352	-1.975176
60	1	0	-5.455323	3.479799	-1.078316
61	1	0	-3.840976	3.862010	-1.688675

IntI1

Thermal correction to Energy=	0.562253
Thermal correction to Enthalpy=	0.563198
Thermal correction to Gibbs Free Energy=	0.473223
Sum of electronic and zero-point Energies=	-1203.801070
Sum of electronic and thermal Energies=	-1203.771932
Sum of electronic and thermal Enthalpies=	-1203.770988
Sum of electronic and thermal Free Energies=	-1203.860962

Esol = -1204.7563835

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.473828	-1.142897	-1.256616
2	6	0	2.945395	-1.491214	0.190373
3	5	0	0.865218	-0.472157	0.263389
4	8	0	1.456070	-0.174642	-1.027877
5	8	0	1.728504	-1.432869	0.926244
6	6	0	3.540140	-2.885331	0.343460
7	1	0	4.407557	-3.017378	-0.312594
8	1	0	3.866534	-3.035118	1.376687
9	1	0	2.796924	-3.648557	0.107493
10	6	0	1.830965	-2.345741	-1.952823
11	1	0	1.330737	-1.993305	-2.858497
12	1	0	2.569941	-3.103998	-2.230829
13	1	0	1.074097	-2.797723	-1.305587
14	6	0	3.550493	-0.534240	-2.145150
15	1	0	4.394566	-1.222058	-2.265011
16	1	0	3.134624	-0.328043	-3.135307
17	1	0	3.919528	0.405438	-1.728195
18	6	0	3.924552	-0.450074	0.746111
19	1	0	4.004898	-0.592214	1.827621
20	1	0	4.921236	-0.553618	0.305104

21	1	0	3.568236	0.566830	0.559322
22	6	0	-2.790488	-1.923007	-0.177286
23	6	0	-2.810665	-1.444189	1.306853
24	5	0	-0.786900	-0.959972	0.354744
25	8	0	-1.390032	-1.866475	-0.496496
26	8	0	-1.668033	-0.570388	1.357902
27	6	0	-4.053894	-0.668239	1.713389
28	1	0	-4.950113	-1.286620	1.597005
29	1	0	-3.975288	-0.374962	2.763608
30	1	0	-4.169662	0.236193	1.114174
31	6	0	-3.503877	-0.953647	-1.119856
32	1	0	-3.264108	-1.228917	-2.149489
33	1	0	-4.589656	-0.987186	-0.989800
34	1	0	-3.159015	0.070507	-0.951652
35	6	0	-3.295424	-3.340454	-0.399628
36	1	0	-4.338215	-3.434934	-0.078513
37	1	0	-3.240761	-3.583488	-1.463746
38	1	0	-2.689902	-4.065622	0.146020
39	6	0	-2.547043	-2.580142	2.295414
40	1	0	-2.367481	-2.150125	3.284098
41	1	0	-3.397582	-3.264740	2.361633
42	1	0	-1.658407	-3.145894	2.001639
43	6	0	1.252802	2.132003	0.523153
44	6	0	1.322257	3.321942	1.215492
45	6	0	0.809413	2.086298	3.216783
46	6	0	0.754398	0.950299	2.440879
47	1	0	1.435163	2.058931	-0.544126
48	1	0	1.554523	4.228226	0.673167
49	1	0	0.626981	2.001780	4.279142
50	7	0	0.973157	0.966529	1.119532
51	1	0	0.529743	-0.025220	2.858355
52	6	0	1.098273	3.331803	2.611630
53	7	0	1.157532	4.481474	3.336975
54	6	0	0.923201	4.446135	4.768173
55	1	0	1.009410	5.455441	5.167719
56	1	0	-0.080203	4.070566	4.999646
57	1	0	1.657068	3.811780	5.278662
58	6	0	1.457246	5.737404	2.675936
59	1	0	1.455984	6.537542	3.414531
60	1	0	2.443760	5.713270	2.198568
61	1	0	0.708307	5.975439	1.911770

TSI2

Thermal correction to Energy= 0.735897
Thermal correction to Enthalpy= 0.736841
Thermal correction to Gibbs Free Energy= 0.629453
Sum of electronic and zero-point Energies= -1585.745315
Sum of electronic and thermal Energies= -1585.707383
Sum of electronic and thermal Enthalpies= -1585.706439
Sum of electronic and thermal Free Energies= -1585.813827

Esol = -1586.9903615

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.805441	0.520905	-2.372168
2	6	0	2.558100	1.536710	-0.328733
3	6	0	0.518271	0.598026	-1.881046
4	1	0	1.962484	0.098688	-3.355467
5	6	0	1.240910	1.577055	0.076231
6	1	0	3.317622	1.922474	0.337760
7	1	0	-0.337378	0.216546	-2.429642
8	1	0	0.932005	1.983986	1.033623
9	7	0	0.238404	1.097805	-0.669306
10	6	0	-2.681984	-2.433383	-1.249305
11	6	0	-3.095987	-2.550854	0.250292
12	5	0	-1.665397	-0.775511	-0.023462
13	8	0	-1.527560	-1.588658	-1.185712
14	8	0	-2.708456	-1.276716	0.769189
15	6	0	-4.589539	-2.735742	0.482689
16	1	0	-4.953202	-3.646728	-0.005240
17	1	0	-4.783610	-2.820480	1.555396
18	1	0	-5.151186	-1.880725	0.102499
19	6	0	-3.728766	-1.690743	-2.083059
20	1	0	-3.303105	-1.478184	-3.067517
21	1	0	-4.642196	-2.278242	-2.216682
22	1	0	-3.974723	-0.735037	-1.610229
23	6	0	-2.309015	-3.750428	-1.913771
24	1	0	-3.157217	-4.443409	-1.909333
25	1	0	-2.023529	-3.568357	-2.953760
26	1	0	-1.467221	-4.224752	-1.404741
27	6	0	-2.315340	-3.637141	0.992993
28	1	0	-2.472956	-3.502770	2.066468
29	1	0	-2.653538	-4.639559	0.711501
30	1	0	-1.244445	-3.551860	0.795694

31	6	0	-2.527309	2.878273	-0.277222
32	6	0	-2.345927	2.557971	1.240780
33	5	0	-1.317622	0.913062	-0.030541
34	8	0	-2.246545	1.626809	-0.888039
35	8	0	-1.260877	1.636969	1.236681
36	6	0	-1.977475	3.759214	2.102059
37	1	0	-2.755227	4.529243	2.054947
38	1	0	-1.872769	3.444419	3.144403
39	1	0	-1.029963	4.198427	1.781248
40	6	0	-1.517636	3.920859	-0.772760
41	1	0	-1.512547	3.904714	-1.866213
42	1	0	-1.775748	4.931141	-0.438510
43	1	0	-0.507985	3.687643	-0.423037
44	6	0	-3.936586	3.305852	-0.668013
45	1	0	-4.246018	4.201093	-0.117172
46	1	0	-3.968124	3.533501	-1.737489
47	1	0	-4.648789	2.502927	-0.470304
48	6	0	-3.569399	1.845134	1.823675
49	1	0	-3.307872	1.464429	2.814880
50	1	0	-4.428301	2.516978	1.921418
51	1	0	-3.840124	0.988643	1.200022
52	6	0	1.074336	-1.899747	0.142398
53	6	0	2.432169	-1.819744	0.394694
54	6	0	1.880000	-0.705264	2.444461
55	6	0	0.545328	-0.830116	2.087610
56	1	0	0.695237	-2.349389	-0.773178
57	1	0	3.125390	-2.227334	-0.329595
58	1	0	2.129606	-0.218243	3.378154
59	7	0	0.136861	-1.405812	0.954174
60	1	0	-0.242148	-0.411178	2.708904
61	6	0	2.885992	0.949316	-1.567944
62	6	0	2.876802	-1.166403	1.560861
63	7	0	4.217619	-0.952469	1.795320
64	7	0	4.187283	0.781079	-1.954959
65	6	0	4.632649	-0.483189	3.103995
66	1	0	4.352098	-1.176452	3.908745
67	1	0	5.716116	-0.363143	3.110868
68	1	0	4.187218	0.492394	3.320966
69	6	0	5.187780	-1.646794	0.969535
70	1	0	5.060724	-1.369244	-0.082830
71	1	0	6.191145	-1.348276	1.275122
72	1	0	5.106749	-2.739712	1.050619
73	6	0	5.248212	1.356348	-1.149229
74	1	0	6.210560	1.049324	-1.558791

75	1	0	5.209679	2.453721	-1.130214
76	1	0	5.184560	0.989645	-0.118542
77	6	0	4.479254	0.331541	-3.303212
78	1	0	5.558895	0.247547	-3.423424
79	1	0	4.041699	-0.655120	-3.486494
80	1	0	4.097876	1.025572	-4.063243

IntI2

Thermal correction to Energy= 0.737048
Thermal correction to Enthalpy= 0.737992
Thermal correction to Gibbs Free Energy= 0.626179
Sum of electronic and zero-point Energies= -1585.749788
Sum of electronic and thermal Energies= -1585.710999
Sum of electronic and thermal Enthalpies= -1585.710055
Sum of electronic and thermal Free Energies= -1585.821868

Esol = -1586.9958053

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.013940	2.129067	-3.091449
2	6	0	-1.690862	3.374436	-1.146927
3	6	0	-0.926286	1.012501	-2.288402
4	1	0	-0.778636	2.034235	-4.142666
5	6	0	-1.584378	2.203114	-0.424136
6	1	0	-2.000383	4.276774	-0.637081
7	1	0	-0.615657	0.043283	-2.662923
8	1	0	-1.804440	2.143968	0.638033
9	7	0	-1.210915	1.044145	-0.978776
10	6	0	2.427537	-1.277011	-1.356399
11	6	0	2.674560	-1.760864	0.107564
12	5	0	0.861460	-0.316215	0.059322
13	8	0	1.636533	-0.109742	-1.169776
14	8	0	1.436020	-1.464301	0.736662
15	6	0	2.944223	-3.253956	0.243868
16	1	0	3.817808	-3.554867	-0.345256
17	1	0	3.137663	-3.498287	1.292540
18	1	0	2.076888	-3.829340	-0.084446
19	6	0	1.594437	-2.286759	-2.152746
20	1	0	1.305241	-1.823154	-3.101575
21	1	0	2.153811	-3.200989	-2.376376

22	1	0	0.681716	-2.536195	-1.602170
23	6	0	3.691184	-0.910710	-2.124036
24	1	0	4.364185	-1.771229	-2.206735
25	1	0	3.425535	-0.588121	-3.135099
26	1	0	4.224537	-0.092529	-1.635274
27	6	0	3.794573	-0.966215	0.790719
28	1	0	3.742759	-1.150624	1.867719
29	1	0	4.785202	-1.265302	0.432433
30	1	0	3.671859	0.106996	0.618990
31	6	0	-2.684244	-1.757444	-0.110270
32	6	0	-2.436827	-1.284937	1.357338
33	5	0	-0.869772	-0.314923	-0.050960
34	8	0	-1.445401	-1.457235	-0.737085
35	8	0	-1.644782	-0.116990	1.179587
36	6	0	-3.700146	-0.923308	2.127725
37	1	0	-4.373954	-1.783795	2.203938
38	1	0	-3.434185	-0.608623	3.141196
39	1	0	-4.232715	-0.100950	1.645164
40	6	0	-3.803485	-0.956541	-0.787345
41	1	0	-3.751939	-1.132847	-1.865717
42	1	0	-4.794393	-1.257333	-0.431266
43	1	0	-3.679640	0.115207	-0.607466
44	6	0	-2.955227	-3.249210	-0.257898
45	1	0	-3.829068	-3.553816	0.328940
46	1	0	-3.148870	-3.485444	-1.308386
47	1	0	-2.088389	-3.827799	0.066071
48	6	0	-1.604653	-2.301461	2.145998
49	1	0	-1.315200	-1.845414	3.098408
50	1	0	-2.164815	-3.216911	2.362539
51	1	0	-0.692062	-2.547419	1.593640
52	6	0	1.581327	2.197573	0.451804
53	6	0	1.689832	3.363233	1.183403
54	6	0	1.007062	2.105241	3.117727
55	6	0	0.917738	0.994860	2.306332
56	1	0	1.802657	2.145633	-0.610489
57	1	0	2.002443	4.268491	0.680669
58	1	0	0.770141	2.003198	4.167905
59	7	0	1.204178	1.035487	0.997351
60	1	0	0.603997	0.023736	2.673245
61	6	0	-1.403132	3.366765	-2.529900
62	6	0	1.400135	3.346086	2.565886
63	7	0	-1.493402	4.498637	-3.287187
64	7	0	1.492156	4.472086	3.331674
65	6	0	-1.231754	4.435536	-4.711844

66	1	0	-1.926942	3.757509	-5.221838
67	1	0	-1.348617	5.430326	-5.139702
68	1	0	-0.209462	4.096087	-4.913333
69	6	0	-1.948758	5.733769	-2.682407
70	1	0	-1.280286	6.051277	-1.873402
71	1	0	-1.960870	6.517950	-3.438177
72	1	0	-2.961540	5.635209	-2.272495
73	6	0	1.952594	5.710245	2.737007
74	1	0	1.965525	6.488756	3.498603
75	1	0	2.965919	5.611641	2.328415
76	1	0	1.286762	6.035796	1.929037
77	6	0	1.229075	4.398875	4.755602
78	1	0	1.347244	5.390263	5.190935
79	1	0	0.205965	4.059836	4.953520
80	1	0	1.922507	3.715800	5.261241

TSI3

Thermal correction to Energy= 0.734677
Thermal correction to Enthalpy= 0.735621
Thermal correction to Gibbs Free Energy= 0.630626
Sum of electronic and zero-point Energies= -1585.716362
Sum of electronic and thermal Energies= -1585.679028
Sum of electronic and thermal Enthalpies= -1585.678084
Sum of electronic and thermal Free Energies= -1585.783079

Esol = -1586.9564405

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.177998	-2.981601	1.242340
2	6	0	-2.650104	-1.095304	1.243432
3	6	0	-0.112941	-2.143647	1.232589
4	1	0	-0.997388	-4.047293	1.312910
5	6	0	-1.522151	-0.256240	1.173282
6	1	0	-3.620528	-0.613578	1.242553
7	1	0	0.913362	-2.486496	1.270153
8	1	0	-1.588802	0.813162	1.340761
9	7	0	-0.255548	-0.771102	1.225583
10	6	0	2.046542	-1.864699	-2.024024
11	6	0	2.707156	-0.507008	-2.442146
12	5	0	0.934368	-0.104309	-1.078834

13	8	0	0.782910	-1.447995	-1.488051
14	8	0	2.197428	0.406732	-1.460667
15	6	0	4.225611	-0.494283	-2.375422
16	1	0	4.652199	-1.249278	-3.044331
17	1	0	4.597559	0.486521	-2.684452
18	1	0	4.567993	-0.686747	-1.356820
19	6	0	2.825758	-2.576742	-0.919295
20	1	0	2.222267	-3.416292	-0.560450
21	1	0	3.775101	-2.974566	-1.291077
22	1	0	3.015564	-1.896996	-0.083649
23	6	0	1.787202	-2.818639	-3.181844
24	1	0	2.724083	-3.084290	-3.683042
25	1	0	1.331395	-3.736567	-2.800905
26	1	0	1.107111	-2.378122	-3.912897
27	6	0	2.223194	-0.024049	-3.810508
28	1	0	2.554237	1.007945	-3.952996
29	1	0	2.623135	-0.634705	-4.625406
30	1	0	1.129938	-0.043774	-3.860784
31	6	0	2.706951	0.506375	2.442427
32	6	0	2.046567	1.864198	2.024317
33	5	0	0.934064	0.104051	1.079055
34	8	0	2.196845	-0.407402	1.461188
35	8	0	0.782889	1.447751	1.488270
36	6	0	1.787334	2.818105	3.182197
37	1	0	2.724235	3.083534	3.683475
38	1	0	1.331732	3.736150	2.801299
39	1	0	1.107113	2.377669	3.913176
40	6	0	2.223159	0.023630	3.810926
41	1	0	2.554098	-1.008389	3.953468
42	1	0	2.623293	0.634321	4.625703
43	1	0	1.129913	0.043482	3.861355
44	6	0	4.225392	0.493315	2.375392
45	1	0	4.652290	1.248323	3.044089
46	1	0	4.597198	-0.487521	2.684490
47	1	0	4.567581	0.685545	1.356680
48	6	0	2.825925	2.576268	0.919701
49	1	0	2.222671	3.416109	0.561132
50	1	0	3.775410	2.973709	1.291526
51	1	0	3.015486	1.896731	0.083827
52	6	0	-1.521706	0.256689	-1.173876
53	6	0	-2.649392	1.096095	-1.244314
54	6	0	-1.176743	2.981953	-1.242645
55	6	0	-0.111924	2.143702	-1.232689
56	1	0	-1.588615	-0.812682	-1.341434

57	1	0	-3.619957	0.614656	-1.243841
58	1	0	-0.995839	4.047606	-1.313049
59	7	0	-0.254927	0.771186	-1.225767
60	1	0	0.914487	2.486257	-1.269969
61	6	0	-2.516679	-2.468334	1.240444
62	6	0	-2.515571	2.469070	-1.241119
63	7	0	-3.596459	3.362676	-1.306261
64	7	0	-3.597860	-3.361551	1.305544
65	6	0	-3.594681	4.444084	-0.329615
66	1	0	-4.321879	5.201670	-0.633281
67	1	0	-3.858135	4.088747	0.680044
68	1	0	-2.615526	4.918754	-0.276514
69	6	0	-4.905460	2.761734	-1.444896
70	1	0	-5.642200	3.552828	-1.601034
71	1	0	-4.920518	2.100175	-2.314278
72	1	0	-5.206792	2.180262	-0.555537
73	6	0	-4.906759	-2.760584	1.444858
74	1	0	-5.208817	-2.179635	0.555417
75	1	0	-5.643340	-3.551646	1.601974
76	1	0	-4.921181	-2.098551	2.313888
77	6	0	-3.596595	-4.443767	0.329832
78	1	0	-2.616943	-4.917217	0.275224
79	1	0	-4.322308	-5.202012	0.635430
80	1	0	-3.862388	-4.089576	-0.679603

IntI3

Thermal correction to Energy= 0.739456
Thermal correction to Enthalpy= 0.740400
Thermal correction to Gibbs Free Energy= 0.635813
Sum of electronic and zero-point Energies= -1585.786827
Sum of electronic and thermal Energies= -1585.749799
Sum of electronic and thermal Enthalpies= -1585.748855
Sum of electronic and thermal Free Energies= -1585.853443

Esol = -1587.0358582

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.190144	2.844882	-0.132879
2	6	0	-2.213200	0.758465	-0.820533
3	6	0	0.036360	2.325051	-0.310602
4	1	0	-1.305449	3.845986	0.262089

5	6	0	-0.896744	0.093825	-0.516588
6	1	0	-3.021849	0.142374	-1.192073
7	1	0	0.946571	2.893083	-0.150066
8	1	0	-0.742806	-0.778937	-1.159064
9	7	0	0.216750	1.018565	-0.750201
10	6	0	2.498587	1.505292	2.961863
11	6	0	3.355301	0.195766	3.059612
12	5	0	1.437890	-0.211141	1.937930
13	8	0	1.214174	1.005593	2.537364
14	8	0	2.742596	-0.650755	2.066889
15	6	0	4.824569	0.369116	2.714500
16	1	0	5.303526	1.065734	3.410022
17	1	0	5.333109	-0.595609	2.788712
18	1	0	4.947434	0.748053	1.698174
19	6	0	3.001019	2.459977	1.883314
20	1	0	2.263863	3.257641	1.760019
21	1	0	3.954779	2.914205	2.167893
22	1	0	3.119555	1.950595	0.921497
23	6	0	2.320047	2.243019	4.279598
24	1	0	3.289292	2.563495	4.675197
25	1	0	1.705697	3.131890	4.116205
26	1	0	1.823521	1.617148	5.022480
27	6	0	3.200391	-0.511774	4.404325
28	1	0	3.651976	-1.504124	4.332684
29	1	0	3.692682	0.040918	5.209176
30	1	0	2.143188	-0.633961	4.657744
31	6	0	3.486710	0.747696	-2.262941
32	6	0	3.021929	-0.748950	-2.240491
33	5	0	1.445673	0.581383	-1.311445
34	8	0	2.582350	1.367659	-1.327726
35	8	0	1.617824	-0.633192	-1.933094
36	6	0	3.171663	-1.475929	-3.567495
37	1	0	4.222785	-1.504587	-3.872640
38	1	0	2.817412	-2.503995	-3.460146
39	1	0	2.588080	-0.994424	-4.353454
40	6	0	3.255685	1.418378	-3.615772
41	1	0	3.406590	2.494646	-3.503419
42	1	0	3.948736	1.043849	-4.374008
43	1	0	2.231718	1.249858	-3.961911
44	6	0	4.911882	0.979041	-1.790627
45	1	0	5.622368	0.459317	-2.441415
46	1	0	5.138005	2.048102	-1.819049
47	1	0	5.048396	0.623819	-0.767604
48	6	0	3.671568	-1.552510	-1.117472

49	1	0	3.176797	-2.525729	-1.059553
50	1	0	4.735593	-1.718474	-1.310210
51	1	0	3.556946	-1.051753	-0.150381
52	6	0	-0.880259	-0.408303	0.961350
53	6	0	-1.970404	-1.425558	1.173683
54	6	0	-0.342767	-3.125921	0.598511
55	6	0	0.665919	-2.278514	0.863834
56	1	0	-1.033035	0.466484	1.601411
57	1	0	-2.947572	-1.071776	1.476102
58	1	0	-0.135365	-4.116584	0.214907
59	7	0	0.431056	-0.976759	1.291554
60	1	0	1.709840	-2.564038	0.789180
61	6	0	-2.366840	2.070260	-0.540983
62	6	0	-1.720140	-2.723745	0.901588
63	7	0	-3.591374	2.761363	-0.615326
64	7	0	-2.697092	-3.737522	0.890755
65	6	0	-4.756601	1.945688	-0.881258
66	1	0	-4.759255	1.519787	-1.899515
67	1	0	-4.799559	1.122866	-0.163120
68	1	0	-5.653322	2.560471	-0.765999
69	6	0	-3.589231	3.974637	-1.421108
70	1	0	-2.717530	4.586778	-1.191141
71	1	0	-3.575752	3.752396	-2.500676
72	1	0	-4.488012	4.556730	-1.198413
73	6	0	-4.064779	-3.293747	1.052156
74	1	0	-4.282624	-2.508456	0.323773
75	1	0	-4.734862	-4.138258	0.870701
76	1	0	-4.272157	-2.899736	2.062087
77	6	0	-2.411298	-4.907879	1.709020
78	1	0	-3.084850	-5.721020	1.423433
79	1	0	-1.385363	-5.242796	1.557291
80	1	0	-2.548083	-4.703280	2.783582

TSI4

Thermal correction to Energy= 0.734242
Thermal correction to Enthalpy= 0.735186
Thermal correction to Gibbs Free Energy= 0.626211
Sum of electronic and zero-point Energies= -1585.723320
Sum of electronic and thermal Energies= -1585.685360
Sum of electronic and thermal Enthalpies= -1585.684416
Sum of electronic and thermal Free Energies= -1585.793392

Esol = -1586.9686268

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.273459	3.165505	-0.424968
2	6	0	2.724034	1.576625	0.646653
3	6	0	0.195147	2.485413	0.015233
4	1	0	1.119520	4.036933	-1.051904
5	6	0	1.610507	0.827371	1.003958
6	1	0	3.693705	1.167973	0.910015
7	1	0	-0.820293	2.798146	-0.185853
8	1	0	1.670447	-0.057578	1.623002
9	7	0	0.311881	1.330539	0.801354
10	6	0	-2.083346	0.546726	-2.804357
11	6	0	-2.880529	-0.726213	-2.349312
12	5	0	-0.836977	-0.724428	-1.403983
13	8	0	-0.740901	0.252344	-2.366312
14	8	0	-2.128566	-1.177499	-1.203269
15	6	0	-4.313092	-0.457068	-1.921699
16	1	0	-4.898148	-0.068412	-2.761260
17	1	0	-4.774150	-1.389848	-1.585325
18	1	0	-4.348923	0.263267	-1.103132
19	6	0	-2.541907	1.815552	-2.092786
20	1	0	-1.818637	2.607745	-2.303670
21	1	0	-3.523527	2.136253	-2.454334
22	1	0	-2.593169	1.662334	-1.010798
23	6	0	-2.058106	0.769320	-4.309334
24	1	0	-3.073722	0.905330	-4.694693
25	1	0	-1.483571	1.671884	-4.531136
26	1	0	-1.590787	-0.068414	-4.828744
27	6	0	-2.832432	-1.854721	-3.378635
28	1	0	-3.236269	-2.762196	-2.923610
29	1	0	-3.422574	-1.615169	-4.267200
30	1	0	-1.802093	-2.056252	-3.686580
31	6	0	-2.864441	0.752072	2.386464
32	6	0	-2.071474	-0.524980	2.837329
33	5	0	-0.825889	0.739781	1.430482
34	8	0	-2.116156	1.199511	1.236511
35	8	0	-0.729834	-0.237519	2.392277
36	6	0	-2.039520	-0.747749	4.342153
37	1	0	-3.053797	-0.878527	4.732812
38	1	0	-1.468501	-1.653274	4.560946
39	1	0	-1.565174	0.087545	4.859118

40	6	0	-2.805141	1.880283	3.415529
41	1	0	-3.206661	2.789845	2.962627
42	1	0	-3.391859	1.643751	4.307165
43	1	0	-1.772180	2.076483	3.718086
44	6	0	-4.300591	0.490343	1.966343
45	1	0	-4.883250	0.104694	2.808952
46	1	0	-4.758574	1.425501	1.632381
47	1	0	-4.344423	-0.229778	1.147977
48	6	0	-2.540295	-1.791400	2.128160
49	1	0	-1.820046	-2.587331	2.335276
50	1	0	-3.521663	-2.107028	2.494820
51	1	0	-2.596398	-1.637892	1.046453
52	6	0	1.601119	-0.824527	-0.990125
53	6	0	2.712624	-1.579484	-0.638575
54	6	0	1.259494	-3.160852	0.440670
55	6	0	0.182416	-2.475242	0.006039
56	1	0	1.662386	0.060090	-1.609513
57	1	0	3.683001	-1.175829	-0.906996
58	1	0	1.104341	-4.031451	1.068457
59	7	0	0.300996	-1.321016	-0.780755
60	1	0	-0.833558	-2.782736	0.212433
61	6	0	2.612042	2.748701	-0.089831
62	6	0	2.598441	-2.750948	0.098547
63	7	0	3.701533	3.507607	-0.575580
64	7	0	3.686526	-3.515431	0.578663
65	6	0	5.000141	2.883872	-0.445134
66	1	0	5.328544	2.781274	0.604824
67	1	0	4.979216	1.889873	-0.899678
68	1	0	5.740806	3.491393	-0.971869
69	6	0	3.727637	4.889924	-0.114161
70	1	0	2.749217	5.353089	-0.249970
71	1	0	3.997281	4.966600	0.952755
72	1	0	4.457902	5.455112	-0.700637
73	6	0	4.987629	-2.898388	0.441427
74	1	0	4.974183	-1.904281	0.896019
75	1	0	5.727891	-3.509695	0.964333
76	1	0	5.311086	-2.797510	-0.610232
77	6	0	3.703120	-4.897879	0.117194
78	1	0	4.433508	-5.466798	0.699896
79	1	0	2.723050	-5.356000	0.258117
80	1	0	3.966813	-4.975973	-0.951106

IntI4

Thermal correction to Energy= 0.365952
Thermal correction to Enthalpy= 0.366896
Thermal correction to Gibbs Free Energy= 0.301101
Sum of electronic and zero-point Energies= -792.856252
Sum of electronic and thermal Energies= -792.837715
Sum of electronic and thermal Enthalpies= -792.836771
Sum of electronic and thermal Free Energies= -792.902566

Esol = -793.4812021

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.308805	1.026990	-0.204064
2	6	0	3.660858	0.999646	-0.160193
3	6	0	3.589306	-1.292991	0.584916
4	6	0	2.225680	-1.251134	0.549173
5	7	0	1.534993	-0.096966	0.132979
6	1	0	1.740002	1.904649	-0.482564
7	1	0	4.204467	1.907563	-0.399592
8	1	0	4.052267	-2.219682	0.904997
9	1	0	1.597111	-2.087035	0.824321
10	5	0	0.111836	-0.060611	0.072841
11	8	0	-0.685125	-1.116175	0.455783
12	8	0	-0.594459	1.034815	-0.372965
13	6	0	-2.016726	-0.786838	0.007624
14	6	0	-1.973758	0.777118	-0.035905
15	6	0	-3.022859	-1.369594	0.985836
16	1	0	-4.038108	-1.053583	0.725638
17	1	0	-2.982649	-2.460888	0.943810
18	1	0	-2.805587	-1.058605	2.008724
19	6	0	-2.192343	-1.406952	-1.377039
20	1	0	-1.996894	-2.479582	-1.307822
21	1	0	-3.207032	-1.259430	-1.756732
22	1	0	-1.484413	-0.973676	-2.089666
23	6	0	-2.864508	1.409669	-1.091598
24	1	0	-3.913150	1.150758	-0.913519
25	1	0	-2.768283	2.497340	-1.046193
26	1	0	-2.583633	1.082799	-2.093821
27	6	0	-2.229672	1.407308	1.331635
28	1	0	-1.974451	2.468459	1.283056
29	1	0	-3.278292	1.311801	1.626525
30	1	0	-1.605919	0.938069	2.098256

31	6	0	4.377815	-0.175991	0.224851
32	7	0	5.789804	-0.145699	0.268186
33	6	0	6.422549	-1.256087	0.946696
34	1	0	6.323641	-2.212836	0.402600
35	1	0	7.489381	-1.043177	1.056672
36	1	0	5.990276	-1.377010	1.942953
37	6	0	6.434143	0.137516	-1.007968
38	1	0	5.966776	1.000761	-1.484019
39	1	0	7.489684	0.370354	-0.838595
40	1	0	6.369297	-0.715162	-1.705106

Isobutyraldehyde

Thermal correction to Energy= 0.120121
Thermal correction to Enthalpy= 0.121065
Thermal correction to Gibbs Free Energy= 0.084076
Sum of electronic and zero-point Energies= -232.234642
Sum of electronic and thermal Energies= -232.228281
Sum of electronic and thermal Enthalpies= -232.227337
Sum of electronic and thermal Free Energies= -232.264326

Esol= -232.4358346

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.422361	-0.845789	-0.000839
2	6	0	1.109581	-0.833946	-0.012566
3	1	0	1.480217	-0.285627	-0.884188
4	1	0	-0.832709	0.166352	-0.040370
5	1	0	-0.803610	-1.404937	-0.859433
6	1	0	-0.796859	-1.331894	0.906890
7	6	0	1.670104	-2.259993	-0.001822
8	1	0	2.762275	-2.262513	-0.039324
9	1	0	1.357646	-2.790824	0.904389
10	1	0	1.295486	-2.821274	-0.861928
11	6	0	1.606512	-0.102365	1.212766
12	8	0	2.290799	0.889005	1.199928
13	1	0	1.285058	-0.561160	2.177705

TS1

Thermal correction to Energy= 0.496988

Thermal correction to Enthalpy=	0.497932
Thermal correction to Gibbs Free Energy=	0.408984
Sum of electronic and zero-point Energies=	-1214.375561
Sum of electronic and thermal Energies=	-1214.348053
Sum of electronic and thermal Enthalpies=	-1214.347109
Sum of electronic and thermal Free Energies=	-1214.436057

Esol=-1215.2686411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.900116	3.437318	-0.225306
2	1	0	1.588343	4.294991	-0.162416
3	6	0	1.716804	2.228846	0.103601
4	8	0	1.949549	1.343533	-0.721213
5	1	0	2.110457	2.107491	1.125435
6	5	0	2.292535	-0.298850	-0.120688
7	8	0	3.054420	-0.901757	-1.122031
8	8	0	3.017965	-0.134604	1.069806
9	6	0	4.253033	-1.370342	-0.480697
10	6	0	4.393556	-0.384909	0.726473
11	6	0	5.400185	-1.318894	-1.476202
12	1	0	6.346141	-1.574847	-0.987763
13	1	0	5.222227	-2.042184	-2.275943
14	1	0	5.489000	-0.328566	-1.925304
15	6	0	4.000682	-2.807630	-0.026827
16	1	0	3.699831	-3.399039	-0.894907
17	1	0	4.896661	-3.258605	0.409162
18	1	0	3.192264	-2.842203	0.709579
19	6	0	5.098865	-0.963108	1.942240
20	1	0	6.115129	-1.278516	1.684934
21	1	0	5.166120	-0.203064	2.725284
22	1	0	4.552501	-1.818709	2.341824
23	6	0	5.036520	0.941111	0.318855
24	1	0	4.898920	1.662853	1.129512
25	1	0	6.109506	0.826783	0.141127
26	1	0	4.573598	1.339270	-0.588484
27	6	0	0.146918	-0.230344	1.131620
28	6	0	-1.217780	-0.212503	1.163635
29	6	0	-1.239685	-1.107046	-1.071689
30	6	0	0.119232	-1.113274	-1.059554
31	7	0	0.846518	-0.681381	0.029442

32	1	0	0.757366	0.071991	1.974803
33	1	0	-1.695133	0.164087	2.061703
34	1	0	-1.740275	-1.504637	-1.946472
35	1	0	0.716949	-1.459011	-1.895038
36	6	0	-1.996932	-0.643508	0.054749
37	6	0	-3.444347	-0.607429	0.060621
38	6	0	-4.180141	-0.528659	1.266525
39	6	0	-4.186848	-0.645326	-1.142818
40	6	0	-5.560173	-0.483913	1.271787
41	1	0	-3.658830	-0.540204	2.217373
42	6	0	-5.567521	-0.601363	-1.144028
43	1	0	-3.667724	-0.674301	-2.094343
44	6	0	-6.273861	-0.518003	0.064489
45	1	0	-6.102757	-0.434394	2.210022
46	1	0	-6.114994	-0.619475	-2.080527
47	6	0	-7.706345	-0.466377	0.066783
48	7	0	-8.864410	-0.421233	0.069378
49	6	0	0.297790	3.340894	-1.622174
50	1	0	-0.291903	4.233711	-1.841026
51	1	0	1.071811	3.233822	-2.384338
52	1	0	-0.356655	2.465901	-1.684435
53	6	0	-0.168916	3.613507	0.866006
54	1	0	0.275801	3.654041	1.864745
55	1	0	-0.717279	4.543531	0.699995
56	1	0	-0.876882	2.780188	0.836158

Int2

Thermal correction to Energy= 0.498434
Thermal correction to Enthalpy= 0.499378
Thermal correction to Gibbs Free Energy= 0.411669
Sum of electronic and zero-point Energies= -1214.381721
Sum of electronic and thermal Energies= -1214.354114
Sum of electronic and thermal Enthalpies= -1214.353170
Sum of electronic and thermal Free Energies= -1214.440879

Esol= -1215.2748828

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.003582	-1.744582	4.618121
2	1	0	2.998275	-1.676081	5.093480

3	6	0	2.127458	-2.418307	3.291178
4	8	0	2.769883	-1.744769	2.318695
5	1	0	2.062851	-3.501574	3.187194
6	5	0	2.339750	-1.987351	0.960219
7	8	0	3.197121	-1.401083	-0.009779
8	8	0	2.033538	-3.335781	0.581296
9	6	0	3.238527	-2.296423	-1.122056
10	6	0	2.967655	-3.679468	-0.444489
11	6	0	4.596864	-2.176578	-1.796914
12	1	0	4.711332	-2.931628	-2.581958
13	1	0	4.694472	-1.188720	-2.255614
14	1	0	5.401139	-2.294443	-1.069207
15	6	0	2.127127	-1.910322	-2.101812
16	1	0	2.238583	-0.852625	-2.357761
17	1	0	2.175831	-2.496944	-3.024010
18	1	0	1.141594	-2.056518	-1.649106
19	6	0	2.341901	-4.723038	-1.357348
20	1	0	2.993747	-4.935222	-2.211256
21	1	0	2.193355	-5.653513	-0.802657
22	1	0	1.371125	-4.389166	-1.728744
23	6	0	4.221670	-4.242427	0.227428
24	1	0	3.927238	-5.081651	0.863109
25	1	0	4.952697	-4.599070	-0.504500
26	1	0	4.689110	-3.480531	0.857966
27	6	0	-0.227392	-1.796943	1.381631
28	6	0	-1.398242	-1.097968	1.639893
29	6	0	-0.261958	0.913237	0.993857
30	6	0	0.869332	0.153274	0.758883
31	7	0	0.872946	-1.169794	0.950576
32	1	0	-0.132923	-2.871161	1.495020
33	1	0	-2.268085	-1.627301	2.012562
34	1	0	-0.244131	1.979712	0.800806
35	1	0	1.810318	0.565004	0.407796
36	6	0	-1.428893	0.285511	1.451249
37	6	0	-2.656438	1.067125	1.728618
38	6	0	-3.915716	0.549407	1.405245
39	6	0	-2.570325	2.332648	2.320536
40	6	0	-5.067367	1.278089	1.663032
41	1	0	-3.991527	-0.420598	0.923995
42	6	0	-3.716157	3.067340	2.587563
43	1	0	-1.599705	2.730273	2.600058
44	6	0	-4.968421	2.540217	2.257149
45	1	0	-6.042795	0.881978	1.403539
46	1	0	-3.650228	4.042787	3.056518

47	6	0	-6.160319	3.298663	2.532817
48	7	0	-7.117711	3.908600	2.756368
49	6	0	1.482192	-0.314461	4.436963
50	1	0	1.417248	0.205878	5.397447
51	1	0	2.139531	0.251277	3.772756
52	1	0	0.480402	-0.336955	3.987843
53	6	0	1.087196	-2.558601	5.530401
54	1	0	1.468811	-3.574081	5.673419
55	1	0	0.989149	-2.090037	6.513402
56	1	0	0.088481	-2.633683	5.085115

TS2

Thermal correction to Energy= 0.497486
Thermal correction to Enthalpy= 0.498430
Thermal correction to Gibbs Free Energy= 0.408002
Sum of electronic and zero-point Energies= -1214.373765
Sum of electronic and thermal Energies= -1214.346017
Sum of electronic and thermal Enthalpies= -1214.345073
Sum of electronic and thermal Free Energies= -1214.435501

Esol= -1215.2660111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.951472	4.469372	0.954407
2	6	0	1.559327	3.670776	-0.197645
3	1	0	0.600277	5.446692	0.612567
4	1	0	0.108941	3.935153	1.402940
5	1	0	1.699483	4.638650	1.737249
6	1	0	0.789528	3.504902	-0.964537
7	6	0	2.001389	2.330999	0.286511
8	8	0	2.370470	1.454029	-0.690155
9	1	0	2.510435	2.226529	1.244948
10	5	0	2.767864	0.182773	-0.327941
11	8	0	3.174531	-0.719663	-1.290021
12	8	0	3.204421	-0.145809	0.948589
13	6	0	3.745563	-1.838982	-0.591362
14	6	0	4.163987	-1.205211	0.781878
15	6	0	4.904933	-2.380103	-1.414946
16	1	0	5.430348	-3.171525	-0.870507
17	1	0	4.521828	-2.802451	-2.347513

18	1	0	5.614680	-1.590478	-1.665589
19	6	0	2.670173	-2.914394	-0.441995
20	1	0	2.274166	-3.150545	-1.433792
21	1	0	3.083588	-3.829624	-0.008413
22	1	0	1.847273	-2.563027	0.183258
23	6	0	4.075742	-2.148706	1.970635
24	1	0	4.737260	-3.009575	1.829017
25	1	0	4.387021	-1.623516	2.877365
26	1	0	3.055482	-2.507486	2.115463
27	6	0	5.543788	-0.550104	0.727220
28	1	0	5.689196	0.035133	1.638467
29	1	0	6.343029	-1.293214	0.656372
30	1	0	5.615207	0.126664	-0.129275
31	6	0	-0.067957	-0.101759	1.028978
32	6	0	-1.456068	-0.073563	1.099036
33	6	0	-1.498448	-0.755368	-1.194753
34	6	0	-0.109573	-0.752783	-1.168404
35	7	0	0.590675	-0.439991	-0.078951
36	1	0	0.551537	0.159176	1.883495
37	1	0	-1.949234	0.232144	2.015837
38	1	0	-2.026351	-1.045655	-2.096970
39	1	0	0.479444	-1.011117	-2.045417
40	6	0	-2.200035	-0.408400	-0.035844
41	6	0	-3.682677	-0.394190	-0.013011
42	6	0	-4.379887	-0.828464	1.120383
43	6	0	-4.406170	0.053313	-1.124602
44	6	0	-5.766632	-0.819081	1.147020
45	1	0	-3.829090	-1.199615	1.978933
46	6	0	-5.793060	0.069427	-1.108563
47	1	0	-3.875238	0.415353	-1.999393
48	6	0	-6.476802	-0.368454	0.029919
49	1	0	-6.306180	-1.163180	2.022483
50	1	0	-6.352538	0.423952	-1.967185
51	6	0	-7.915833	-0.354736	0.052869
52	7	0	-9.072708	-0.343535	0.072642
53	6	0	2.719999	4.434815	-0.855550
54	1	0	3.501832	4.641445	-0.116615
55	1	0	3.159129	3.841484	-1.661010
56	1	0	2.379113	5.389677	-1.268710

Int3

Thermal correction to Energy= 0.314934

Thermal correction to Enthalpy= 0.315878
Thermal correction to Gibbs Free Energy= 0.254923
Sum of electronic and zero-point Energies= -643.173531
Sum of electronic and thermal Energies= -643.157324
Sum of electronic and thermal Enthalpies= -643.156380
Sum of electronic and thermal Free Energies= -643.217336

Esol= -643.7036558

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.407319	-2.494311	-1.691486
2	6	0	-3.198303	-3.264091	-0.620676
3	1	0	-3.262180	-4.313198	-0.942589
4	1	0	-1.391233	-2.887227	-1.774538
5	1	0	-2.892402	-2.575104	-2.669363
6	1	0	-2.346411	-1.432927	-1.427211
7	6	0	-4.610748	-2.702247	-0.465829
8	1	0	-5.182175	-3.264345	0.277569
9	1	0	-4.571400	-1.655984	-0.142411
10	1	0	-5.150019	-2.736848	-1.416054
11	6	0	-2.492618	-3.239587	0.692555
12	8	0	-1.272419	-3.867849	0.703060
13	1	0	-2.605451	-2.404141	1.381179
14	5	0	-0.387408	-3.658766	1.715852
15	8	0	-0.614083	-2.816912	2.779290
16	8	0	0.833239	-4.281390	1.753151
17	6	0	0.650718	-2.687710	3.462159
18	6	0	1.378109	-4.014951	3.061468
19	6	0	0.395486	-2.525275	4.950937
20	1	0	1.340759	-2.529737	5.502883
21	1	0	-0.104480	-1.571253	5.135561
22	1	0	-0.240599	-3.325257	5.332471
23	6	0	1.338963	-1.447661	2.896336
24	1	0	0.674278	-0.589525	3.020401
25	1	0	2.279743	-1.240118	3.413422
26	1	0	1.546231	-1.571944	1.829344
27	6	0	2.889515	-3.904078	2.953562
28	1	0	3.321968	-3.609490	3.915221
29	1	0	3.307097	-4.873698	2.671510
30	1	0	3.179207	-3.173908	2.196480
31	6	0	0.989192	-5.189488	3.957049

32	1	0	1.353375	-6.113262	3.501852
33	1	0	1.425606	-5.093743	4.954967
34	1	0	-0.098082	-5.260635	4.055684

TS3

Thermal correction to Energy= 0.545020
Thermal correction to Enthalpy= 0.545964
Thermal correction to Gibbs Free Energy= 0.459717
Sum of electronic and zero-point Energies= -1183.438709
Sum of electronic and thermal Energies= -1183.411101
Sum of electronic and thermal Enthalpies= -1183.410157
Sum of electronic and thermal Free Energies= -1183.496405

Esol=-1184.3600389

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.801005	-0.088485	-0.764596
2	6	0	3.824933	0.032830	0.219042
3	6	0	2.515360	0.404823	-0.110879
4	6	0	2.210611	0.664177	-1.450433
5	6	0	3.190013	0.546833	-2.434940
6	6	0	4.485406	0.167532	-2.097118
7	1	0	5.811520	-0.374185	-0.489203
8	1	0	4.075080	-0.151592	1.260583
9	1	0	1.191908	0.930938	-1.711664
10	1	0	2.937415	0.751392	-3.471308
11	1	0	5.246434	0.074008	-2.865388
12	6	0	1.491989	0.584392	0.963138
13	6	0	-0.318802	4.854024	0.559656
14	6	0	-1.345664	3.756737	0.835517
15	1	0	-0.677026	5.814133	0.940543
16	1	0	0.644606	4.645615	1.029861
17	1	0	-0.156058	4.964641	-0.518380
18	1	0	-1.417010	3.591180	1.920661
19	6	0	-0.943158	2.456812	0.206861
20	8	0	-1.803690	1.432722	0.513189
21	1	0	-0.577687	2.462598	-0.821454
22	5	0	-1.795914	0.275282	-0.213622
23	8	0	-2.771739	-0.671029	-0.087165
24	8	0	-0.857564	-0.010202	-1.171371
25	6	0	-2.341887	-1.814498	-0.857276

26	6	0	-1.313418	-1.188262	-1.869890
27	6	0	-3.562244	-2.447141	-1.507696
28	1	0	-3.262975	-3.274905	-2.158477
29	1	0	-4.219739	-2.843706	-0.730347
30	1	0	-4.126763	-1.721465	-2.095308
31	6	0	-1.695313	-2.788227	0.120310
32	1	0	-2.413967	-3.020599	0.910167
33	1	0	-1.402249	-3.718745	-0.374514
34	1	0	-0.814230	-2.343354	0.586745
35	6	0	-0.105280	-2.061178	-2.169837
36	1	0	-0.417584	-3.013766	-2.609794
37	1	0	0.549946	-1.549982	-2.880424
38	1	0	0.470099	-2.254464	-1.261482
39	6	0	-1.965850	-0.703626	-3.161964
40	1	0	-1.235591	-0.117872	-3.726009
41	1	0	-2.296096	-1.540367	-3.783436
42	1	0	-2.827292	-0.064250	-2.947793
43	6	0	0.991135	-0.597426	1.695654
44	6	0	1.604841	-1.855793	1.564648
45	6	0	-0.118430	-0.503848	2.557663
46	6	0	1.165263	-2.951809	2.301300
47	1	0	2.438443	-1.976679	0.881691
48	6	0	-0.556901	-1.600812	3.287914
49	1	0	-0.659639	0.433108	2.638308
50	6	0	0.089283	-2.830979	3.175482
51	1	0	1.666688	-3.907808	2.184802
52	1	0	-1.417134	-1.496152	3.941812
53	1	0	-0.252896	-3.686655	3.748391
54	6	0	1.086827	1.851146	1.252777
55	1	0	1.587146	2.681170	0.766111
56	1	0	0.531785	2.079533	2.157336
57	6	0	-2.737522	4.177047	0.333938
58	1	0	-2.704944	4.385733	-0.741107
59	1	0	-3.467669	3.384404	0.509253
60	1	0	-3.074182	5.084131	0.845091

Int4

Thermal correction to Energy=	0.548575
Thermal correction to Enthalpy=	0.549519
Thermal correction to Gibbs Free Energy=	0.462746
Sum of electronic and zero-point Energies=	-1183.489372
Sum of electronic and thermal Energies=	-1183.462137
Sum of electronic and thermal Enthalpies=	-1183.461192

Sum of electronic and thermal Free Energies= -1183.547965

Esol= -1184.4127396

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.430798	2.881099	1.147027
2	6	0	1.322443	3.377325	-0.141598
3	6	0	2.353490	4.157113	-0.725710
4	6	0	3.491780	4.413859	0.079205
5	6	0	3.584438	3.920147	1.372311
6	6	0	2.562147	3.146245	1.918751
7	1	0	0.617325	2.293111	1.561014
8	1	0	0.416588	3.187788	-0.706723
9	1	0	4.317964	4.997980	-0.313462
10	1	0	4.467717	4.144241	1.964247
11	1	0	2.642229	2.762365	2.930187
12	6	0	2.209198	4.713532	-2.045649
13	6	0	3.078205	6.184842	-5.645746
14	6	0	3.678161	4.944294	-4.983288
15	1	0	2.837180	5.972761	-6.690942
16	1	0	2.157531	6.516217	-5.160541
17	1	0	3.794209	7.015751	-5.632283
18	1	0	2.906988	4.168094	-4.905978
19	6	0	4.189159	5.255036	-3.571012
20	8	0	4.790605	4.062532	-3.065066
21	1	0	4.963109	6.033268	-3.663034
22	5	0	5.898753	4.133708	-2.294949
23	8	0	6.716986	3.054516	-2.074927
24	8	0	6.338477	5.288738	-1.675524
25	6	0	7.659909	3.446346	-1.060751
26	6	0	7.668218	5.009955	-1.190706
27	6	0	8.996747	2.781616	-1.348625
28	1	0	9.758753	3.129047	-0.643489
29	1	0	8.894515	1.699399	-1.237602
30	1	0	9.333211	2.990167	-2.365161
31	6	0	7.103851	2.965268	0.276510
32	1	0	6.951574	1.884820	0.223165
33	1	0	7.787065	3.184915	1.101705
34	1	0	6.135261	3.429505	0.479376
35	6	0	7.878507	5.755266	0.116625
36	1	0	8.844615	5.491543	0.558473

37	1	0	7.868200	6.832206	-0.068815
38	1	0	7.088003	5.523149	0.833123
39	6	0	8.639994	5.509222	-2.257579
40	1	0	8.450543	6.570390	-2.436003
41	1	0	9.680170	5.386920	-1.943925
42	1	0	8.491770	4.970799	-3.198569
43	6	0	1.161272	4.237150	-2.961937
44	6	0	0.984473	2.862896	-3.201616
45	6	0	0.351466	5.138665	-3.670233
46	6	0	0.045093	2.414047	-4.121577
47	1	0	1.621000	2.155789	-2.677637
48	6	0	-0.593007	4.688023	-4.585739
49	1	0	0.450337	6.204535	-3.483697
50	6	0	-0.746943	3.324025	-4.819664
51	1	0	-0.062459	1.349124	-4.302753
52	1	0	-1.212827	5.404622	-5.115631
53	1	0	-1.478275	2.971347	-5.539590
54	6	0	3.143489	5.774013	-2.558049
55	1	0	3.684575	6.242116	-1.732479
56	1	0	2.578839	6.577814	-3.044808
57	6	0	4.829071	4.403485	-5.835054
58	1	0	5.625355	5.153665	-5.922893
59	1	0	5.255884	3.499906	-5.397433
60	1	0	4.480860	4.169665	-6.845088

TS4

Thermal correction to Energy= 0.763514
Thermal correction to Enthalpy= 0.764458
Thermal correction to Gibbs Free Energy= 0.655589
Sum of electronic and zero-point Energies= -1534.476977
Sum of electronic and thermal Energies= -1534.439035
Sum of electronic and thermal Enthalpies= -1534.438090
Sum of electronic and thermal Free Energies= -1534.546960

Esol= -1535.7146854

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.591260	-1.943216	-2.647837
2	6	0	-1.672040	-0.767750	-1.912908
3	6	0	-0.923264	-0.580280	-0.734922

4	6	0	-0.104616	-1.646072	-0.319063
5	6	0	-0.031883	-2.826934	-1.050263
6	6	0	-0.768757	-2.983877	-2.222013
7	1	0	-2.181810	-2.049410	-3.552798
8	1	0	-2.333492	0.026029	-2.247779
9	1	0	0.499299	-1.550739	0.578555
10	1	0	0.609562	-3.631602	-0.703395
11	1	0	-0.706277	-3.905343	-2.791812
12	6	0	0.683578	3.667893	2.186431
13	6	0	1.268574	2.961235	0.963608
14	1	0	0.927337	4.733530	2.158578
15	1	0	-0.405436	3.585298	2.231122
16	1	0	1.098990	3.256575	3.114690
17	1	0	0.725436	3.286990	0.069511
18	6	0	1.151932	1.432133	1.080742
19	8	0	1.690366	0.862382	-0.112070
20	1	0	1.775433	1.131380	1.935490
21	5	0	2.768156	0.049895	-0.064281
22	8	0	3.404042	-0.393463	-1.198522
23	8	0	3.354172	-0.405095	1.101887
24	6	0	4.344888	-1.394452	-0.769662
25	6	0	4.620303	-0.975391	0.712378
26	6	0	5.560251	-1.353998	-1.680653
27	1	0	6.335967	-2.035713	-1.317318
28	1	0	5.271640	-1.667382	-2.686960
29	1	0	5.974172	-0.346264	-1.742371
30	6	0	3.641866	-2.746339	-0.866918
31	1	0	3.244787	-2.864631	-1.877944
32	1	0	4.325014	-3.572796	-0.651250
33	1	0	2.801575	-2.790908	-0.167498
34	6	0	4.959245	-2.120987	1.650850
35	1	0	5.867519	-2.633212	1.317822
36	1	0	5.135285	-1.730562	2.656350
37	1	0	4.144339	-2.844444	1.702191
38	6	0	5.663052	0.135411	0.821481
39	1	0	5.647899	0.533934	1.838834
40	1	0	6.668929	-0.235270	0.605649
41	1	0	5.434039	0.951191	0.128818
42	6	0	-1.349108	1.936717	-0.682507
43	6	0	-0.758768	2.192107	-1.927718
44	6	0	-2.097107	2.958671	-0.082270
45	6	0	-0.913323	3.428287	-2.546954
46	1	0	-0.145875	1.423283	-2.387695
47	6	0	-2.251028	4.195505	-0.700167

48	1	0	-2.562676	2.778610	0.884354
49	6	0	-1.657744	4.435670	-1.937067
50	1	0	-0.438117	3.609088	-3.506219
51	1	0	-2.835247	4.971754	-0.215647
52	1	0	-1.774336	5.400225	-2.420615
53	6	0	-0.259661	0.851434	1.310945
54	1	0	-0.170660	-0.107905	1.831391
55	1	0	-0.793906	1.512924	2.002532
56	6	0	2.744417	3.331316	0.792357
57	1	0	3.333635	2.977312	1.648041
58	1	0	3.159856	2.890465	-0.117138
59	1	0	2.865645	4.416231	0.726754
60	6	0	-1.103727	0.658719	0.058544
61	1	0	-2.336897	0.383271	0.660810
62	6	0	-3.070477	-1.099704	2.153562
63	6	0	-3.484269	-0.012533	1.247777
64	6	0	-4.312759	-0.396833	0.091798
65	6	0	-4.346822	-1.677020	-0.309747
66	6	0	-3.599768	-2.789601	0.371594
67	6	0	-3.093096	-2.371308	1.724759
68	1	0	-3.797089	0.908254	1.750750
69	1	0	-4.921405	-1.945478	-1.195875
70	1	0	-2.728662	-3.041944	-0.260894
71	1	0	-2.755166	-3.166812	2.388270
72	6	0	-5.015046	0.705732	-0.651054
73	1	0	-4.289022	1.432840	-1.035206
74	1	0	-5.590446	0.314961	-1.493587
75	1	0	-5.696349	1.254385	0.009001
76	6	0	-2.631687	-0.724844	3.543921
77	1	0	-2.258443	-1.593491	4.091347
78	1	0	-1.843293	0.034565	3.525540
79	1	0	-3.470335	-0.299896	4.107326
80	6	0	-4.466075	-4.053928	0.478150
81	1	0	-4.801938	-4.379806	-0.510664
82	1	0	-3.904647	-4.875241	0.933295
83	1	0	-5.349203	-3.858903	1.093658

Int5

Thermal correction to Energy=	0.562215
Thermal correction to Enthalpy=	0.563159
Thermal correction to Gibbs Free Energy=	0.476251
Sum of electronic and zero-point Energies=	-1184.112521
Sum of electronic and thermal Energies=	-1184.085254

Sum of electronic and thermal Enthalpies= -1184.084309
Sum of electronic and thermal Free Energies= -1184.171217

Esol= -1185.0489518

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.406634	2.748696	1.177580
2	6	0	1.151944	3.412149	-0.016344
3	6	0	2.033049	4.378761	-0.517277
4	6	0	3.179409	4.664382	0.226798
5	6	0	3.433861	4.007844	1.430427
6	6	0	2.553124	3.046018	1.910386
7	1	0	0.706447	2.001774	1.538684
8	1	0	0.254316	3.174910	-0.581816
9	1	0	3.893118	5.403076	-0.126568
10	1	0	4.328084	4.252972	1.995348
11	1	0	2.755321	2.534542	2.845902
12	6	0	3.141456	6.742174	-5.306797
13	6	0	3.634011	5.460188	-4.634578
14	1	0	3.169731	6.632846	-6.394434
15	1	0	2.111216	6.983802	-5.032175
16	1	0	3.777245	7.596075	-5.042259
17	1	0	2.890452	4.671119	-4.790122
18	6	0	3.845062	5.661469	-3.122166
19	8	0	4.295660	4.424274	-2.570946
20	1	0	4.646786	6.407821	-3.020070
21	5	0	5.548116	4.293875	-2.083161
22	8	0	6.068534	3.074630	-1.722084
23	8	0	6.432242	5.339944	-1.901632
24	6	0	7.304615	3.350384	-1.037806
25	6	0	7.715242	4.733898	-1.641779
26	6	0	8.282958	2.219895	-1.308291
27	1	0	9.263615	2.448590	-0.878589
28	1	0	7.912924	1.299937	-0.848987
29	1	0	8.397435	2.044318	-2.379092
30	6	0	6.983251	3.441590	0.452242
31	1	0	6.465456	2.528887	0.756719
32	1	0	7.888661	3.557164	1.054879
33	1	0	6.318829	4.288744	0.647612
34	6	0	8.509930	5.629536	-0.706733
35	1	0	9.442230	5.139171	-0.409130

36	1	0	8.761851	6.562433	-1.217349
37	1	0	7.937777	5.873974	0.189446
38	6	0	8.423813	4.597440	-2.987954
39	1	0	8.481516	5.583048	-3.456352
40	1	0	9.437803	4.205119	-2.871595
41	1	0	7.864398	3.932888	-3.653723
42	6	0	1.173291	4.214448	-2.917634
43	6	0	1.716690	2.943776	-3.122614
44	6	0	0.241234	4.702135	-3.837213
45	6	0	1.352162	2.193249	-4.236674
46	1	0	2.447536	2.559374	-2.418984
47	6	0	-0.119788	3.956661	-4.955928
48	1	0	-0.197407	5.685815	-3.679693
49	6	0	0.440896	2.698904	-5.161414
50	1	0	1.789962	1.211274	-4.387108
51	1	0	-0.840509	4.355614	-5.662989
52	1	0	0.163741	2.113358	-6.032252
53	6	0	2.643791	6.169835	-2.306540
54	1	0	3.011981	6.746717	-1.451742
55	1	0	2.094708	6.886496	-2.924425
56	6	0	4.956359	5.005920	-5.258312
57	1	0	5.750117	5.737674	-5.059788
58	1	0	5.272381	4.039805	-4.856246
59	1	0	4.857248	4.901284	-6.342374
60	6	0	1.632240	5.124109	-1.787065
61	1	0	0.749336	5.712001	-1.496553

1,3,5-trimethyl-1,4-cyclohexadiene

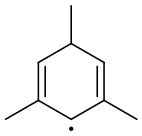
Thermal correction to Energy= 0.217385
Thermal correction to Enthalpy= 0.218329
Thermal correction to Gibbs Free Energy= 0.173125
Sum of electronic and zero-point Energies= -351.001801
Sum of electronic and thermal Energies= -350.991981
Sum of electronic and thermal Enthalpies= -350.991037
Sum of electronic and thermal Free Energies= -351.036240

Esol= -351.3241491

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.478336	-3.083807	-0.050790

2	6	0	-1.077152	-3.437182	0.373414
3	6	0	-0.156642	-2.257963	0.546600
4	6	0	-0.569847	-1.008019	0.338168
5	6	0	-1.967172	-0.621096	-0.060452
6	6	0	-2.853855	-1.820560	-0.249967
7	1	0	-1.114403	-4.011664	1.313267
8	1	0	-0.640328	-4.137268	-0.357169
9	1	0	0.134633	-0.188080	0.478860
10	1	0	-1.914859	-0.076679	-1.016968
11	1	0	-3.880677	-1.615244	-0.553243
12	6	0	1.249227	-2.586907	0.962790
13	1	0	1.728020	-3.247316	0.230107
14	1	0	1.859477	-1.686675	1.064275
15	1	0	1.258125	-3.119568	1.921024
16	6	0	-3.414433	-4.244883	-0.233812
17	1	0	-4.406990	-3.915540	-0.548885
18	1	0	-3.027659	-4.942904	-0.985561
19	1	0	-3.518944	-4.811814	0.698833
20	6	0	-2.576587	0.344454	0.970642
21	1	0	-1.958801	1.240930	1.080565
22	1	0	-3.580226	0.657818	0.667575
23	1	0	-2.648888	-0.146190	1.945218

1,3,5-trimethyl-1,4-cyclohexadiene radical

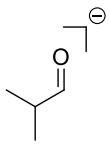


Thermal correction to Energy= 0.203695
Thermal correction to Enthalpy= 0.204639
Thermal correction to Gibbs Free Energy= 0.158675
Sum of electronic and zero-point Energies= -350.382037
Sum of electronic and thermal Energies= -350.372200
Sum of electronic and thermal Enthalpies= -350.371256
Sum of electronic and thermal Free Energies= -350.417220

Esol= -350.6914158

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.467755	-3.070503	0.010505
2	6	0	-1.132401	-3.323330	0.430678

3	6	0	-0.198019	-2.263031	0.593925
4	6	0	-0.584902	-0.980235	0.353573
5	6	0	-1.976058	-0.600182	-0.055350
6	6	0	-2.867156	-1.792212	-0.233147
7	1	0	-0.818412	-4.346064	0.624092
8	1	0	0.129980	-0.169413	0.481289
9	1	0	-1.921744	-0.058470	-1.017605
10	1	0	-3.890095	-1.598544	-0.551129
11	6	0	1.206245	-2.594788	1.031046
12	1	0	1.683179	-3.278581	0.321756
13	1	0	1.822639	-1.696394	1.105835
14	1	0	1.203385	-3.090064	2.007236
15	6	0	-3.409979	-4.236106	-0.152746
16	1	0	-4.390930	-3.908654	-0.503497
17	1	0	-3.013443	-4.959826	-0.871653
18	1	0	-3.545009	-4.762859	0.797262
19	6	0	-2.590517	0.395100	0.955651
20	1	0	-1.965682	1.288430	1.047651
21	1	0	-3.589461	0.705012	0.634778
22	1	0	-2.672118	-0.075217	1.938845

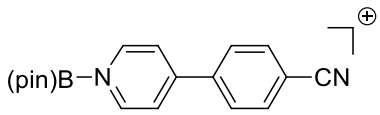


Thermal correction to Energy= 0.116177
Thermal correction to Enthalpy= 0.117121
Thermal correction to Gibbs Free Energy= 0.080047
Sum of electronic and zero-point Energies= -232.180257
Sum of electronic and thermal Energies= -232.173929
Sum of electronic and thermal Enthalpies= -232.172985
Sum of electronic and thermal Free Energies= -232.210059

Esol = -232.4455291

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.481495	-0.914189	0.029711
2	6	0	1.038664	-0.794838	-0.004034
3	1	0	1.326884	-0.287246	-0.943465
4	1	0	-0.934636	0.083587	0.068246

5	1	0	-0.892060	-1.458740	-0.831177
6	1	0	-0.789081	-1.445542	0.940568
7	6	0	1.708022	-2.176887	-0.034933
8	1	0	2.783368	-2.012110	0.085794
9	1	0	1.361631	-2.774089	0.820253
10	1	0	1.520169	-2.753154	-0.956399
11	6	0	1.567280	0.036301	1.164904
12	8	0	2.846935	0.192151	1.270741
13	1	0	0.946459	-0.140211	2.090998

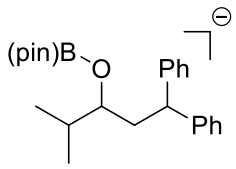


Thermal correction to Energy= 0.378019
Thermal correction to Enthalpy= 0.378964
Thermal correction to Gibbs Free Energy= 0.306909
Sum of electronic and zero-point Energies= -981.942635
Sum of electronic and thermal Energies= -981.921989
Sum of electronic and thermal Enthalpies= -981.921045
Sum of electronic and thermal Free Energies= -981.993099

Esol = -982.6663108

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.308613	1.176440	-0.025872
2	6	0	3.683267	1.203041	-0.028043
3	6	0	3.683325	-1.202825	0.027986
4	6	0	2.308670	-1.176289	0.025824
5	7	0	1.637767	0.000060	-0.000022
6	1	0	1.691482	2.067915	-0.034890
7	1	0	4.190354	2.160410	-0.019439
8	1	0	4.190456	-2.160170	0.019379
9	1	0	1.691580	-2.067793	0.034846
10	5	0	0.133157	0.000023	-0.000019
11	8	0	-0.551874	-1.149754	0.078789
12	8	0	-0.551930	1.149768	-0.078826
13	6	0	-1.949934	-0.762072	-0.189926
14	6	0	-1.949972	0.762017	0.189885
15	6	0	-2.861563	-1.626398	0.658903
16	1	0	-3.897789	-1.293583	0.548858

17	1	0	-2.801065	-2.663822	0.323545
18	1	0	-2.589208	-1.586125	1.714059
19	6	0	-2.178469	-1.012203	-1.674921
20	1	0	-1.962401	-2.059191	-1.897243
21	1	0	-3.216512	-0.809313	-1.948108
22	1	0	-1.529373	-0.384101	-2.292383
23	6	0	-2.861641	1.626298	-0.658946
24	1	0	-3.897851	1.293430	-0.548906
25	1	0	-2.801197	2.663724	-0.323588
26	1	0	-2.589280	1.586039	-1.714101
27	6	0	-2.178523	1.012136	1.674880
28	1	0	-1.962501	2.059134	1.897203
29	1	0	-3.216558	0.809200	1.948063
30	1	0	-1.529401	0.384062	2.292343
31	6	0	4.412200	0.000126	-0.000031
32	6	0	5.884457	0.000160	-0.000036
33	6	0	6.590051	0.992793	-0.694095
34	6	0	6.590103	-0.992439	0.694017
35	6	0	7.976004	0.991169	-0.702972
36	1	0	6.057228	1.748483	-1.262383
37	6	0	7.976057	-0.990748	0.702885
38	1	0	6.057320	-1.748155	1.262308
39	6	0	8.669834	0.000227	-0.000046
40	1	0	8.526415	1.746899	-1.251499
41	1	0	8.526507	-1.746453	1.251409
42	6	0	10.108893	0.000263	-0.000051
43	7	0	11.265168	0.000294	-0.000055



Thermal correction to Energy= 0.546336
Thermal correction to Enthalpy= 0.547281
Thermal correction to Gibbs Free Energy= 0.461425
Sum of electronic and zero-point Energies= -1183.525814
Sum of electronic and thermal Energies= -1183.498530
Sum of electronic and thermal Enthalpies= -1183.497586
Sum of electronic and thermal Free Energies= -1183.583442

Esol = -1184.4918736

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.537652	2.769267	1.141237
2	6	0	1.377834	3.243755	-0.146052
3	6	0	2.370507	4.032547	-0.820339
4	6	0	3.529895	4.293263	-0.016742
5	6	0	3.662333	3.827007	1.284763
6	6	0	2.685711	3.042503	1.894682
7	1	0	0.729951	2.187072	1.583222
8	1	0	0.436492	3.051641	-0.648532
9	1	0	4.338047	4.897303	-0.416387
10	1	0	4.563083	4.088965	1.841261
11	1	0	2.804656	2.669447	2.906755
12	6	0	2.169619	4.602844	-2.112162
13	6	0	3.166338	6.151425	-5.710914
14	6	0	3.712080	4.917065	-4.993198
15	1	0	2.850807	5.889252	-6.725801
16	1	0	2.302969	6.581060	-5.201672
17	1	0	3.942573	6.923908	-5.791721
18	1	0	2.909592	4.176474	-4.890771
19	6	0	4.200831	5.263941	-3.580188
20	8	0	4.891957	4.104042	-3.096816
21	1	0	4.934915	6.084969	-3.673169
22	5	0	5.974451	4.198564	-2.315905
23	8	0	6.831309	3.131739	-2.108822
24	8	0	6.409916	5.353350	-1.680540
25	6	0	7.723761	3.510068	-1.056175
26	6	0	7.708531	5.077530	-1.143796
27	6	0	9.084864	2.878492	-1.313361
28	1	0	9.813986	3.213079	-0.567319
29	1	0	8.995792	1.791285	-1.243494
30	1	0	9.456467	3.127400	-2.308876
31	6	0	7.132364	2.980604	0.248015
32	1	0	7.029737	1.895584	0.166106
33	1	0	7.768117	3.211186	1.108614
34	1	0	6.132835	3.391585	0.411131
35	6	0	7.841867	5.786149	0.195330
36	1	0	8.788013	5.525046	0.681764
37	1	0	7.819407	6.868229	0.040232
38	1	0	7.014751	5.518569	0.855744
39	6	0	8.728044	5.622884	-2.144191
40	1	0	8.528453	6.686043	-2.300373

41	1	0	9.754813	5.505591	-1.784599
42	1	0	8.629615	5.111912	-3.106672
43	6	0	1.080389	4.217900	-2.979988
44	6	0	0.604896	2.878006	-3.082001
45	6	0	0.427120	5.138316	-3.848182
46	6	0	-0.412283	2.509623	-3.947197
47	1	0	1.094227	2.114062	-2.486032
48	6	0	-0.585088	4.762376	-4.719319
49	1	0	0.701422	6.188229	-3.802048
50	6	0	-1.029138	3.441767	-4.786251
51	1	0	-0.715490	1.464783	-3.986453
52	1	0	-1.048096	5.521662	-5.347588
53	1	0	-1.821638	3.147822	-5.467484
54	6	0	3.101673	5.694310	-2.584045
55	1	0	3.611246	6.157515	-1.731601
56	1	0	2.563972	6.525194	-3.062673
57	6	0	4.846746	4.311025	-5.822298
58	1	0	5.685033	5.017661	-5.895711
59	1	0	5.218605	3.389507	-5.372966
60	1	0	4.506061	4.093588	-6.840246

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