

Mild reductive rearrangement of oximes and oxime ethers to secondary amines with hydrosilanes catalyzed by $B(C_6F_5)_3$

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Supporting Information

Table of Contents

1	General Experimental Information	S2
2	Experiment Details for the Reductive Rearrangement of Oximes	S5
2.1	Optimization Study.....	S5
2.2	General Procedure for the Reductive Rearrangement of Oximes.....	S6
2.3	Characterization Data.....	S7
3	Scale-Up Experiment	S19
4	Mechanistic Control Experiments	S20
4.1	Reductive Rearrangement of Hydroxylamine 6aa.....	S20
4.2	Reductive Rearrangement of O-Silylated Hydroxylamine 7de	S20
4.3	² H-Labeling Experiments	S20
5	NMR Spectra.....	S23
6	Computational Data	S86
6.1	Results of the DFT Calculations.....	S86
6.2	Cartesian Coordinates of the Optimized Stationary Point.....	S97
7	References.....	S138

1 General Experimental Information

Reagents and Solvents

Toluene, benzene, fluorobenzene, chlorobenzene, and 1,2-difluorobenzene were purified by distillation over LiAlH_4 and freshly distilled prior to use. CH_2Cl_2 was dried over CaH_2 and freshly distilled prior to use. $\text{B}(\text{C}_6\text{F}_5)_3$ was purchased from Boulder Scientific Company, sublimed under vacuum at 130 °C prior to use, and stored in a nitrogen-filled glovebox.

(*E*)-3,4-Dihydronaphthalen-1(2*H*)-one oxime ((*E*)-**1aa**),^[1] (*E*)-thiochroman-4-one oxime ((*E*)-**1ba**),^[2] (*E*)-2,3-dihydro-1*H*-inden-1-one oxime ((*E*)-**1ca**),^[3] (*E*)-1-phenylethan-1-one oxime ((*E*)-**1da**),^[1] (*E*)-1-([1,1'-biphenyl]-4-yl)ethan-1-one oxime ((*E*)-**1ea**),^[1] (*E/Z*)-1-(*o*-tolyl)ethan-1-one oxime ((*E/Z*)-**1fa**),^[4] (*E*)-1-(*m*-tolyl)ethan-1-one oxime ((*E*)-**1ga**),^[5] (*E*)-1-(*p*-tolyl)ethan-1-one oxime ((*E*)-**1ha**),^[1] (*E*)-1-(4-fluorophenyl)ethan-1-one oxime ((*E*)-**1ia**),^[1] (*E*)-1-(4-chlorophenyl)ethan-1-one oxime ((*E*)-**1ja**),^[1] (*E*)-1-(4-bromophenyl)ethan-1-one oxime ((*E*)-**1ka**),^[1] (*Z*)-1-(4-bromophenyl)ethan-1-one oxime ((*Z*)-**1ka**),^[6] (*E*)-1-(4-iodophenyl)ethan-1-one oxime ((*E*)-**1la**),^[7] (*E*)-1-(4-(trifluoromethyl)phenyl)ethan-1-one oxime ((*E*)-**1ma**),^[1] (*E*)-1-(4-(methylthio)phenyl)ethan-1-one oxime ((*E*)-**1na**),^[6] (*E*)-1-(4-(dimethylamino)phenyl)ethan-1-one oxime ((*E*)-**1pa**),^[8] (*E*)-1-(naphthalen-2-yl)ethan-1-one oxime ((*E*)-**1qa**),^[1] (*E*)-1-phenylbutan-1-one oxime ((*E*)-**1ra**),^[9] (*E*)-1,2-diphenylethan-1-one oxime ((*E*)-**1sa**),^[10] (*E/Z*)-2-methyl-1-phenylpropan-1-one oxime ((*E/Z*)-**S1a**),^[4] (*E/Z*)-cyclohexyl(phenyl)methanone oxime ((*E/Z*)-**S1b**),^[4] (*Z*)-2,2-dimethyl-1-phenylpropan-1-one oxime ((*Z*)-**S1c**),^[11] 4-phenylcyclohexan-1-one oxime (**1wa**),^[3] (*E/Z*)-4-phenylbutan-2-one oxime ((*E/Z*)-**1ya**),^[1] (1*Z*,2*Z*)-1,2-diphenylethane-1,2-dione dioxime ((*Z,Z*)-**4**),^[12] (*E*)-1-phenylethan-1-one *O*-trimethylsilyl oxime ((*E*)-**1db**),^[13] (*E*)-1-phenylethan-1-one *O*-triethylsilyl oxime ((*E*)-**1dc**),^[14] (*E*)-1-phenylethan-1-one *O*-(*tert*-butyldimethylsilyl) oxime ((*E*)-**1dd**),^[14] (*E*)-1-phenylethan-1-one *O*-triisopropylsilyl oxime ((*E*)-**1de**),^[14] (*E*)-1-phenylethan-1-one *O*-methyl oxime ((*E*)-**1df**),^[14] (*E*)-1-phenylethan-1-one *O*-benzyl oxime ((*E*)-**1dg**),^[15] *N*-(1,2,3,4-tetrahydronaphthalen-1-yl)hydroxylamine (**6aa**),^[16] and *N*-(1-phenylethyl)-*O*-(triisopropylsilyl)hydroxylamine (**7de**)^[14] were prepared according to literature procedures.

PhSiD_3 was prepared according to a literature procedure.^[17]

All other reagents were purchased from commercial sources and used as received unless

specified otherwise.

Reactions

All manipulations were carried out in a nitrogen-filled glovebox or under an atmosphere of dry nitrogen using standard Schlenk techniques, unless otherwise stated.

Chromatography

Analytical thin layer chromatography (TLC) was performed on silica gel 60 F254 glass plates by *Merck*. Flash column chromatography was performed on silica gel 60 (40–63 μm , 230–400 mesh, ASTM) by *Grace* using the indicated solvents.

Nuclear Magnetic Resonance (NMR) Spectroscopy

^1H , ^{13}C , and ^{19}F NMR spectra were recorded in CDCl_3 on Bruker AV500 instruments. Chemical shifts are reported in parts per million (ppm) and are referenced to the residual solvent resonance as the internal standard (CHCl_3 : $\delta = 7.26$ ppm for ^1H NMR and CDCl_3 : $\delta = 77.16$ ppm for ^{13}C NMR). Data are reported as follows: chemical shift, multiplicity (br = broad signal, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), and integration.

Gas chromatography (GC)

Gas chromatography (GC) was performed on an *Agilent Technologies* 7820A gas chromatograph equipped with a HP-5 capillary column (30 m $\times$ 0.32 mm, 0.25 μm film thickness) by *Agilent Technologies/CS-Chromatographie Service* using the following program: N_2 carrier gas, injection temperature 250 $^\circ\text{C}$, detector temperature 300 $^\circ\text{C}$, flow rate: 1.7 mL/min; temperature program: start temperature 40 $^\circ\text{C}$, heating rate 10 $^\circ\text{C}/\text{min}$, end temperature 280 $^\circ\text{C}$ for 10 min.

Gas chromatography–mass spectrometry (GC-MS)

Gas chromatography–mass spectrometry (GC-MS) was performed on an *Agilent Technologies* 5975C gas chromatograph equipped with an *Agilent Technologies* HP-5 column (30 m $\times$ 0.32 mm, 0.25 μm film thickness) using the following program: N_2 carrier gas, injection

temperature 280 °C, detector temperature 280 °C, flow rate: 0.8 mL/min; temperature program: start temperature 40 °C, heating rate 10 °C/min, end temperature 280 °C for 10 min.

Infrared Spectroscopy

Infrared (IR) spectra were recorded on an Agilent Technologies Cary 630 FT-IR spectrometer equipped with an ATR unit or a Jasco FT/IR-4100 spectrometer, and the bands are reported in wavenumbers (cm^{-1}).

Mass Spectrometry

High resolution mass spectrometry (HRMS) analysis was performed by the Analytical Facility at the *Institut für Chemie, Technische Universität Berlin*.

Compound Naming

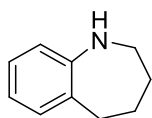
The compound names were generated by the computer program *ChemDraw* according to the guidelines specified by the *International Union of Pure and Applied Chemistry* (IUPAC).

Entry	B(C ₆ F ₅) ₃ [mol%]	Hydrosilane [equiv]	Solvent	T [°C]	Yield [%] ^b
1	10	MePhSiH ₂ (6.0)	1,2-C ₆ H ₄ F ₂	120	66
2	10	PhSiH ₃ (6.0)	1,2-C ₆ H ₄ F ₂	120	57
3	10	Et ₂ SiH ₂ (6.0)	1,2-C ₆ H ₄ F ₂	120	0
4	10	Me ₂ PhSiH (6.0)	1,2-C ₆ H ₄ F ₂	120	0
5	10	Et ₃ SiH (6.0)	1,2-C ₆ H ₄ F ₂	120	0
6	10	(EtO) ₃ SiH (6.0)	1,2-C ₆ H ₄ F ₂	120	0
7	10	Ph ₃ SiH (6.0)	1,2-C ₆ H ₄ F ₂	120	0
8	10	<i>i</i> Pr ₃ SiH (6.0)	1,2-C ₆ H ₄ F ₂	120	0
9	10	MePhSiH ₂ (6.0)	toluene	RT	70
10	10	MePhSiH ₂ (6.0)	benzene	RT	63
11	10	MePhSiH ₂ (6.0)	C ₆ H ₅ F	RT	55
12	10	MePhSiH ₂ (6.0)	C ₆ H ₅ Cl	RT	57
13	10	MePhSiH ₂ (6.0)	CH ₂ Cl ₂	RT	48
14	10	MePhSiH ₂ (6.0)	neat	RT	51
15	10	PhSiH ₃ (6.0)	toluene	RT	85
16	10	PhSiH ₃ (4.0)	toluene	RT	93
17	10	PhSiH ₃ (4.0)	1,2-C ₆ H ₄ F ₂	RT	40
18	10	PhSiH ₃ (4.0)	C ₆ H ₅ F	RT	64
19	10	PhSiH ₃ (4.0)	C ₆ H ₅ Cl	RT	69
20	10	PhSiH ₃ (4.0)	CH ₂ Cl ₂	RT	66
21	10	PhSiH ₃ (4.0)	benzene	RT	88
22	10	PhSiH ₃ (4.0)	toluene- <i>d</i> ₈	RT	95 (88)
23	10	MePhSiH ₂ (4.0)	toluene- <i>d</i> ₈	RT	95
24	10	Ph ₂ SiH ₂ (4.0)	toluene- <i>d</i> ₈	RT	77
25	10	Et ₂ SiH ₂ (4.0)	toluene- <i>d</i> ₈	RT	0
26	10	Me ₂ PhSiH (4.0)	toluene- <i>d</i> ₈	RT	0
27 ^c	10	PhSiH ₃ (4.0)	toluene- <i>d</i> ₈	RT	67
28	10	PhSiH ₃ (2.0)	toluene- <i>d</i> ₈	RT	80
29	5.0	PhSiH ₃ (4.0)	toluene- <i>d</i> ₈	RT	78

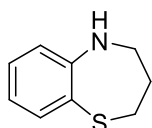
^a All reactions were performed on a 0.10 mmol scale in a GC vial. ^b Yields determined by ¹H NMR spectroscopy using mesitylene as an internal standard; isolated yield in parenthesis. ^c 8 h.

2.2 General Procedure for the Reductive Rearrangement of Oximes: In a nitrogen-filled glovebox, a 2-mL GC vial or a dried 1-mL sealed tube equipped with a magnetic stir bar was charged with the desired amount of oxime, hydrosilane, toluene-*d*₈, and B(C₆F₅)₃. The GC vial or sealed tube was fitted with a cap and the reaction stirred at RT for 20 h in the glove box or 120 °C for 20 h in a preheated oil bath. After that, mesitylene (0.500 equiv) was added as an internal standard, and the yield was determined by ¹H NMR spectroscopy. The generated *N*-silylated products were rapidly converted into their N–H form upon exposure of the reaction mixture to air. Methyl *tert*-butyl ether (2 mL) was added to the residue, and the mixture was transferred to a 10-mL sample bottle by pipette. 1 M aqueous HCl solution (4 mL) was added, and the mixture was stirred at RT for 12 h. The organic layer was extracted with 4 × 10 mL of 1 M aqueous HCl solution. To the combined aqueous phases was added NaOH (10.0 g), and the mixture was stirred at RT for 4 h. The product was extracted into 4 × 15 mL of methyl *tert*-butyl ether. Removal of the solvent under reduced pressure yielded the crude amine. Further purification by flash column chromatography on silica gel with methyl *tert*-butyl ether : cyclohexane = 1 : 20 for arylamines or MeOH : *tert*-butyl ether = 1 : 10 for alkylamines as the eluent gave the corresponding amines.

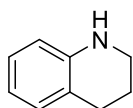
2.3 Characterization Data



2,3,4,5-Tetrahydro-1H-benzo[b]azepine (2a). The general procedure was followed with (*E*)-3,4-dihydronaphthalen-1(2*H*)-one oxime ((*E*)-**1aa**, 32.2 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (25.9 mg, 88% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.12 (d, *J* = 7.4 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 7.4 Hz, 1H), 6.75 (d, *J* = 7.8 Hz, 1H), 3.67 (br, 1H), 3.06 (t, *J* = 5.4 Hz, 2H), 2.79 (t, *J* = 5.6 Hz, 2H), 1.84 – 1.80 (m, 2H), 1.69 – 1.64 (m, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 150.5, 133.9, 130.9, 126.7, 121.0, 119.5, 49.0, 36.2, 32.1, 27.0 ppm. Spectral data is in agreement with published data.^[18]

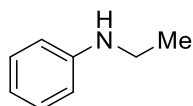


2,3,4,5-Tetrahydrobenzo[b][1,4]thiazepine (2b). The general procedure was followed with (*E*)-thiochroman-4-one oxime ((*E*)-**1ba**, 35.8 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (31.5 mg, 95% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.39 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.06 (dd, *J* = 7.6, 1.5 Hz, 1H), 6.80 (td, *J* = 7.5, 1.2 Hz, 1H), 6.73 (dd, *J* = 7.9, 1.0 Hz, 1H), 3.81 (br, 1H), 3.29 – 3.27 (m, 2H), 2.86 – 2.83 (m, 2H), 2.10 – 2.06 (m, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 151.8, 133.0, 127.9, 125.2, 121.0, 120.1, 47.3, 33.1, 31.9 ppm. Spectral data is in agreement with published data.^[19]



1,2,3,4-Tetrahydroquinoline (2c). The general procedure was followed with (*E*)-2,3-dihydro-1*H*-inden-1-one oxime ((*E*)-**1ca**, 29.4 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (22.4 mg, 84% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.00 – 6.96 (m, 2H), 6.63 (t, *J* = 7.4 Hz, 1H), 6.49 (d, *J* = 7.9 Hz, 1H), 3.76 (br, 1H), 3.32 (t, *J* = 5.5 Hz, 2H), 2.79 (t, *J* = 6.5 Hz, 2H), 1.99 – 1.94 (m, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 144.9, 129.6, 126.8, 121.6, 117.1, 114.3, 42.1, 27.1, 22.3 ppm. Spectral data is in agreement with

published data.^[18]



N-Ethylaniline (2d). The general procedure was followed with (*E*)-1-phenylethan-1-one oxime ((*E*)-**1da**, 27.0 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (16.0 mg, 66% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.21 (t, *J* = 7.4 Hz, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.64 (d, *J* = 7.9 Hz, 2H), 3.49 (br, 1H), 3.18 (q, *J* = 7.2 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.6, 129.3, 117.3, 112.9, 38.6, 15.0 ppm. Spectral data is in agreement with published data.^[20]

The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-trimethylsilyl oxime ((*E*)-**1db**, 41.5 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 99% yield of **2d** was determined by ¹H NMR spectroscopy.

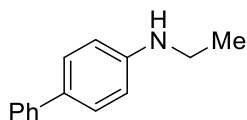
The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-triethylsilyl oxime ((*E*)-**1dc**, 49.9 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and an 89% yield of **2d** was determined by ¹H NMR spectroscopy.

The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-(*tert*-butyldimethylsilyl) oxime ((*E*)-**1dd**, 49.9 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 98% yield of **2d** was determined by ¹H NMR spectroscopy.

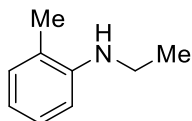
The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-triisopropylsilyl oxime ((*E*)-**1de**, 58.3 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 99% yield of **2d** was determined by ¹H NMR spectroscopy.

The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-methyl oxime ((*E*)-**1df**, 29.8 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and an 85% yield of **2d** was determined by ¹H NMR spectroscopy.

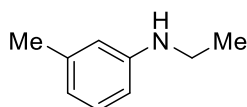
The general procedure was followed with (*E*)-1-phenylethan-1-one *O*-benzyl oxime ((*E*)-**1dg**, 45.0 mg, 0.200 mmol), PhSiH₃ (49.4 μ L, 0.400 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (2.60 mg, 5.00 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 38% yield of **2d** was determined by ¹H NMR spectroscopy.



N-Ethyl-[1,1'-biphenyl]-4-amine (2e). The general procedure was followed with (*E*)-1-([1,1'-biphenyl]-4-yl)ethan-1-one oxime ((*E*)-**1ea**, 42.2 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (36.1 mg, 92% yield). ¹H NMR (500 MHz, CDCl₃): δ 7.58 (dd, *J* = 8.3, 1.0 Hz, 2H), 7.48 (dd, *J* = 8.7, 0.9 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.29 (td, *J* = 7.5, 0.9 Hz, 1H), 6.71 (d, *J* = 8.5 Hz, 2H), 3.41 (br, 1H), 3.23 (q, *J* = 7.2 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H) ppm. ¹³C NMR (125 MHz, CDCl₃): δ 148.0, 141.4, 130.2, 128.7, 128.0, 126.4, 126.1, 113.1, 38.6, 15.0 ppm. Spectral data is in agreement with published data.^[21]

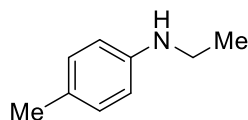


N-Ethyl-2-methylaniline (2f). The general procedure was followed with (*E/Z*)-1-(*o*-tolyl)ethan-1-one oxime (75 : 25 *E/Z* mixture of isomers) ((*E/Z*)-**1fa**, 29.8 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (15.6 mg, 59% yield). ¹H NMR (500 MHz, CDCl₃): δ 7.15 (t, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 7.3 Hz, 1H), 6.67 (t, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 8.1 Hz, 1H), 3.36 (br, 1H), 3.22 (q, *J* = 7.2 Hz, 2H), 2.16 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H) ppm. ¹³C NMR (125 MHz, CDCl₃): δ 146.5, 130.1, 127.3, 121.8, 116.9, 109.8, 38.6, 17.6, 15.1 ppm. Spectral data is in agreement with published data.^[20]



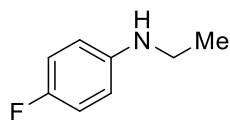
N-Ethyl-3-methylaniline (2g). The general procedure was followed with (*E*)-1-(*m*-tolyl)ethan-1-one oxime ((*E*)-**1ga**, 29.8 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a

colorless liquid (19.6 mg, 73% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.08 (t, *J* = 7.8 Hz, 1H), 6.55 (d, *J* = 7.3 Hz, 1H), 6.45 (d, *J* = 7.6 Hz, 2H), 3.46 (br, 1H), 3.17 (q, *J* = 7.2 Hz, 2H), 2.30 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.6, 139.1, 129.2, 118.3, 113.7, 110.0, 38.6, 21.7, 15.1 ppm. Spectral data is in agreement with published data.^[20]

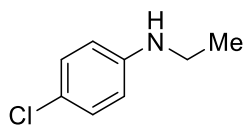


N-Ethyl-4-methylaniline (2h). The general procedure was followed with (*E*)-1-(*p*-tolyl)ethan-1-one oxime ((*E*)-**1ha**, 29.8 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (23.4 mg, 87% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.00 (d, *J* = 7.8 Hz, 2H), 6.57 (d, *J* = 7.5 Hz, 2H), 3.27 (br, 1H), 3.15 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 146.2, 129.8, 126.8, 113.3, 39.1, 20.5, 15.0 ppm. Spectral data is in agreement with published data.^[22]

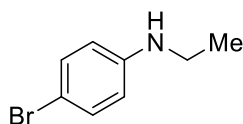
The general procedure was followed with (*E*)-1-(4-(trifluoromethyl)phenyl)ethan-1-one oxime ((*E*)-**1ma**, 40.6 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (20.7 mg, 77% yield).



N-Ethyl-4-fluoroaniline (2i). The general procedure was followed with (*E*)-1-(4-fluorophenyl)ethan-1-one oxime ((*E*)-**1ia**, 30.6 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (25.0 mg, 90% yield). **¹H NMR** (500 MHz, CDCl₃): δ 6.91 – 6.86 (m, 2H), 6.56 – 6.52 (m, 2H), 3.13 (q, *J* = 7.1 Hz, 2H), 3.04 (br, 1H), 1.25 (t, *J* = 7.3 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 155.9 (d, *J* = 233.1 Hz), 144.9, 115.7 (d, *J* = 22.2 Hz), 113.7 (d, *J* = 7.2 Hz), 39.3, 15.0 ppm. **¹⁹F NMR** (471 MHz, CDCl₃): δ –128.3 ppm. Spectral data is in agreement with published data.^[20]

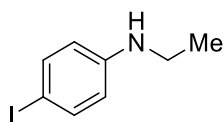


4-Chloro-N-ethylaniline (2j). The general procedure was followed with (*E*)-1-(4-chlorophenyl)ethan-1-one oxime ((*E*)-**1ja**, 34.0 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (27.8 mg, 90% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.12 (d, *J* = 8.5 Hz, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 3.31 (br, 1H), 3.13 (q, *J* = 7.1 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 146.9, 129.1, 122.1, 114.1, 38.9, 14.8 ppm. Spectral data is in agreement with published data.^[22]



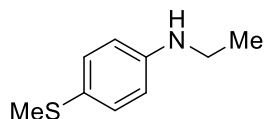
4-Bromo-N-ethylaniline (2k). The general procedure was followed with (*E*)-1-(4-bromophenyl)ethan-1-one oxime ((*E*)-**1ka**, 42.8 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (39.0 mg, 98% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.24 (d, *J* = 8.6 Hz, 2H), 6.48 (d, *J* = 8.7 Hz, 2H), 3.22 (br, 1H), 3.12 (q, *J* = 7.1 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 147.4, 132.0, 114.5, 109.0, 38.7, 14.8 ppm. Spectral data is in agreement with published data.^[20]

The general procedure was followed with (*Z*)-1-(4-bromophenyl)ethan-1-one oxime ((*Z*)-**1ka**, 42.8 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 93% yield of **2k** was determined by ¹H NMR spectroscopy.

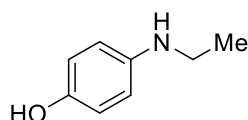


N-Ethyl-4-iodoaniline (2l). The general procedure was followed with (*E*)-1-(4-iodophenyl)ethan-1-one oxime ((*E*)-**1la**, 52.2 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a white solid (28.0 mg, 57% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.41 (d, *J* =

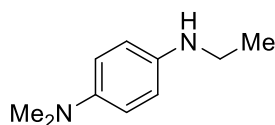
8.8 Hz, 2H), 6.39 (d, J = 8.7 Hz, 2H), 3.46 (br, 1H), 3.12 (q, J = 7.2 Hz, 2H), 1.24 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 148.0, 137.9, 115.1, 77.8, 38.5, 14.8 ppm. Spectral data is in agreement with published data.^[23]



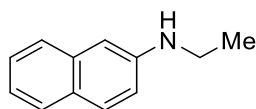
N-Ethyl-4-(methylthio)aniline (2n). The general procedure was followed with (*E*)-1-(4-(methylthio)phenyl)ethan-1-one oxime ((*E*)-**1na**, 36.2 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (28.7 mg, 86% yield). ^1H NMR (500 MHz, CDCl_3): δ 7.24 – 7.21 (m, 2H), 6.57 – 6.54 (m, 2H), 3.58 (br, 1H), 3.14 (q, J = 7.2 Hz, 2H), 2.41 (s, 3H), 1.25 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 147.5, 131.8, 124.0, 113.4, 38.6, 19.4, 14.9 ppm. Spectral data is in agreement with published data.^[20]



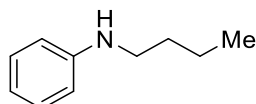
4-(Ethylamino)phenol (2o). The general procedure was followed with (*E*)-1-(4-hydroxyphenyl)ethan-1-one oxime ((*E*)-**1oa**, 30.2 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (14.0 mg, 51% yield). ^1H NMR (500 MHz, CDCl_3): δ 6.69 (d, J = 8.6 Hz, 2H), 6.55 (d, J = 8.6 Hz, 2H), 3.74 (br, 2H), 3.10 (q, J = 7.1 Hz, 2H), 1.24 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 148.1, 142.6, 116.4, 114.8, 39.8, 15.1 ppm. Spectral data is in agreement with published data.^[20]



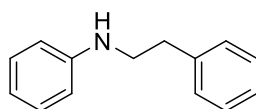
N¹-Ethyl-N⁴,N⁴-dimethylbenzene-1,4-diamine (2p). The general procedure was followed with (*E*)-1-(4-(dimethylamino)phenyl)ethan-1-one oxime ((*E*)-**1pa**, 35.6 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at RT for 20 h. A trace amount of amine product **2p** was detected by GC-MS and a 64% of 4-ethyl-*N,N*-dimethylaniline was formed. The crude NMR is in agreement with published data.^[24]



N-Ethyl-1-naphthalen-2-amine (2q). The general procedure was followed with (*E*)-1-(naphthalen-2-yl)ethan-1-one oxime ((*E*)-**1qa**, 37.0 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (32.2 mg, 94% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.68 (d, *J* = 8.2 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.88 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.81 (d, *J* = 2.1 Hz, 1H), 3.73 (br, 1H), 3.28 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 146.2, 135.4, 129.0, 127.8, 127.6, 126.4, 126.0, 122.0, 118.1, 104.4, 38.7, 14.9 ppm. Spectral data is in agreement with published data.^[25]

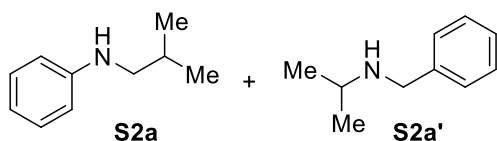


N-Butylaniline (2r). The general procedure was followed with (*E*)-1-phenylbutan-1-one oxime ((*E*)-**1ra**, 32.6 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (23.7 mg, 80% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.20 (t, *J* = 7.6 Hz, 2H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.63 (d, *J* = 8.5 Hz, 2H), 3.57 (br, 1H), 3.14 (t, *J* = 7.2 Hz, 2H), 1.66 – 1.60 (m, 2H), 1.50 – 1.43 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.7, 129.3, 117.2, 112.8, 43.8, 31.8, 20.4, 14.0 ppm. Spectral data is in agreement with published data.^[26]

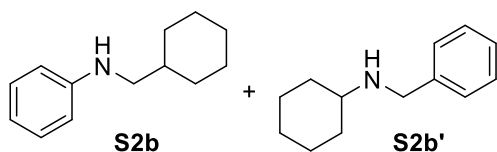


N-Phenethyl-aniline (2s). The general procedure was followed with (*E*)-1,2-diphenylethan-1-one oxime ((*E*)-**1sa**, 42.2 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (34.4 mg, 87% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.33 (t, *J* = 7.8 Hz, 2H), 7.25 (t, *J* = 7.5 Hz, 3H), 7.19 (t, *J* = 7.6 Hz, 2H), 6.72 (t, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 8.2 Hz, 2H), 3.72 (br, 1H), 3.41 (t, *J* = 7.1 Hz, 2H), 2.93 (t, *J* = 7.1 Hz, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.1, 139.4, 129.4, 128.9, 128.7, 126.6, 117.6, 113.2, 45.2, 35.6 ppm. Spectral

data is in agreement with published data.^[20]



N-Isobutylaniline (S2a) + N-benzylpropan-2-amine (S2a'). The general procedure was followed with (*E/Z*)-2-methyl-1-phenylpropan-1-one oxime (40 : 60 *E/Z* mixture of isomers) ((*E/Z*)-**S1a**, 32.6 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at 120 °C for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and an 82% yield of **S2a** and **S2a'** with a ratio of 45 : 55 was determined by ¹H NMR spectroscopy. After work-up, the amine products **S2a** and **S2a'** were afforded as a colorless liquid (19.2 mg, 66% yield, **S2a** : **S2a'** = 58 : 42). Amines **S2a** and **S2a'** can be further isolated by flash column chromatography on silica gel. *NMR data of S2a*: **¹H NMR** (500 MHz, CDCl₃): δ 7.18 (t, *J* = 8.4 Hz, 2H), 6.69 (t, *J* = 7.3 Hz, 1H), 6.61 (d, *J* = 7.8 Hz, 2H), 3.69 (br, 1H), 2.94 (d, *J* = 6.8 Hz, 2H), 1.94 – 1.86 (m, 1H), 1.00 (d, *J* = 6.7 Hz, 6H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.7, 129.4, 117.1, 112.8, 52.0, 28.2, 20.6 ppm. Spectral data is in agreement with published data.^[21] *NMR data of S2a'*: **¹H NMR** (500 MHz, CDCl₃): δ 7.34 – 7.30 (m, 4H), 7.26 – 7.22 (m, 1H), 3.69 (s, 2H), 2.90 – 2.82 (m, 1H), 1.53 (br, 1H), 1.10 (d, *J* = 6.2 Hz, 6H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 140.9, 128.5, 128.3, 127.0, 51.8, 48.2, 23.1 ppm. Spectral data is in agreement with published data.^[27]



N-(Cyclohexylmethyl)aniline (S2b) + N-benzylcyclohexanamine (S2b'). The general procedure was followed with (*E/Z*)-cyclohexyl(phenyl)methanone oxime (27 : 73 *E/Z* mixture of isomers) ((*E/Z*)-**S1b**, 40.6 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at 120 °C for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 92% yield of **S2b** and **S2b'** with a ratio of 32 : 68 was determined by ¹H NMR spectroscopy. After work-up, the amine products **S2b** and **S2b'** were afforded as a colorless liquid (30.1 mg, 80% yield, **S2b** : **S2b'** = 40 : 60). Amines **S2b** and **S2b'** can be further isolated by flash column chromatography on silica gel. *NMR data of S2b*: **¹H NMR** (500 MHz, CDCl₃): δ 7.17 (t, *J* = 8.3 Hz, 2H), 6.68 (t, *J* = 7.3 Hz, 1H), 6.60 (d, *J*

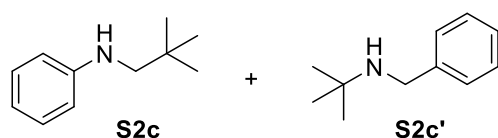
= 7.8 Hz, 2H), 3.70 (br, 1H), 2.96 (d, J = 6.7 Hz, 2H), 1.83 (d, J = 13.2 Hz, 2H), 1.77 – 1.74 (m, 2H), 1.71 – 1.69 (m, 1H), 1.63 – 1.55 (m, 1H), 1.31 – 1.17 (m, 3H), 1.03 – 0.95 (m, 2H) ppm.

¹³C NMR (125 MHz, CDCl₃): δ 148.8, 129.3, 117.0, 112.8, 50.7, 37.7, 31.5, 26.7, 26.1 ppm.

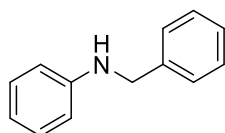
Spectral data is in agreement with published data.^[20] **NMR data of S2b'**: **¹H NMR** (500 MHz, CDCl₃): δ 7.34 – 7.30 (m, 4H), 7.25 – 7.21 (m, 1H), 3.81 (s, 2H), 2.52 – 2.46 (m, 1H), 1.93 – 1.90 (m, 2H), 1.75 – 1.72 (m, 2H), 1.63 – 1.60 (m, 1H), 1.46 (br, 1H), 1.30 – 1.09 (m, 5H) ppm.

¹³C NMR (125 MHz, CDCl₃): δ 141.1, 128.5, 128.2, 126.9, 56.3, 51.2, 33.7, 26.3, 25.2 ppm.

Spectral data is in agreement with published data.^[28]

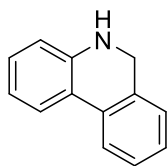


N-Neopentylaniline (S2c) + N-benzyl-2-methylpropan-2-amine (S2c'). The general procedure was followed with (Z)-2,2-dimethyl-1-phenylpropan-1-one oxime ((Z)-**S1c**, 35.4 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at 120 °C for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and a 65% yield of **S2c** and **S2c'** with a ratio of 2 : 98 was determined by ¹H NMR spectroscopy. After work-up, the amine products **S2c** and **S2c'** were afforded as a colorless liquid (19.9 mg, 61% yield, **S2c** : **S2c'** = 2 : 98). Amines **S2c'** can be further isolated by flash column chromatography on silica gel. However, it is difficult to characterize **S2c** by NMR due to its low concentration and the crude spectral data of **S2c** is in agreement with published data.^[29] **NMR data of S2c'**: **¹H NMR** (500 MHz, CDCl₃): δ 7.35 – 7.29 (m, 4H), 7.25 – 7.21 (m, 1H), 3.73 (s, 2H), 1.29 (br, 1H), 1.18 (s, 9H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 141.6, 128.5, 128.4, 126.9, 50.8, 47.4, 29.3 ppm. Spectral data is in agreement with published data.^[30]



N-Benzylaniline (2t). The general procedure was followed with diphenylmethanone oxime (**1ta**, 39.4 mg, 0.200 mmol), PhSiH₃ (98.8 μL, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a colorless liquid (35.7 mg, 98% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.40 – 7.35 (m, 4H), 7.30 (t, J = 7.0 Hz, 1H), 7.20 (t, J = 7.5 Hz, 2H), 6.74 (t, J = 7.4 Hz, 1H), 6.67 (d, J = 7.7 Hz, 2H), 4.35 (s, 2H),

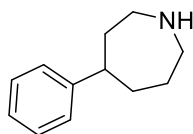
3.79 (br, 1H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 148.2, 139.5, 129.4, 128.8, 127.7, 127.4, 117.8, 113.1, 48.5 ppm. Spectral data is in agreement with published data.^[20]



5,6-Dihydrophenanthridine (2u). The general procedure was followed with 9H-fluoren-9-one oxime (**1ua**, 39.0 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a white solid (32.6 mg, 90% yield). ^1H NMR (500 MHz, CDCl_3): δ 7.72 – 7.69 (m, 2H), 7.33 (t, J = 7.8 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.14 – 7.11 (m, 2H), 6.88 – 6.84 (m, 1H), 6.68 (d, J = 7.9 Hz, 1H), 4.40 (s, 2H), 3.71 (br, 1H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 145.8, 132.9, 132.2, 128.9, 127.8, 127.2, 126.1, 123.7, 122.5, 122.2, 119.4, 115.2, 46.5 ppm. Spectral data is in agreement with published data.^[31]

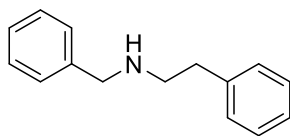


Azepane (2v). The general procedure was followed with cyclohexanone oxime (**1va**, 22.6 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at 120 °C for 20 h. Mesitylene (0.500 equiv) was added as an internal standard and an 80% yield of **2v** was determined by ^1H NMR spectroscopy. The crude spectral data is in agreement with published data.^[32]

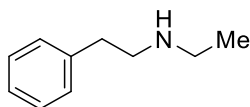


4-Phenylazepane (2w). The general procedure was followed with 4-phenylcyclohexan-1-one oxime (**1wa**, 37.9 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol) at 120 °C for 20 h. The amine product was afforded as a light brown liquid (23.8 mg, 68% yield). ^1H NMR (500 MHz, CDCl_3): δ 7.28 (t, J = 7.6 Hz, 2H), 7.21 – 7.16 (m, 3H), 4.38 (br, 1H), 3.27 – 3.19 (m, 2H), 3.09 – 2.97 (m, 2H), 2.82 – 2.77 (m, 1H), 2.06 – 1.92 (m, 4H), 1.88 – 1.78 (m, 2H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ 148.1, 128.7, 126.8, 126.2, 47.6, 46.5, 46.0, 37.1, 35.2, 27.6 ppm. Spectral data is in agreement with

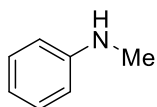
published data.^[33]



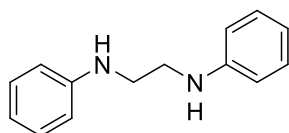
N-Benzyl-2-phenylethan-1-amine (2x). The general procedure was followed with 1,3-diphenylpropan-2-one oxime (**1xa**, 45.0 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at 120 °C for 20 h. The amine product was afforded as a light brown liquid (34.3 mg, 81% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.37 – 7.32 (m, 6H), 7.30 – 7.23 (m, 4H), 3.85 (s, 2H), 2.96 (t, *J* = 6.8 Hz, 2H), 2.88 (t, *J* = 6.8 Hz, 2H), 1.56 (br, 1H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 140.4, 140.2, 128.9, 128.6, 128.5, 128.2, 127.0, 126.3, 54.0, 50.7, 36.5 ppm. Spectral data is in agreement with published data.^[34]



N-Ethyl-2-phenylethan-1-amine (2y). The general procedure was followed with (*E/Z*)-4-phenylbutan-2-one oxime (71 : 29 *E/Z* mixture of isomers) ((*E/Z*)-**1ya**, 32.6 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at 120 °C for 20 h. The amine product was afforded as a colorless liquid (20.2 mg, 68% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.31 – 7.28 (m, 2H), 7.22 – 7.19 (m, 3H), 2.89 (t, *J* = 6.8 Hz, 2H), 2.82 (t, *J* = 7.1 Hz, 2H), 2.67 (q, *J* = 7.2 Hz, 2H), 1.58 (br, 1H), 1.09 (t, *J* = 7.2 Hz, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 140.2, 128.8, 128.6, 126.3, 51.2, 44.1, 36.5, 15.3 ppm. Spectral data is in agreement with published data.^[35]

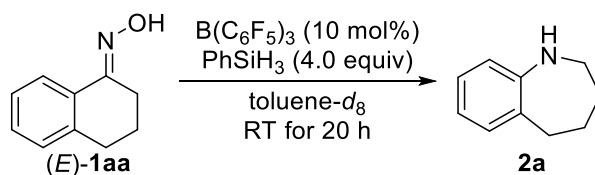


N-Methylaniline (2z). The general procedure was followed with (*E*)-benzaldehyde oxime ((*E*)-**1za**, 24.2 mg, 0.200 mmol), PhSiH₃ (98.8 μ L, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μ mol) at RT for 20 h. The amine product was afforded as a colorless liquid (17.5 mg, 82% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.21 (t, *J* = 7.5 Hz, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.64 (d, *J* = 8.5 Hz, 2H), 3.61 (br, 1H), 2.85 (s, 3H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 149.5, 129.3, 117.4, 112.6, 30.9 ppm. Spectral data is in agreement with published data.^[36]



***N*¹,*N*²-Diphenylethane-1,2-diamine (5).** The general procedure was followed with (1*Z*,2*Z*)-1,2-diphenylethane-1,2-dione dioxime ((*Z,Z*)-**4**, 48.0 mg, 0.200 mmol), PhSiH₃ (197.6 μL, 1.600 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol) at RT for 20 h. The amine product was afforded as a white solid (23.4 mg, 55% yield). **¹H NMR** (500 MHz, CDCl₃): δ 7.22 (t, *J* = 7.5 Hz, 4H), 6.76 (t, *J* = 7.3 Hz, 2H), 6.67 (d, *J* = 7.8 Hz, 4H), 3.86 (br, 1H), 3.41 (s, 4H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 148.2, 129.5, 118.0, 113.2, 43.4 ppm. Spectral data is in agreement with published data.^[37]

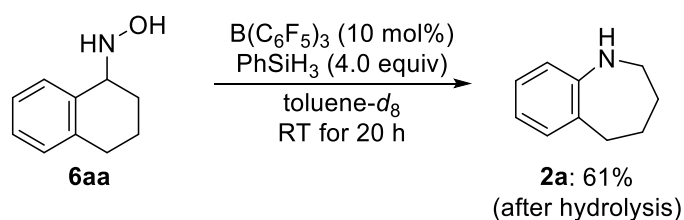
3 Scale-Up Experiment



In a nitrogen-filled glovebox, a 25 mL dried single neck round bottom flask was charged with *(E)*-3,4-dihydronaphthalen-1(2*H*)-one oxime (**(E)-1aa**, 1.13 g, 7.00 mmol), PhSiH_3 (3.46 mL, 28.0 mmol), toluene- d_8 (2.00 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (358 mg, 0.700 mmol) at RT for 20 h. The reaction was then removed from the glove box, diluted with methyl *tert*-butyl ether (10 mL), and transferred to a 100 mL single neck round bottom flask. 1 M aqueous HCl solution (50 mL) was added and the mixture was stirred at RT for 12 h. The organic layer was extracted with 4 $\times$ 10 mL of 1 M aqueous HCl solution. The combined aqueous phase was added NaOH (20.0 g) and the mixture was stirred at RT for 4 h. The product was extracted into 4 $\times$ 15 mL of methyl *tert*-butyl ether. Removal of the solvent under reduced pressure and purification by flash column chromatography on silica gel with methyl *tert*-butyl ether : cyclohexane = 1 : 20 as the eluent yielded amine **2a** as a colorless liquid (0.93 g, 90% yield).

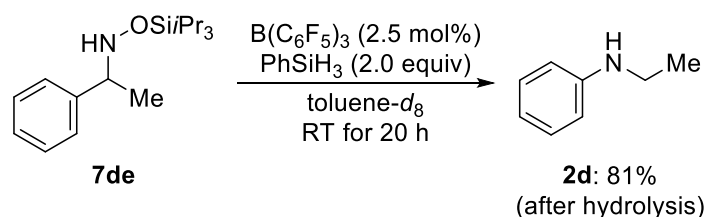
4 Mechanistic Control Experiments

4.1 Reductive Rearrangement of Hydroxylamine 6aa



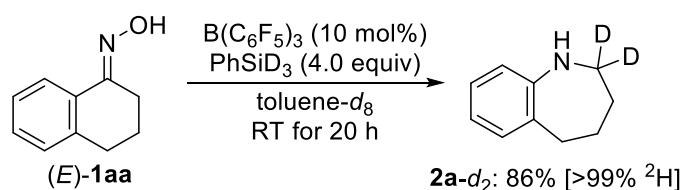
In a nitrogen-filled glovebox, a 2-mL GC vial equipped with a magnetic stir bar was charged with *N*-(1,2,3,4-tetrahydronaphthalen-1-yl)hydroxylamine (**6aa**, 32.6 mg, 0.200 mmol), PhSiH_3 (98.8 μL , 0.800 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (10.2 mg, 20.0 μmol). The GC vial was fitted with a cap and the reaction stirred at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard, and a 61% yield of **2a** was determined by NMR spectroscopy.

4.2 Reductive Rearrangement of O-Silylated Hydroxylamine 7de



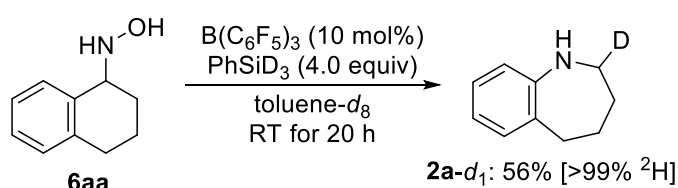
In a nitrogen-filled glovebox, a 2-mL GC vial equipped with a magnetic stir bar was charged with *N*-(1-phenylethyl)-*O*-(triisopropylsilyl)hydroxylamine (**7de**, 29.3 mg, 0.100 mmol), PhSiH_3 (24.7 μL , 0.200 mmol), toluene- d_8 (0.200 mL), and $\text{B}(\text{C}_6\text{F}_5)_3$ (1.30 mg, 2.50 μmol). The GC vial was fitted with a cap and the reaction stirred at RT for 20 h. After that, mesitylene (0.500 equiv) was added as an internal standard and an 81% yield of **2d** was determined by ^1H NMR spectroscopy.

4.3 ^2H -Labeling Experiments



In a nitrogen-filled glovebox, a 2-mL GC vial equipped with a magnetic stir bar was charged

with (*E*)-3,4-dihydronaphthalen-1(2*H*)-one oxime ((*E*)-**1aa**, 32.2 mg, 0.200 mmol), PhSiD₃ (88.8 mg, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol). The GC vial was fitted with a cap and the reaction stirred at RT for 20 h in the glove box. After that, mesitylene (0.500 equiv) was added as an internal standard, and the yield was determined by ¹H NMR spectroscopy. Methyl *tert*-butyl ether (2 mL) was added to the residue, and the mixture was transferred to a 10-mL sample bottle by pipette. 1 M aqueous HCl solution (4 mL) was added and the mixture was stirred at RT for 12 h. The organic layer was extracted with 4 × 10 mL of 1 M aqueous HCl solution. To the combined aqueous phases was added NaOH (10.0 g), and the mixture was stirred at RT for 4 h. The product was extracted into 4 × 15 mL of methyl *tert*-butyl ether. Removal of the solvent under reduced pressure yielded the crude amine. Further purification by flash column chromatography on silica gel with methyl *tert*-butyl ether : cyclohexane = 1 : 20 as the eluent gave the corresponding dideuterated amine as a colorless liquid (25.7 mg, 86%). **¹H NMR** (500 MHz, CDCl₃): δ 7.12 (d, *J* = 7.4 Hz, 1H), 7.05 (td, *J* = 7.6, 1.3 Hz, 1H), 6.84 (td, *J* = 7.4, 0.6 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H), 3.75 (br, 1H), 2.79 (t, *J* = 5.6 Hz, 2H), 1.80 (t, *J* = 6.0 Hz, 2H), 1.68 – 1.64 (m, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 150.5, 133.8, 130.9, 126.7, 120.9, 119.4, 48.3 (p, *J* = 20.4 Hz), 36.2, 31.9, 27.0 ppm. **IR** (ATR): ν = 3358, 2919, 2849, 2069, 1600, 1470, 1254, 1185, 943, 749 cm⁻¹. **HRMS** (APCI) *m/z*: [M+H]⁺ calculated for C₁₀H₁₂D₂N 150.1252, found 150.1245.



In a nitrogen-filled glovebox, a 2-mL GC vial equipped with a magnetic stir bar was charged with *N*-(1,2,3,4-tetrahydronaphthalen-1-yl)hydroxylamine (**6aa**, 32.6 mg, 0.200 mmol), PhSiD₃ (88.8 mg, 0.800 mmol), toluene-*d*₈ (0.200 mL), and B(C₆F₅)₃ (10.2 mg, 20.0 μmol). The GC vial was fitted with a cap and the reaction stirred at RT for 20 h in the glove box. After that, mesitylene (0.500 equiv) was added as an internal standard, and the yield was determined by ¹H NMR spectroscopy. Methyl *tert*-butyl ether (2 mL) was added to the residue, and the mixture was transferred to a 10-mL sample bottle via pipette. 1 M aqueous HCl solution (4 mL) was added, and the mixture was stirred at RT for 12 h. The organic layer was extracted with 4 × 10

mL of 1 M aqueous HCl solution. To the combined aqueous phases was added NaOH (10.0 g), and the mixture was stirred at RT for 4 h. The product was extracted into 4 × 15 mL of methyl *tert*-butyl ether. Removal of the solvent under reduced pressure yielded the crude amine. Further purification by flash column chromatography on silica gel with methyl *tert*-butyl ether : cyclohexane = 1 : 20 as the eluent gave the corresponding monodeuterated amine as a colorless liquid (16.6 mg, 56%). **¹H NMR** (500 MHz, CDCl₃): δ 7.11 (d, *J* = 7.3 Hz, 1H), 7.04 (td, *J* = 7.6, 1.2 Hz, 1H), 6.83 (t, *J* = 7.4, 0.9 Hz, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 3.71 (br, 1H), 3.04 – 3.01 (m, 1H), 2.78 (t, *J* = 5.5 Hz, 2H), 1.80 (q, *J* = 5.8 Hz, 2H), 1.68 – 1.63 (m, 2H) ppm. **¹³C NMR** (125 MHz, CDCl₃): δ 150.5, 133.8, 130.9, 126.7, 120.9, 119.5, 48.6 (p, *J* = 20.5 Hz), 36.2, 32.0, 27.0 ppm. **IR** (ATR): ν = 3359, 2921, 2849, 1601, 1474, 1275, 1255, 1103, 942, 754 cm⁻¹. **HRMS** (APCI) *m/z*: [M+H]⁺ calculated for C₁₀H₁₃DN 149.1189, found 149.1183.

5 NMR Spectra

Figure S1. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **2,3,4,5-tetrahydro-1H-benzo[*b*]azepine (2a)**.

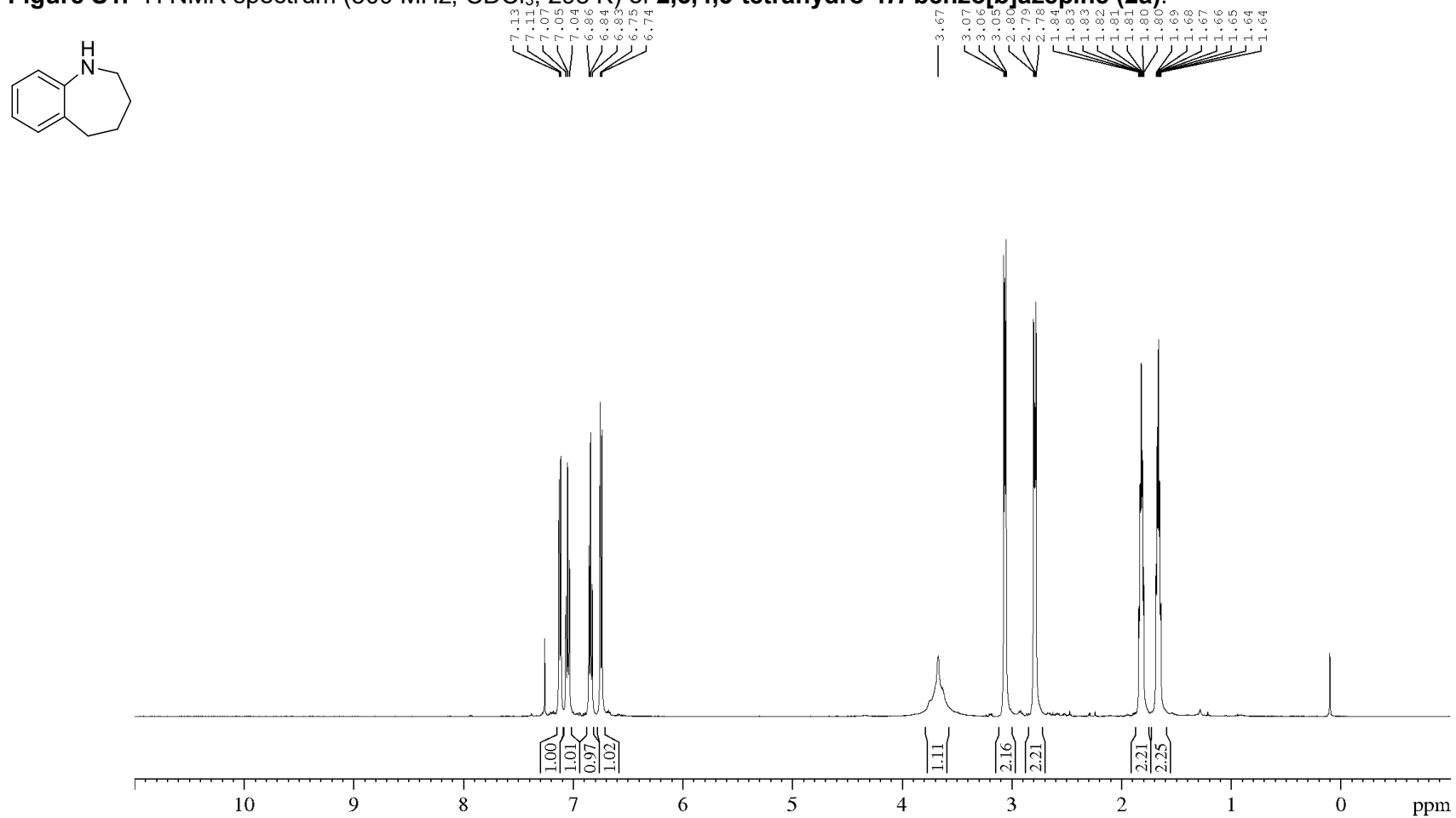


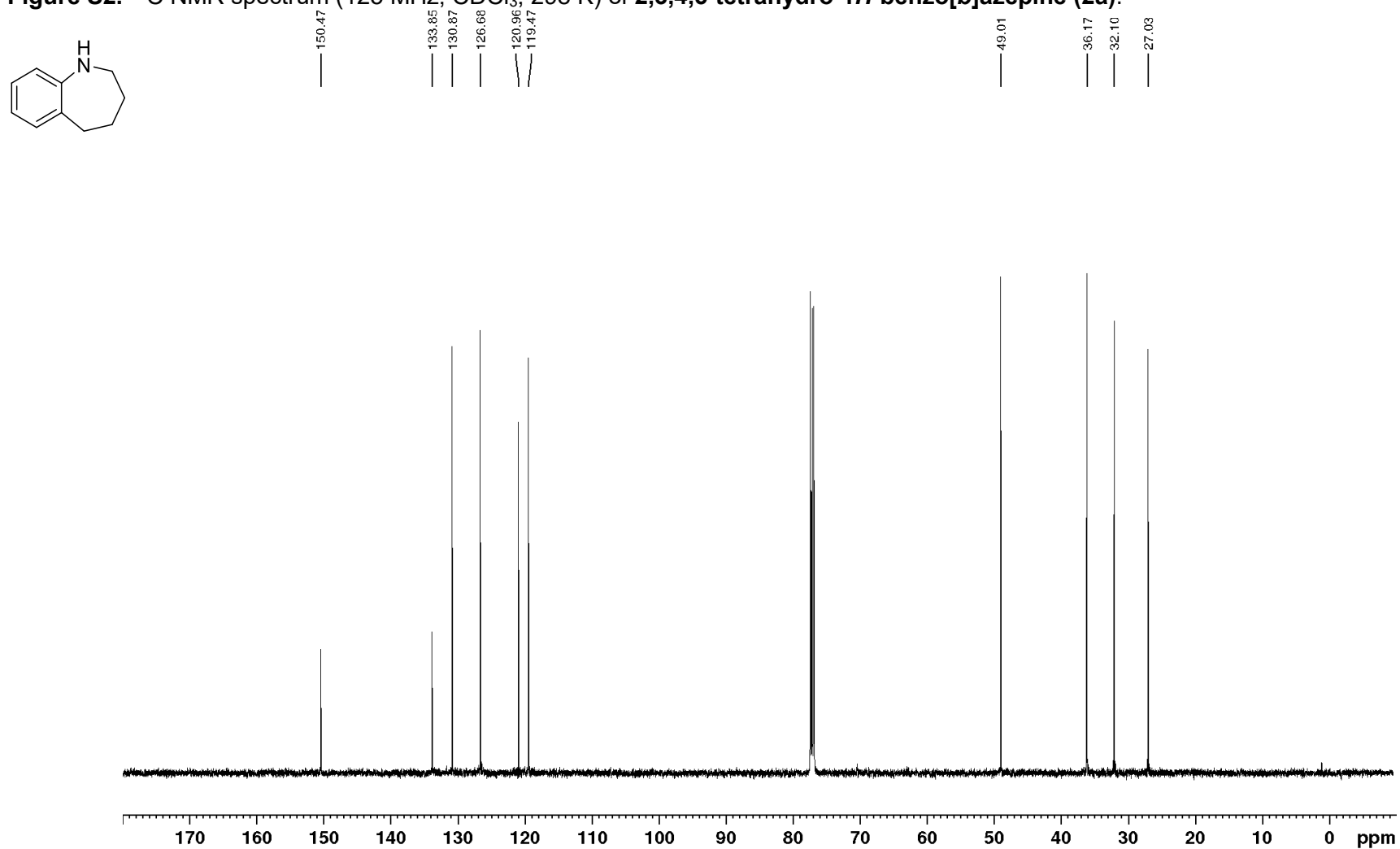
Figure S2. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 2,3,4,5-tetrahydro-1*H*-benzo[*b*]azepine (2a).

Figure S3. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **2,3,4,5-tetrahydrobenzo[*b*][1,4]thiazepine (2b)**.

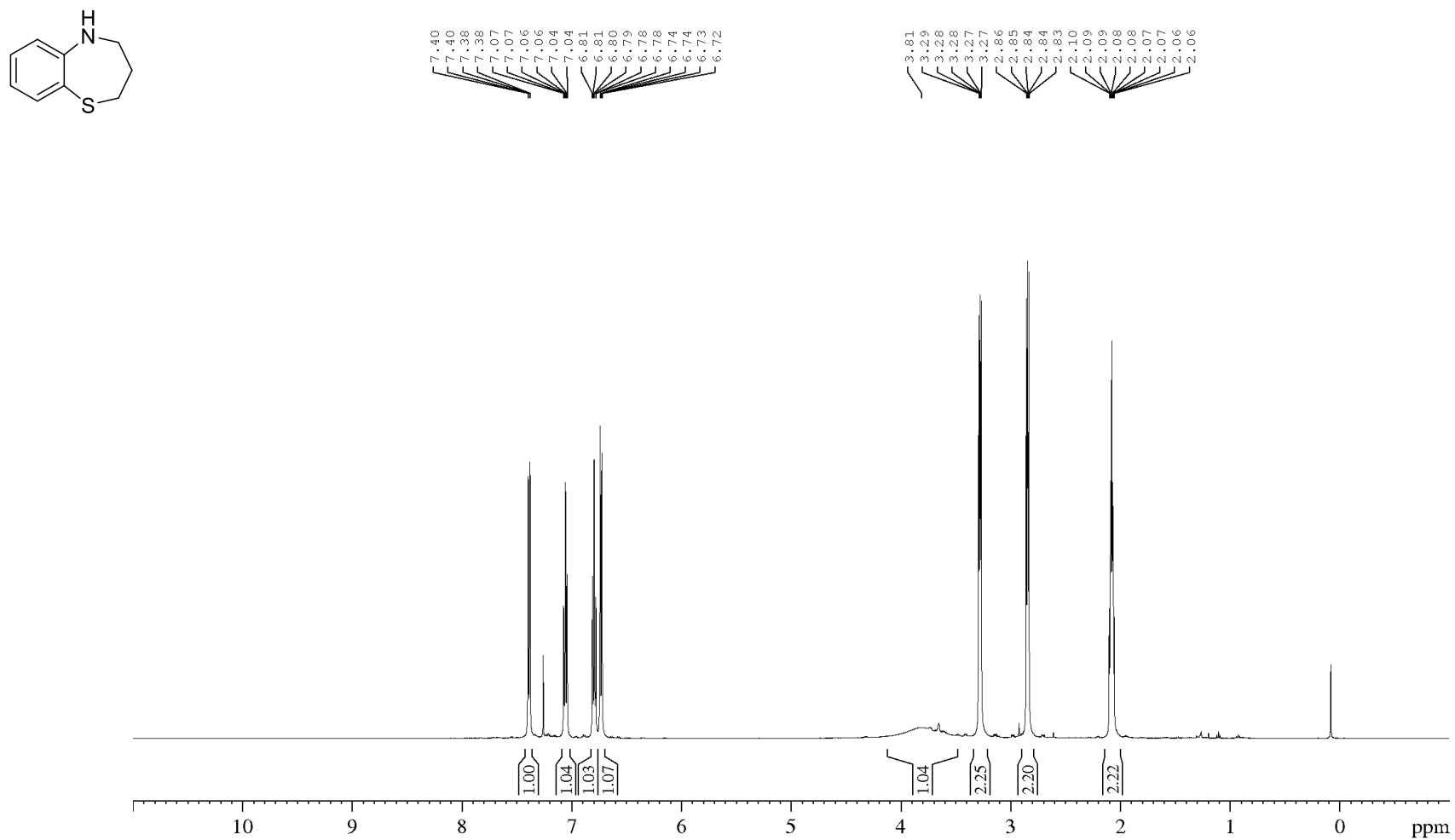


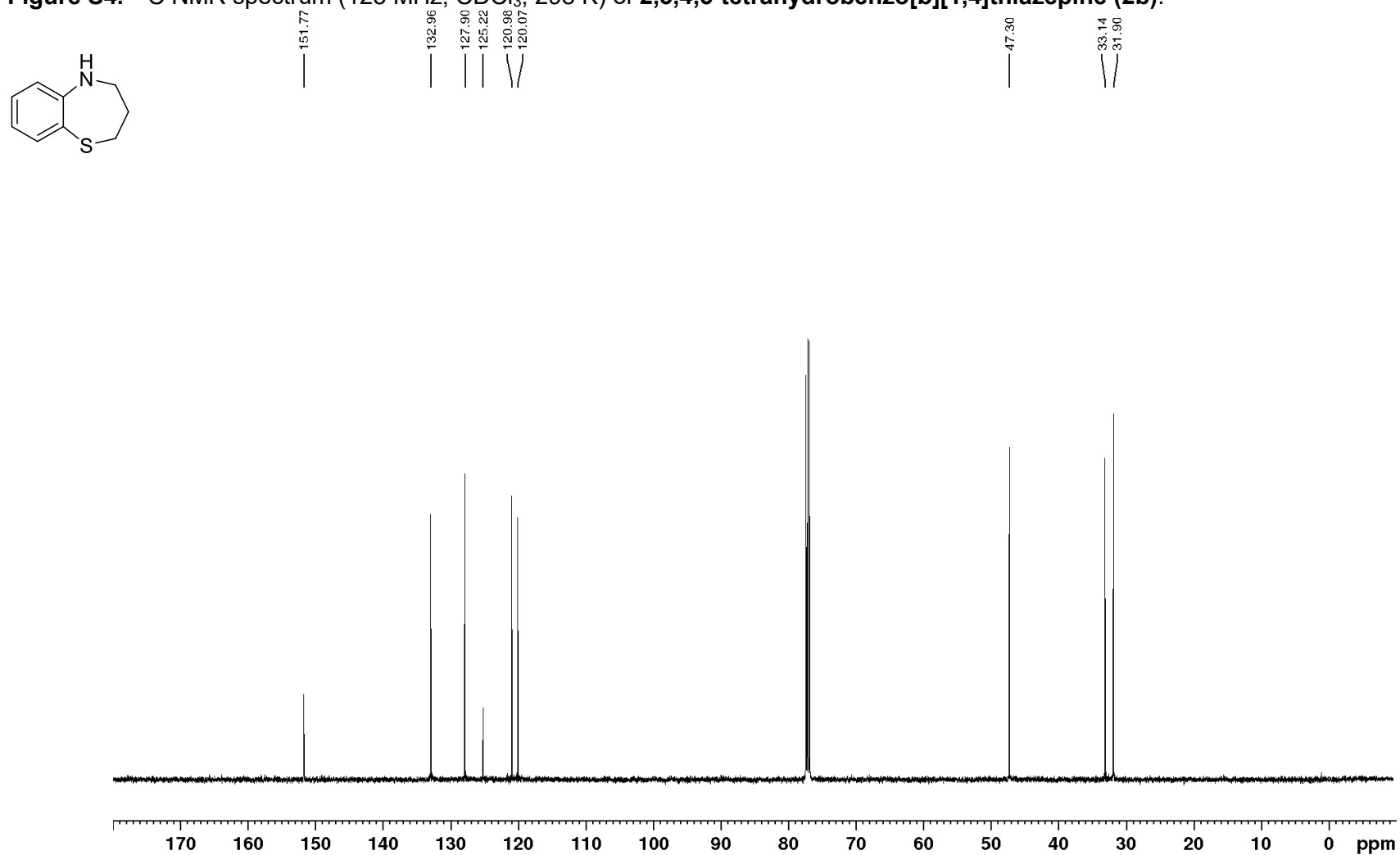
Figure S4. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 2,3,4,5-tetrahydrobenzo[*b*][1,4]thiazepine (2b).

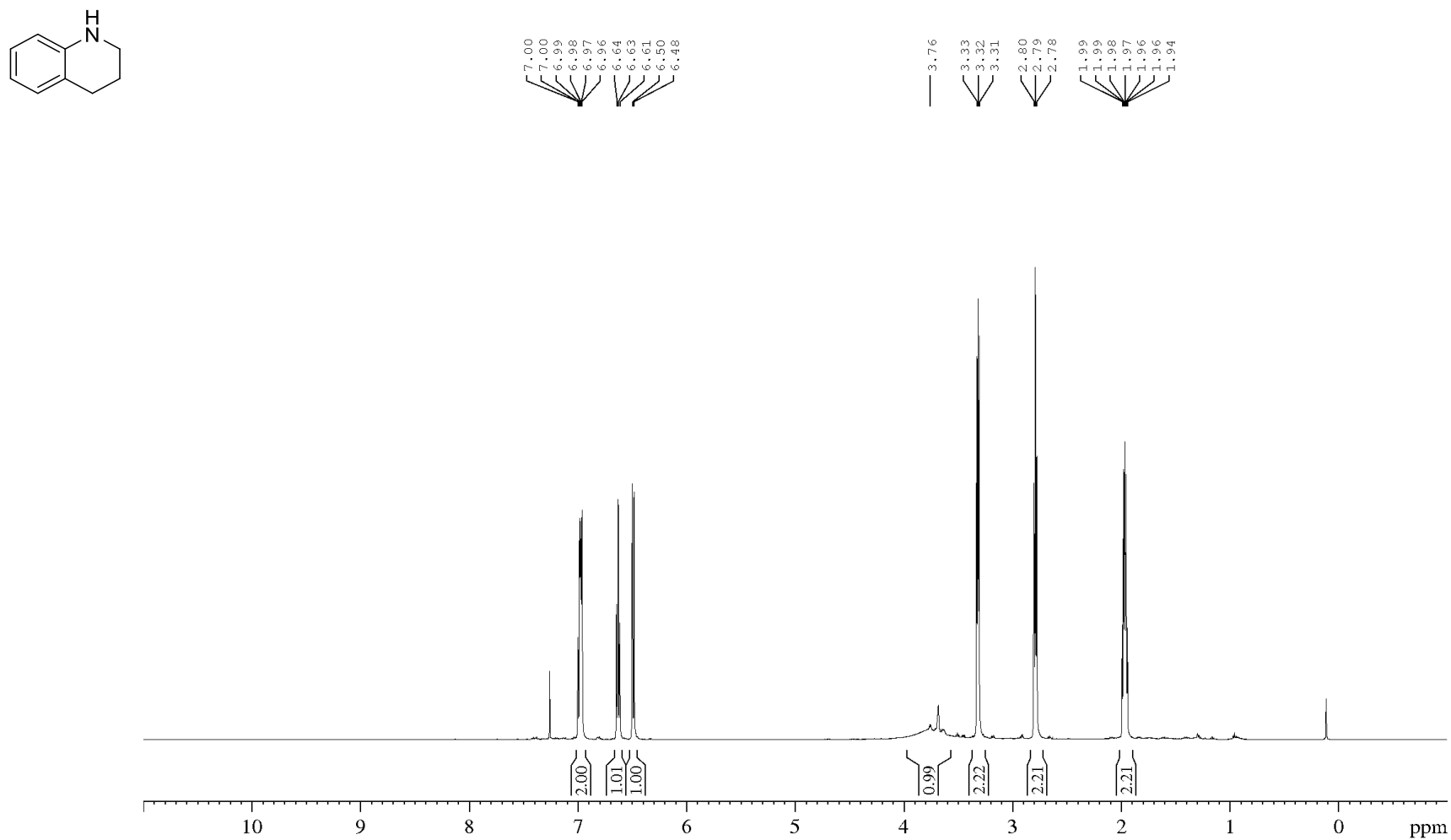
Figure S5. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **1,2,3,4-tetrahydroquinoline (2c)**.

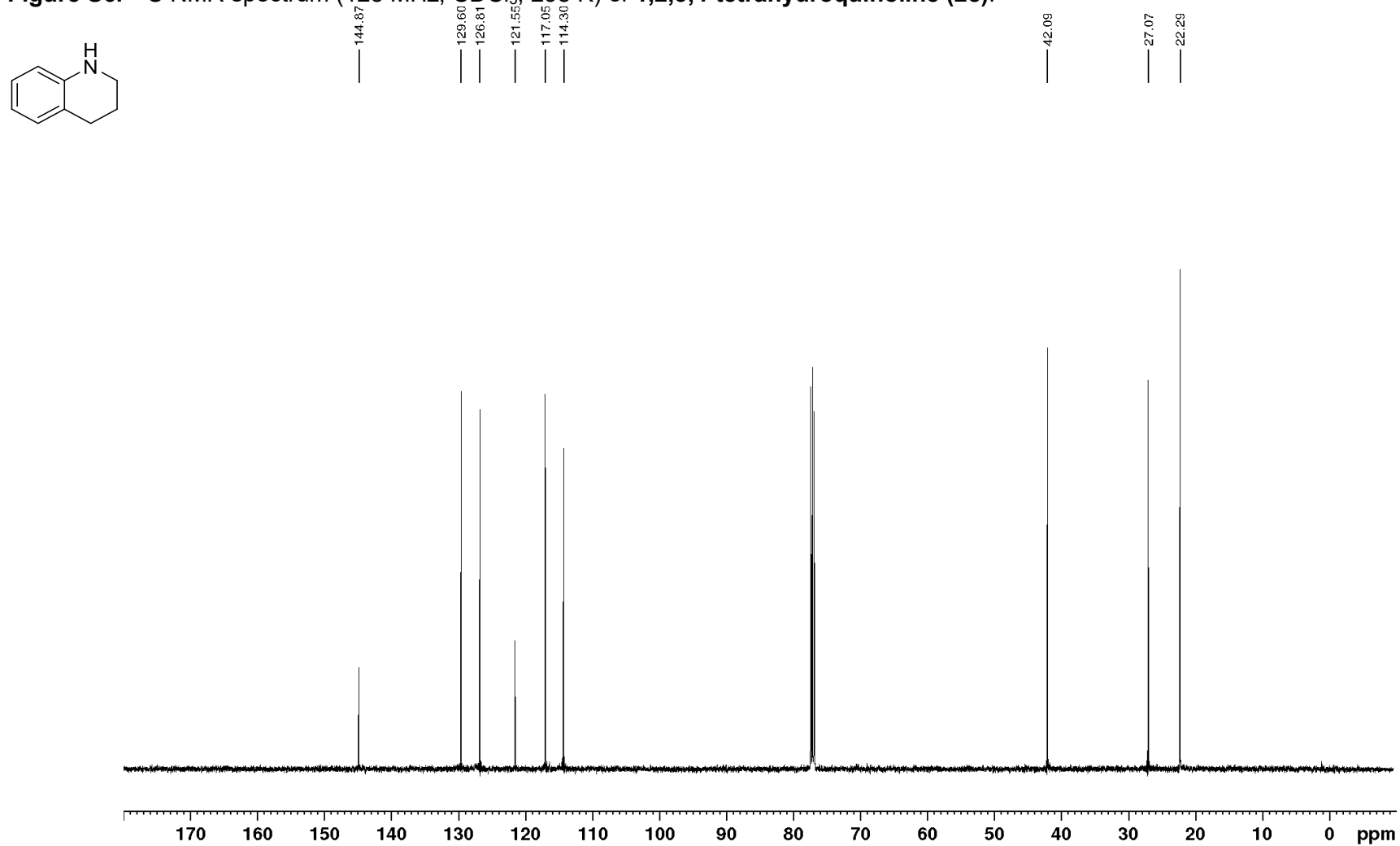
Figure S6. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of **1,2,3,4-tetrahydroquinoline (2c)**.

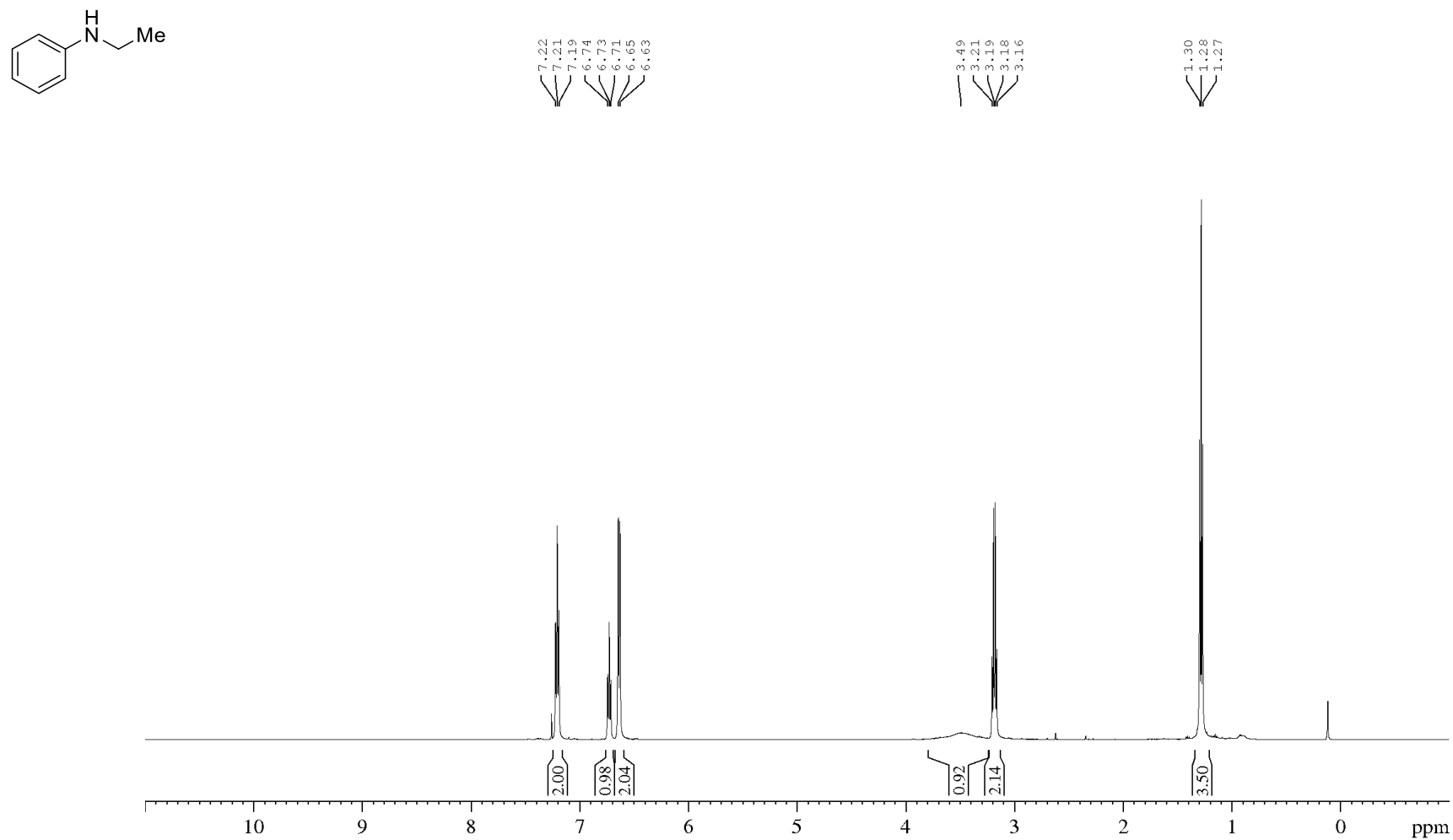
Figure S7. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-ethylaniline (**2d**).

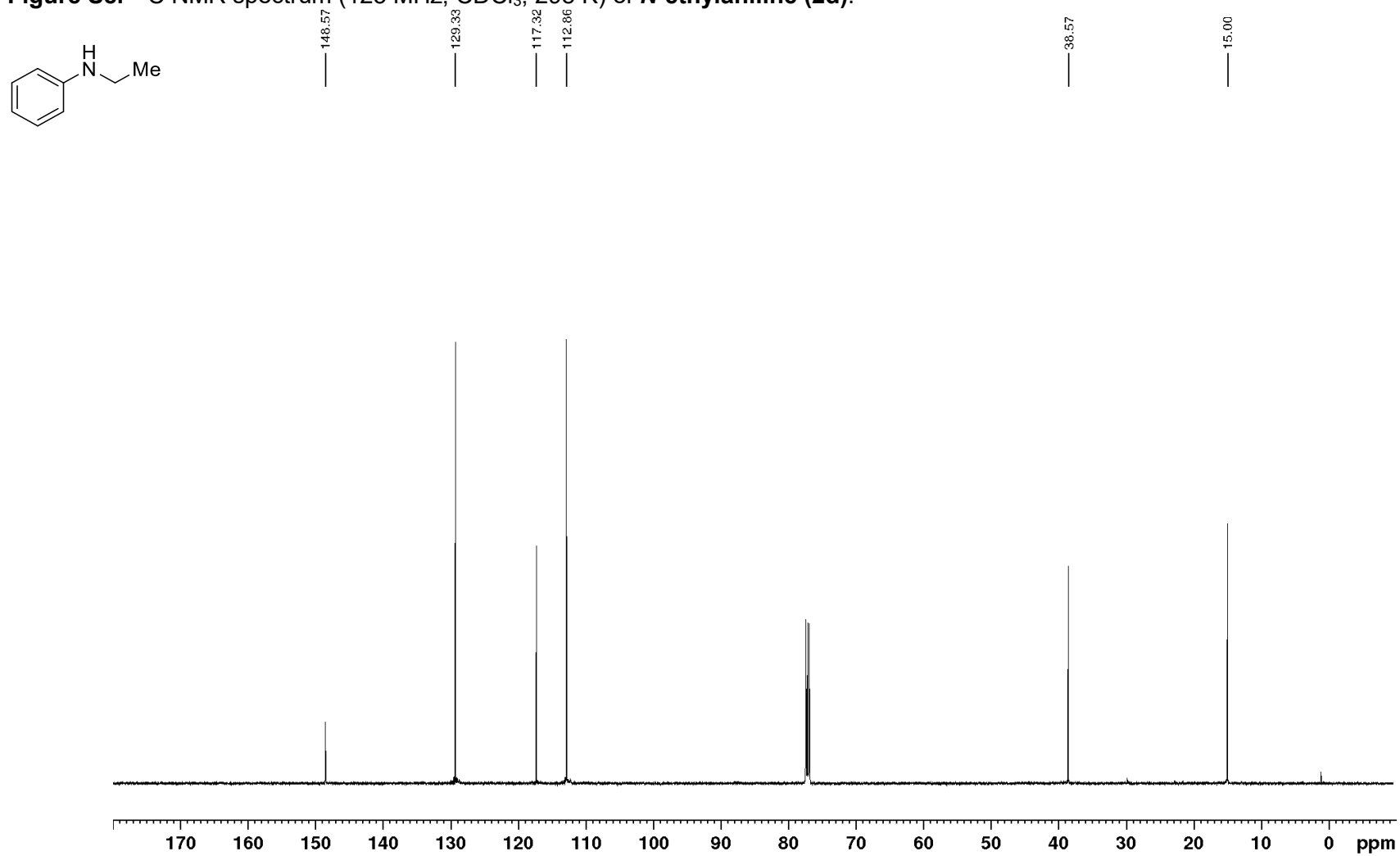
Figure S8. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethylaniline (2d).

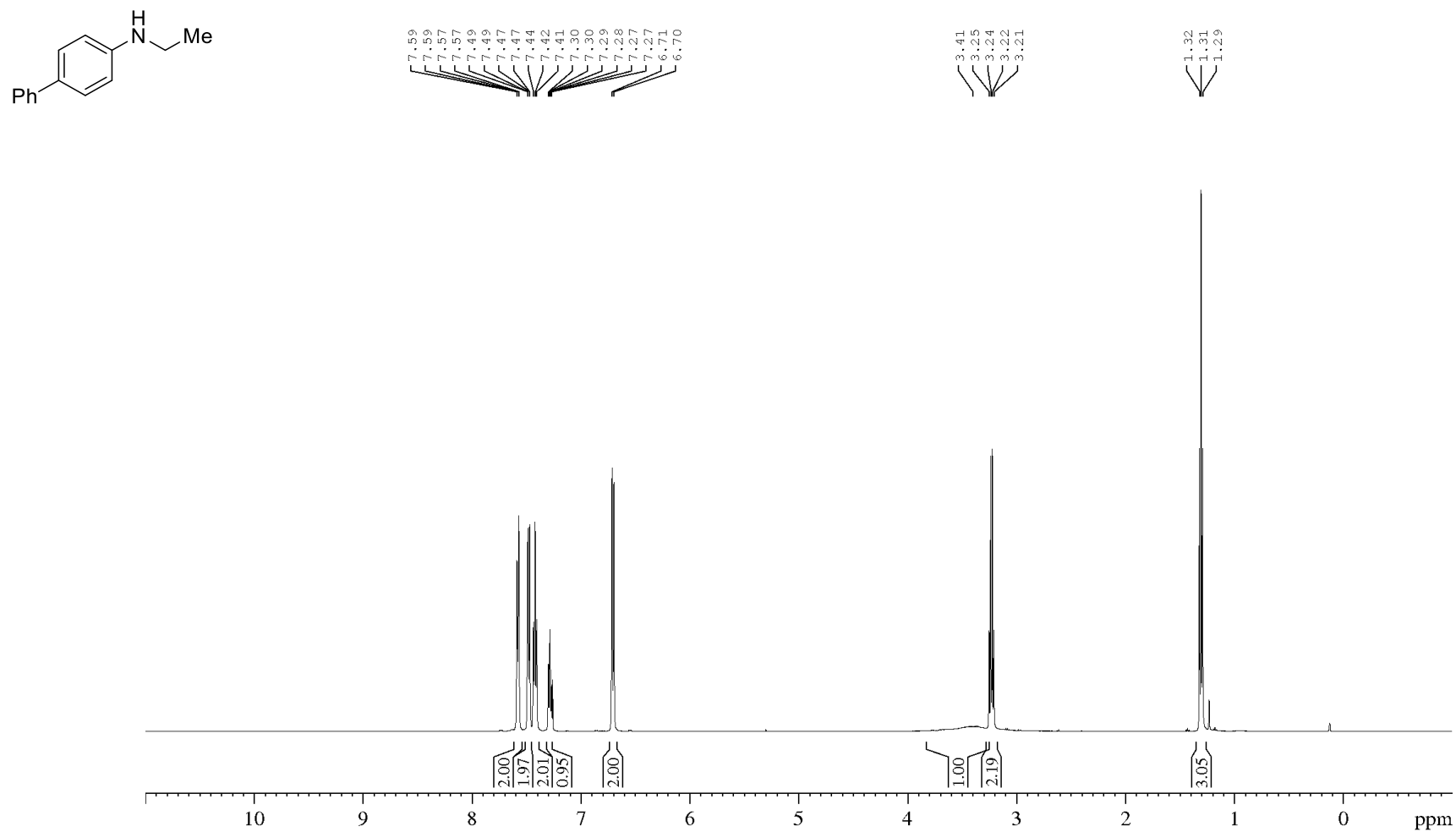
Figure S9. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-ethyl-[1,1'-biphenyl]-4-amine (**2e**).

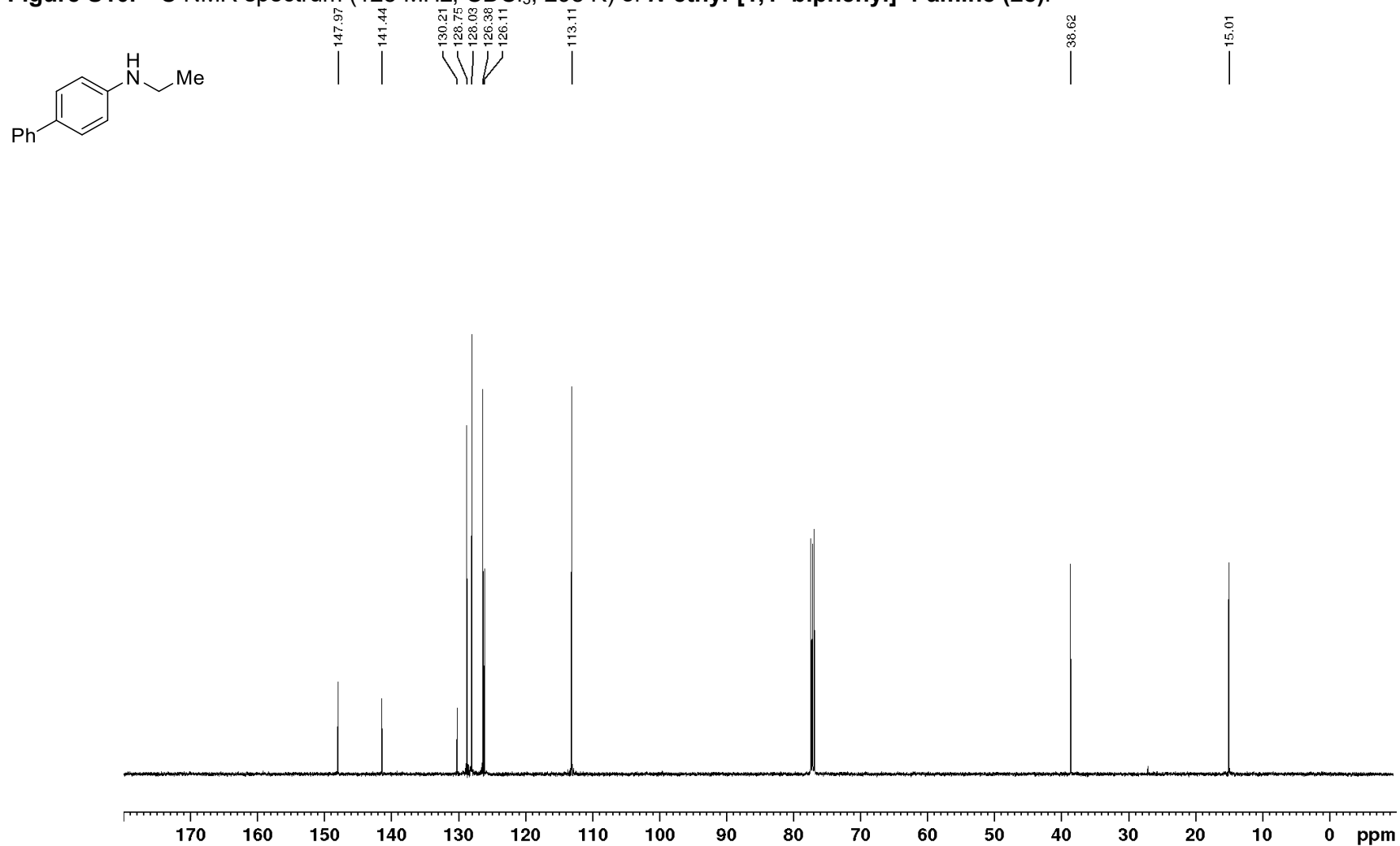
Figure S10. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-[1,1'-biphenyl]-4-amine (**2e**).

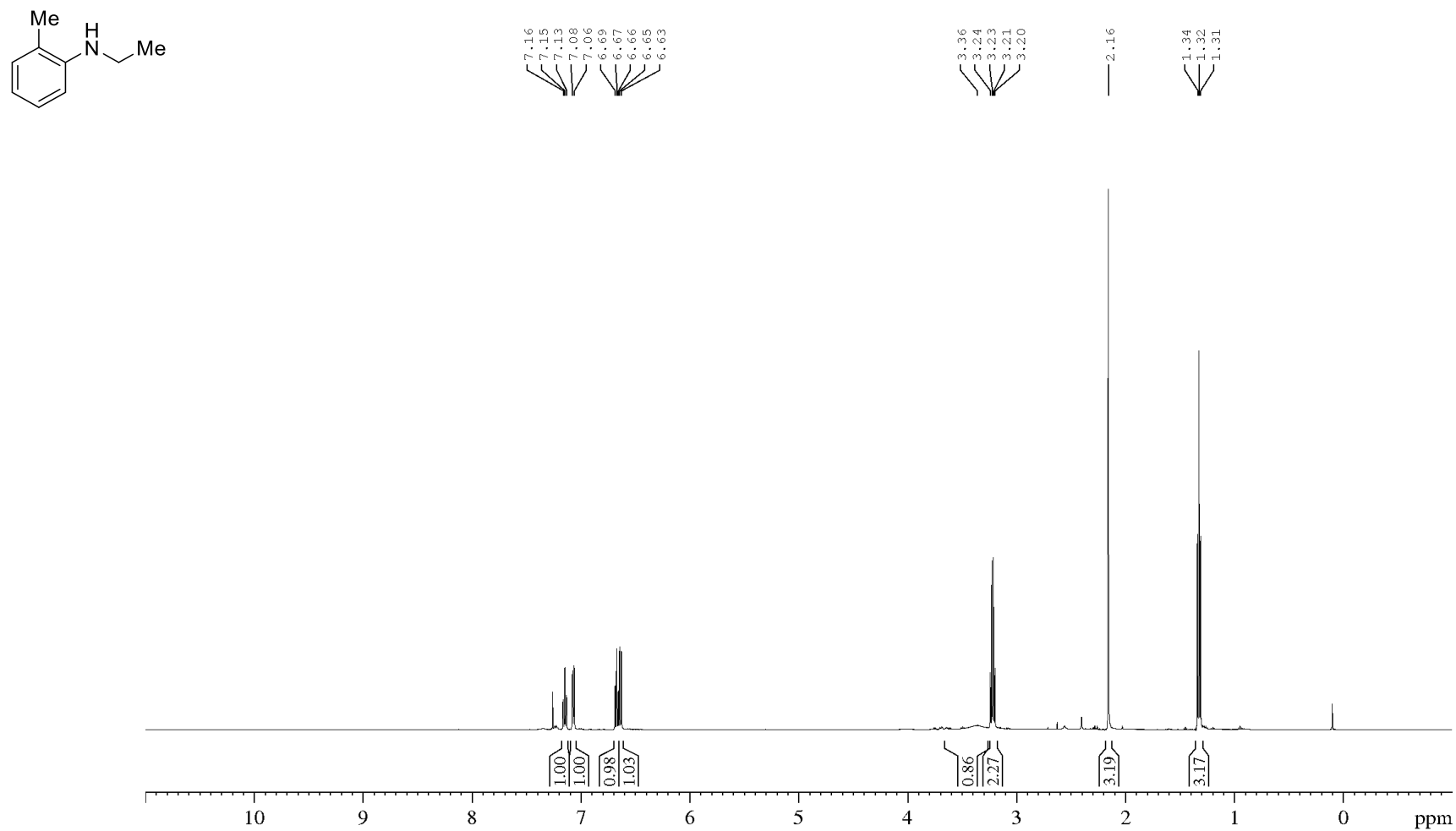
Figure S11. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-ethyl-2-methylaniline (**2f**).

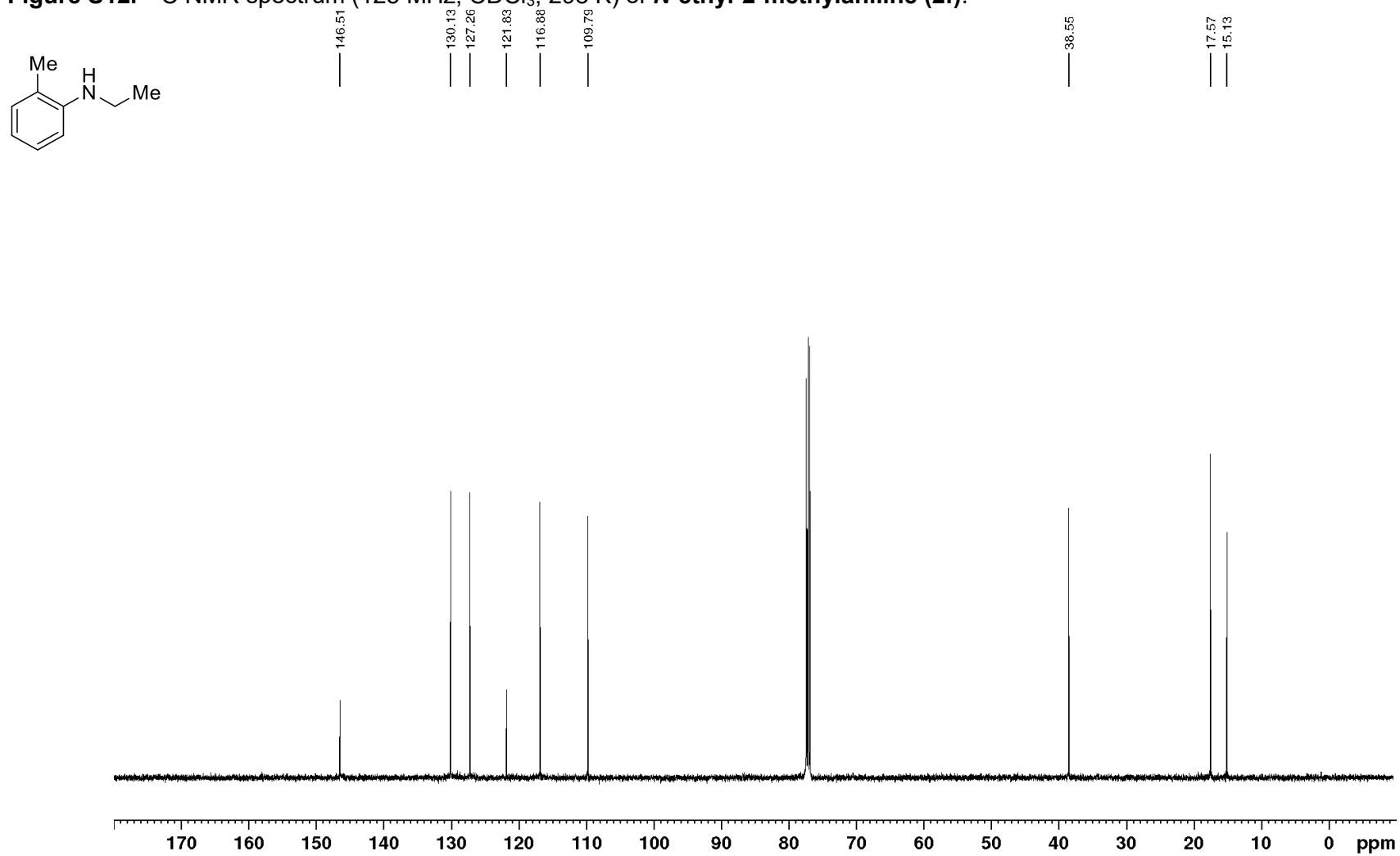
Figure S12. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-2-methylaniline (**2f**).

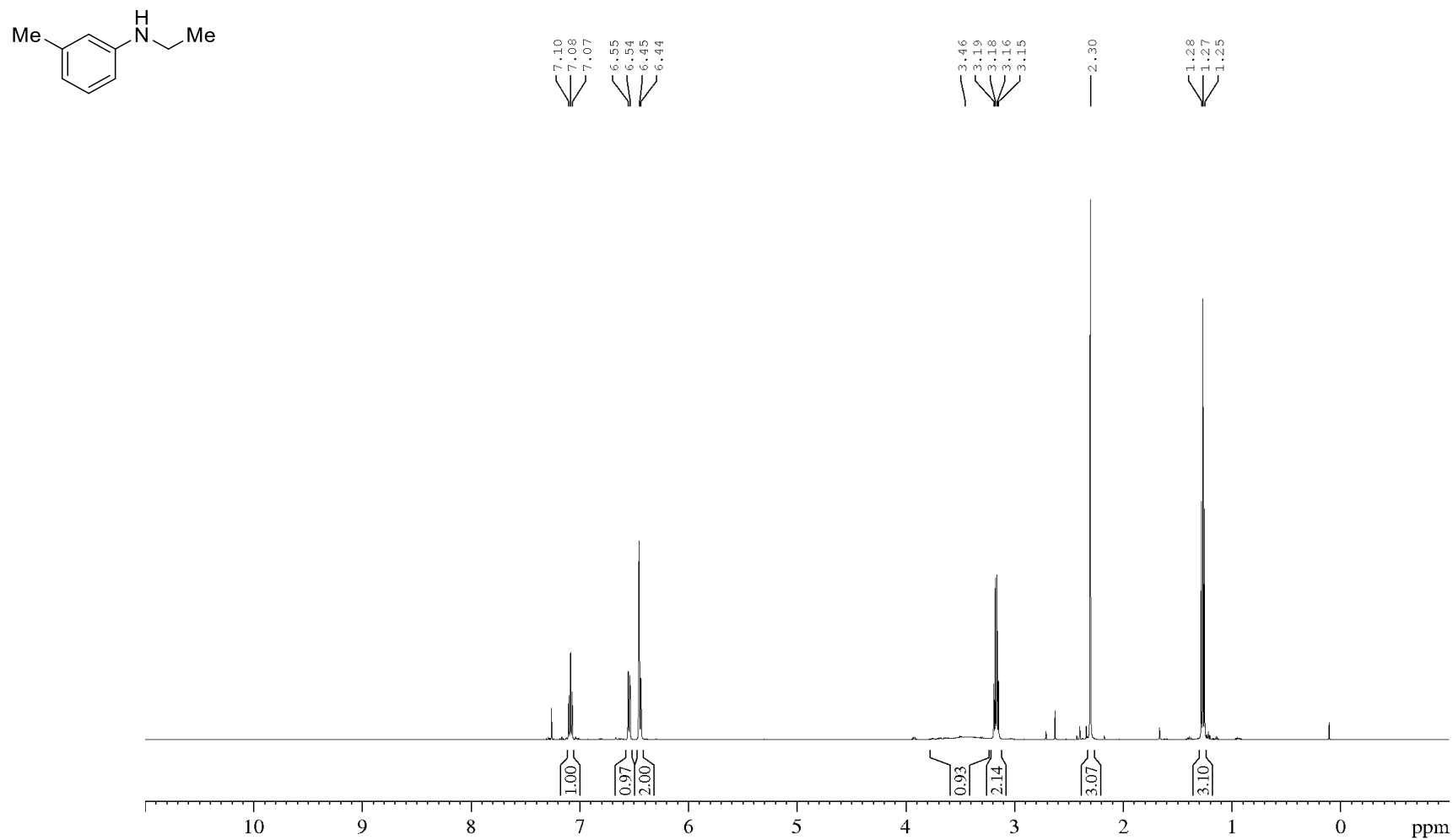
Figure S13. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethyl-3-methylaniline (2g)**.

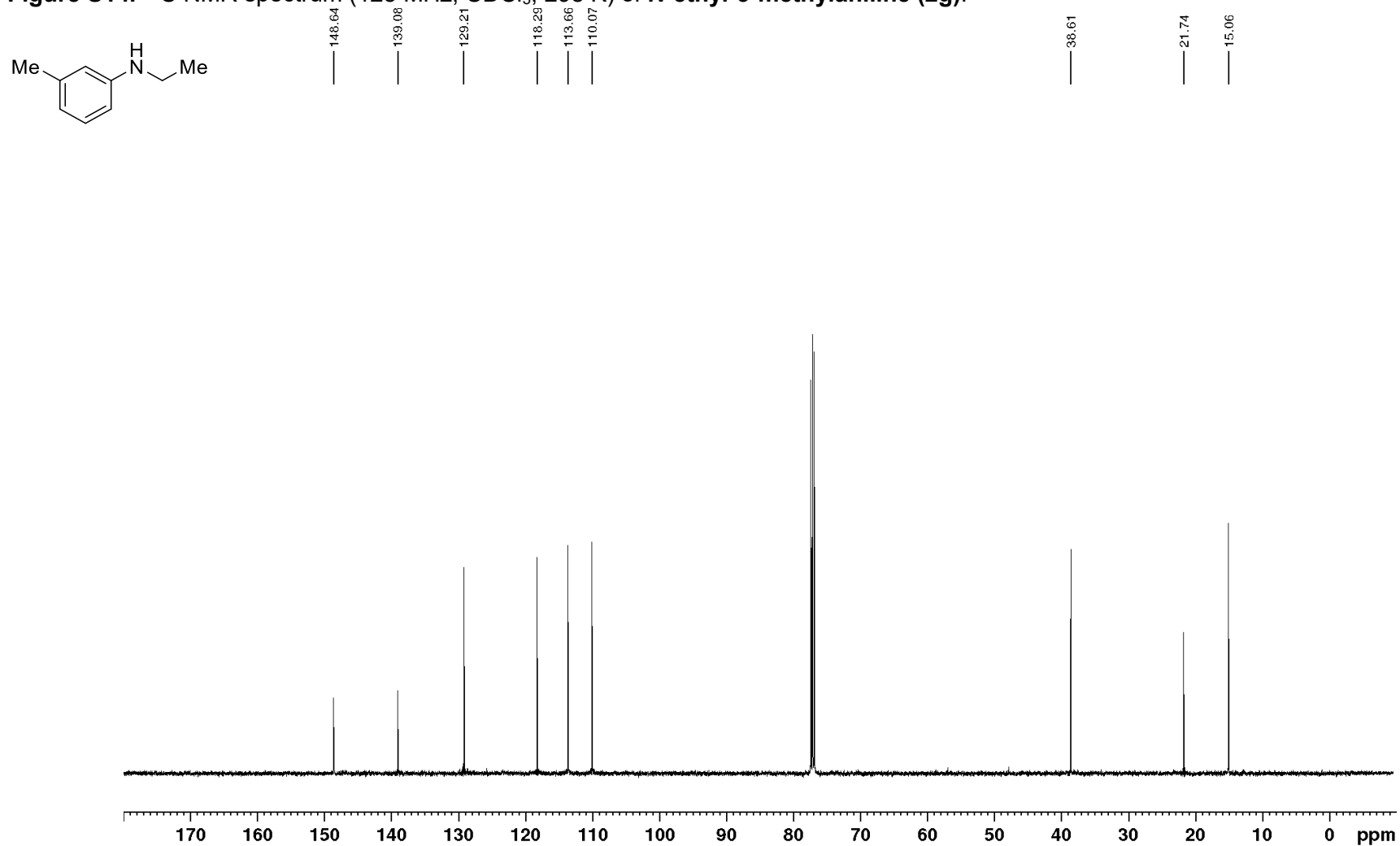
Figure S14. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-3-methylaniline (2g).

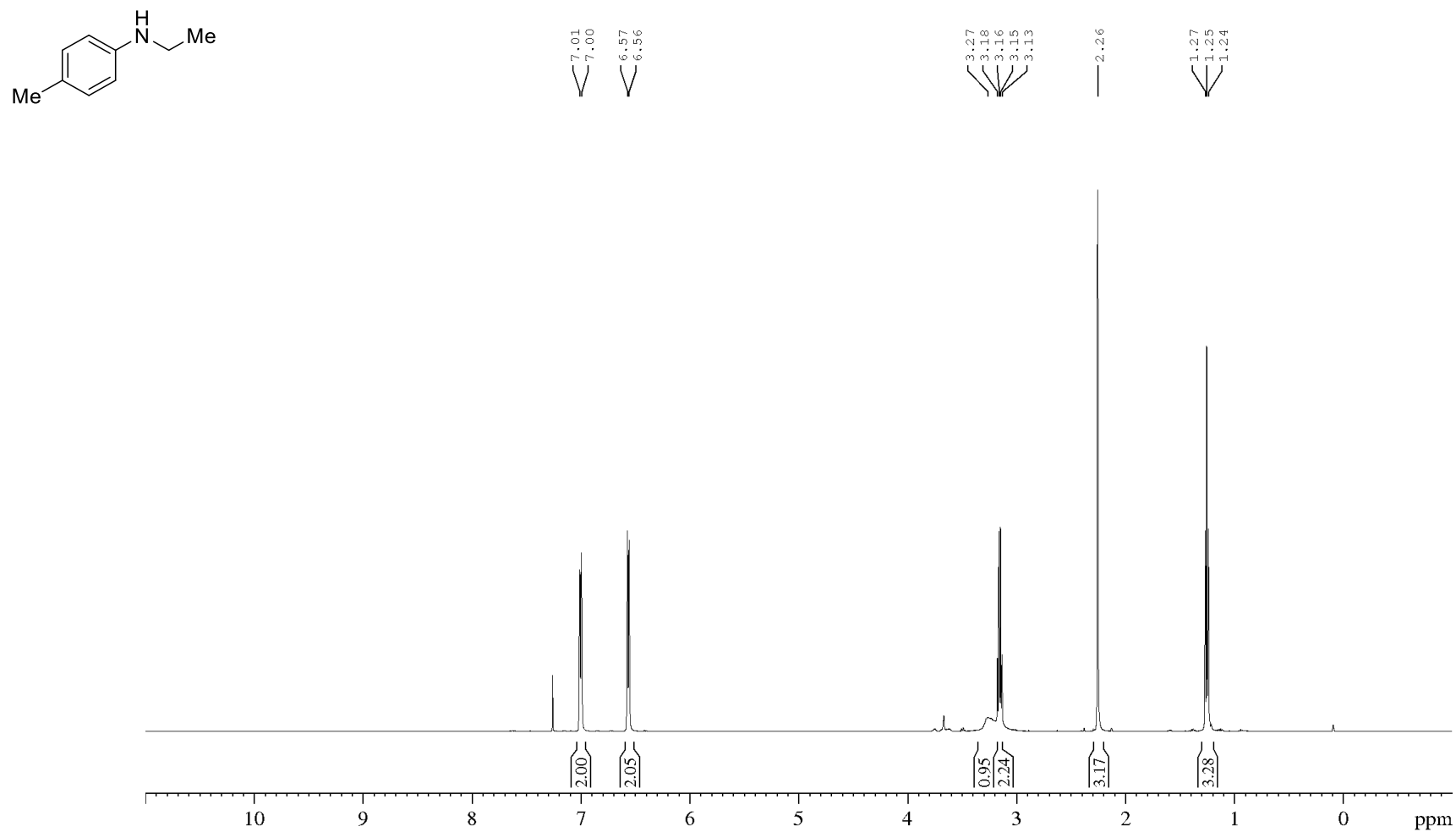
Figure S15. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethyl-4-methylaniline (2h)**.

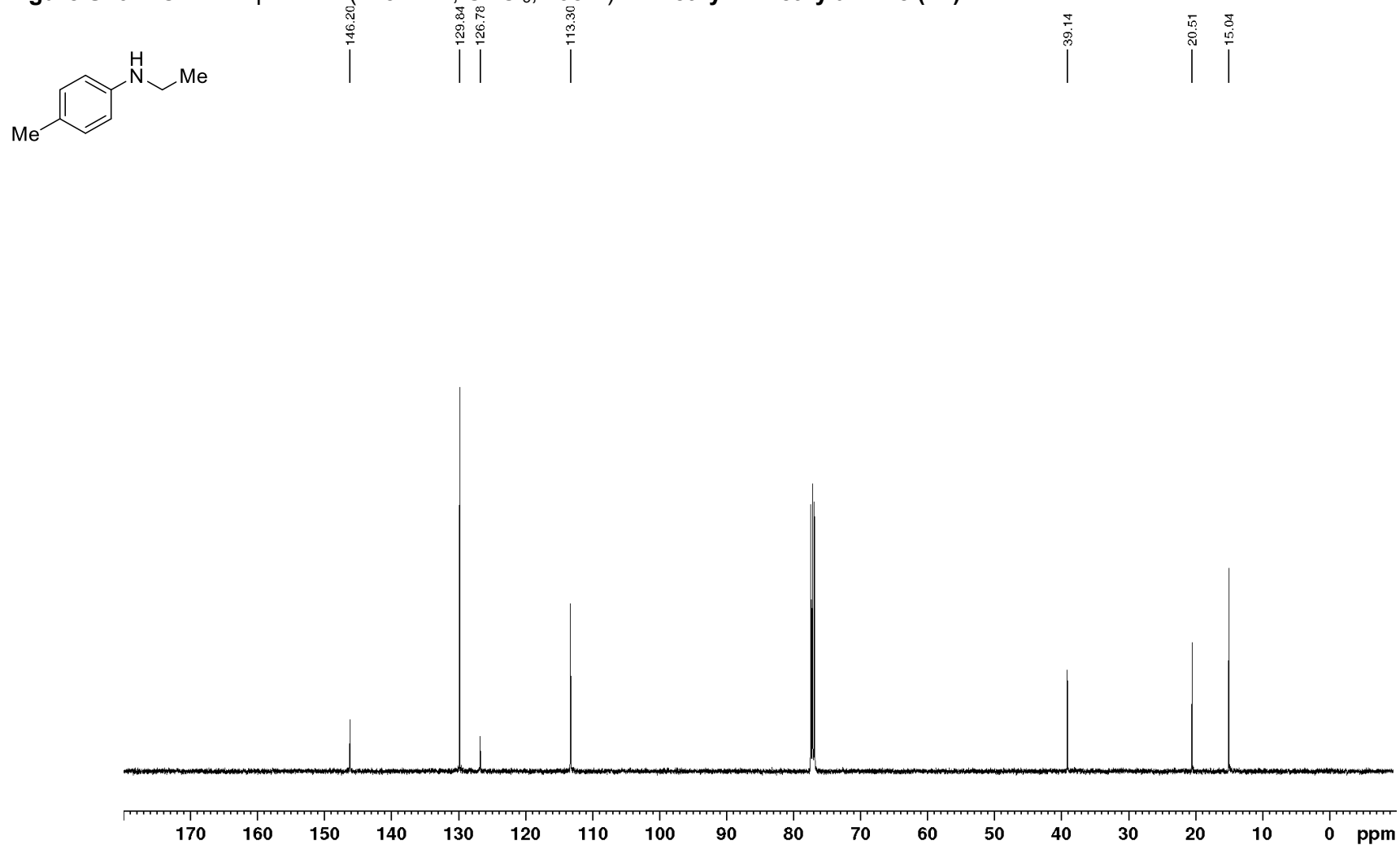
Figure S16. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-4-methylaniline (2h).

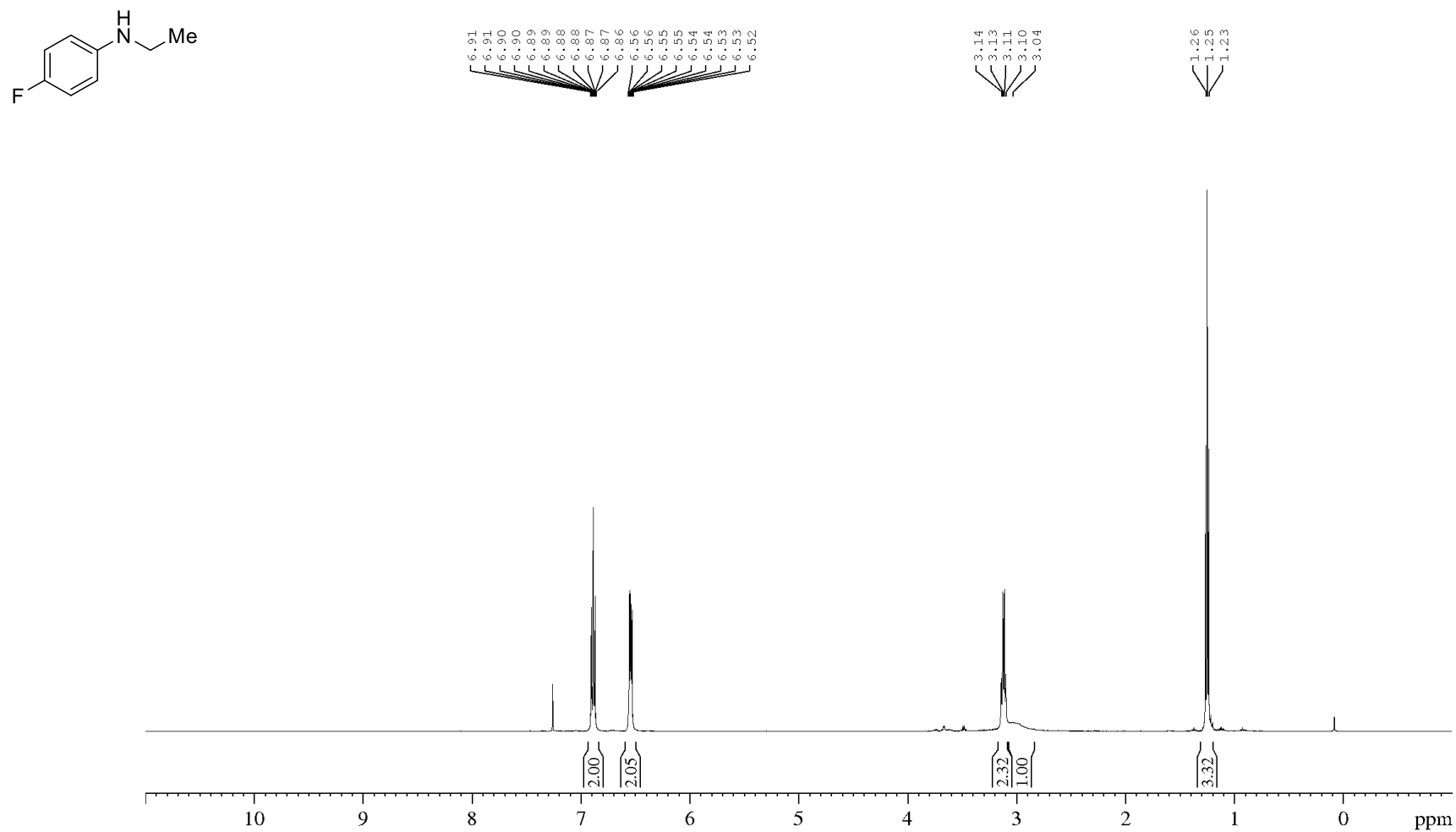
Figure S17. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethyl-4-fluoroaniline (2i)**.

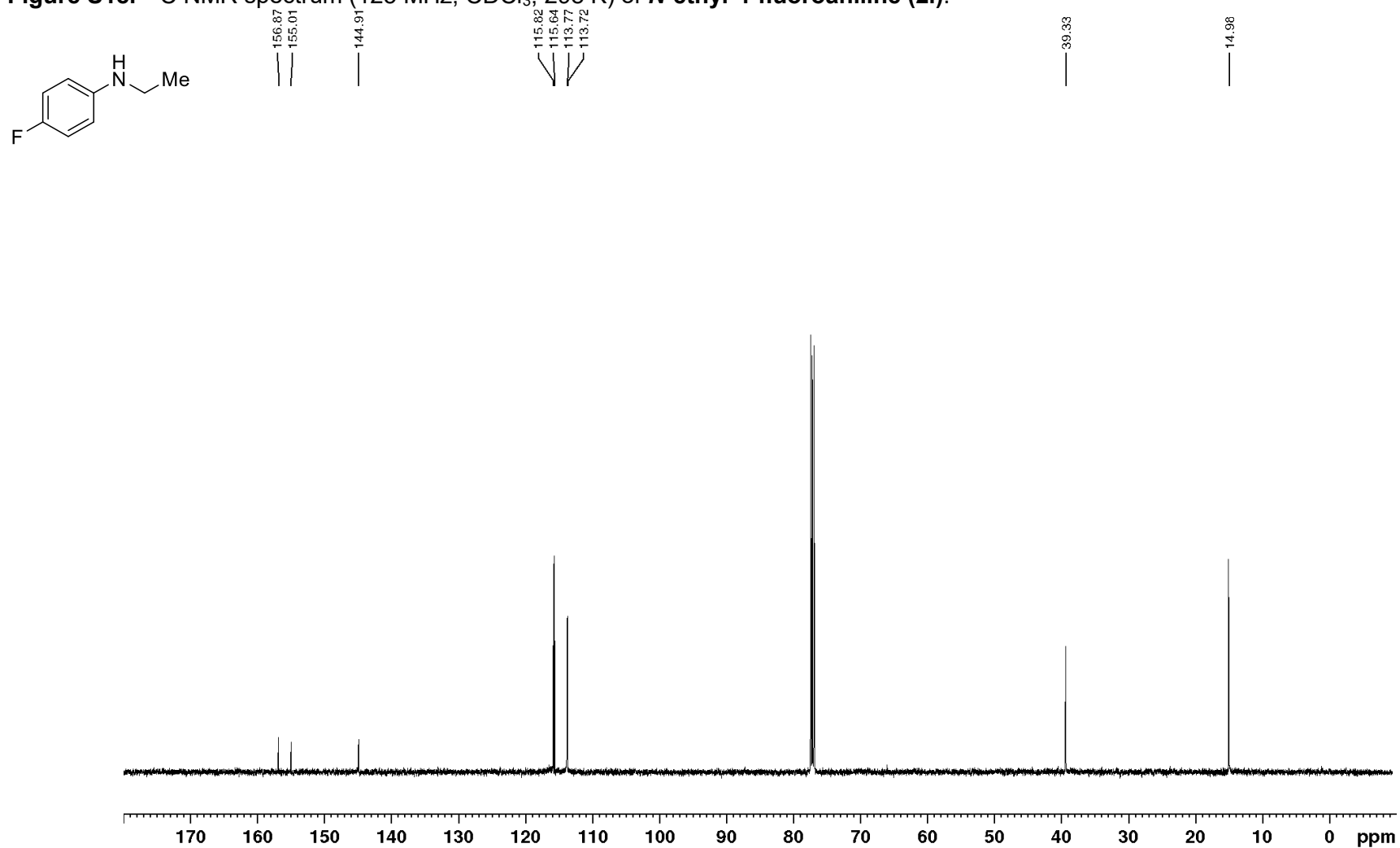
Figure S18. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-4-fluoroaniline (**2i**).

Figure S19. ^{19}F NMR spectrum (471 MHz, CDCl_3 , 298 K) of ***N*-ethyl-4-fluoroaniline (2i)**.

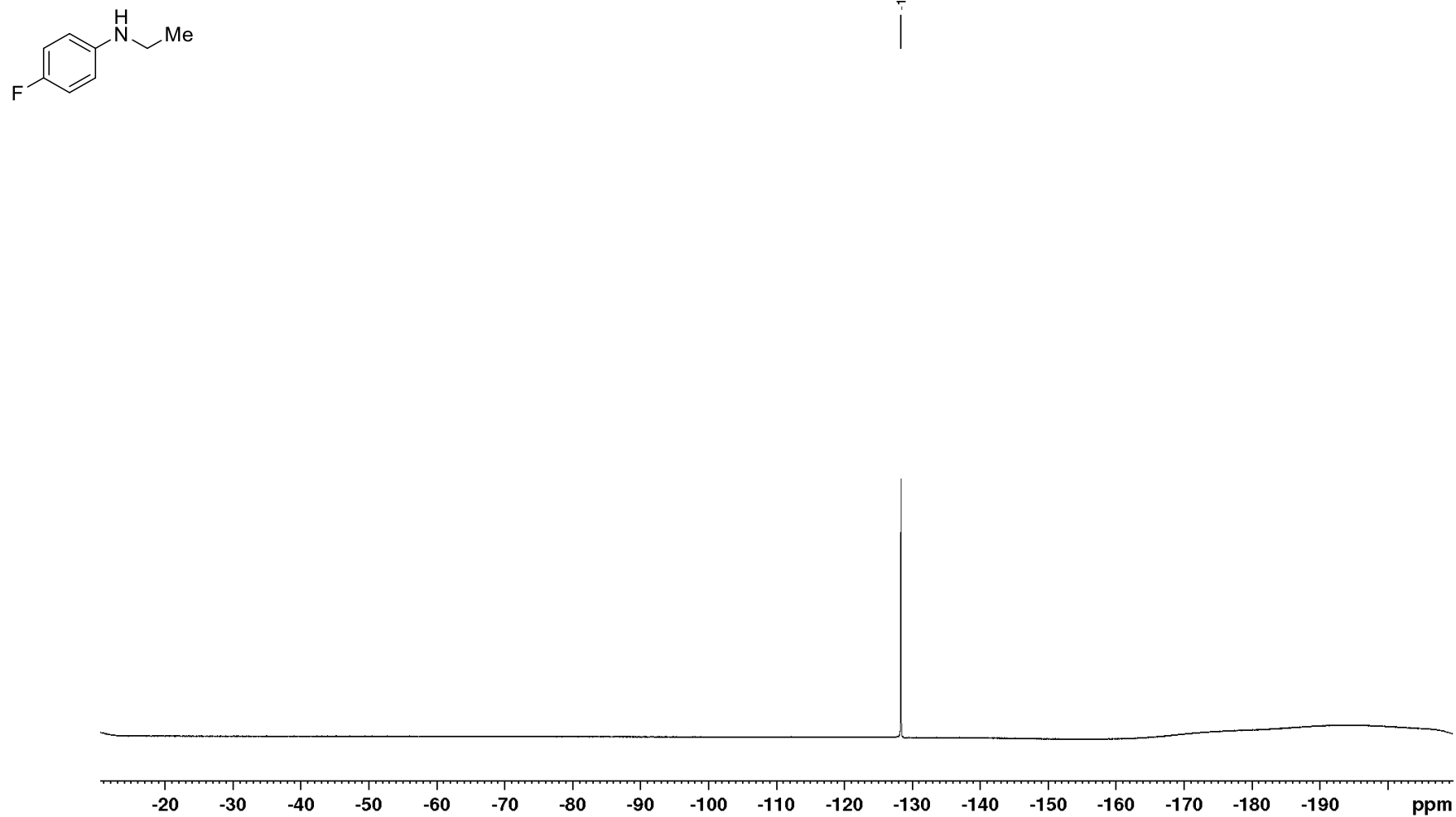


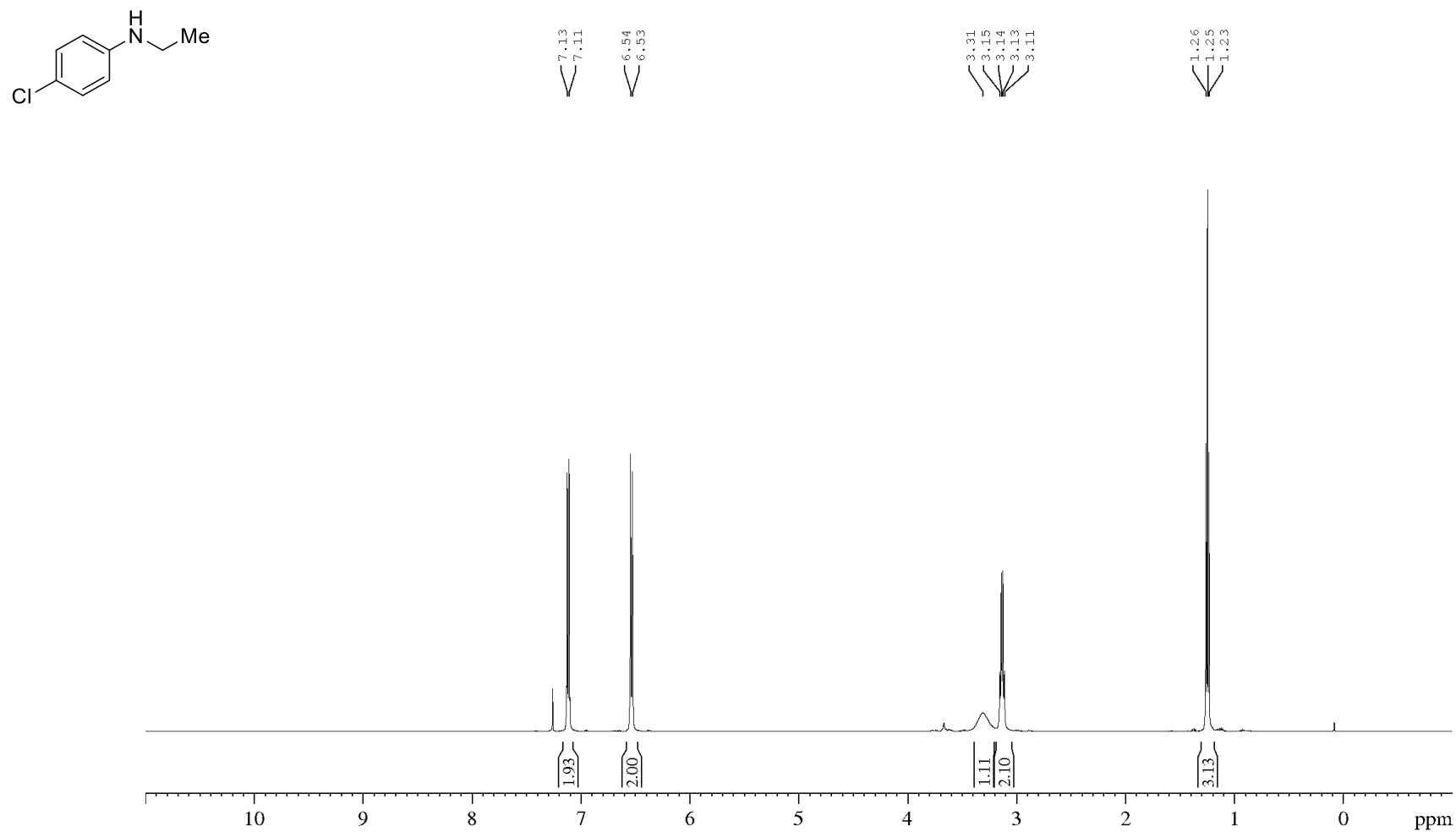
Figure S20. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **4-chloro-*N*-ethylaniline (2j)**.

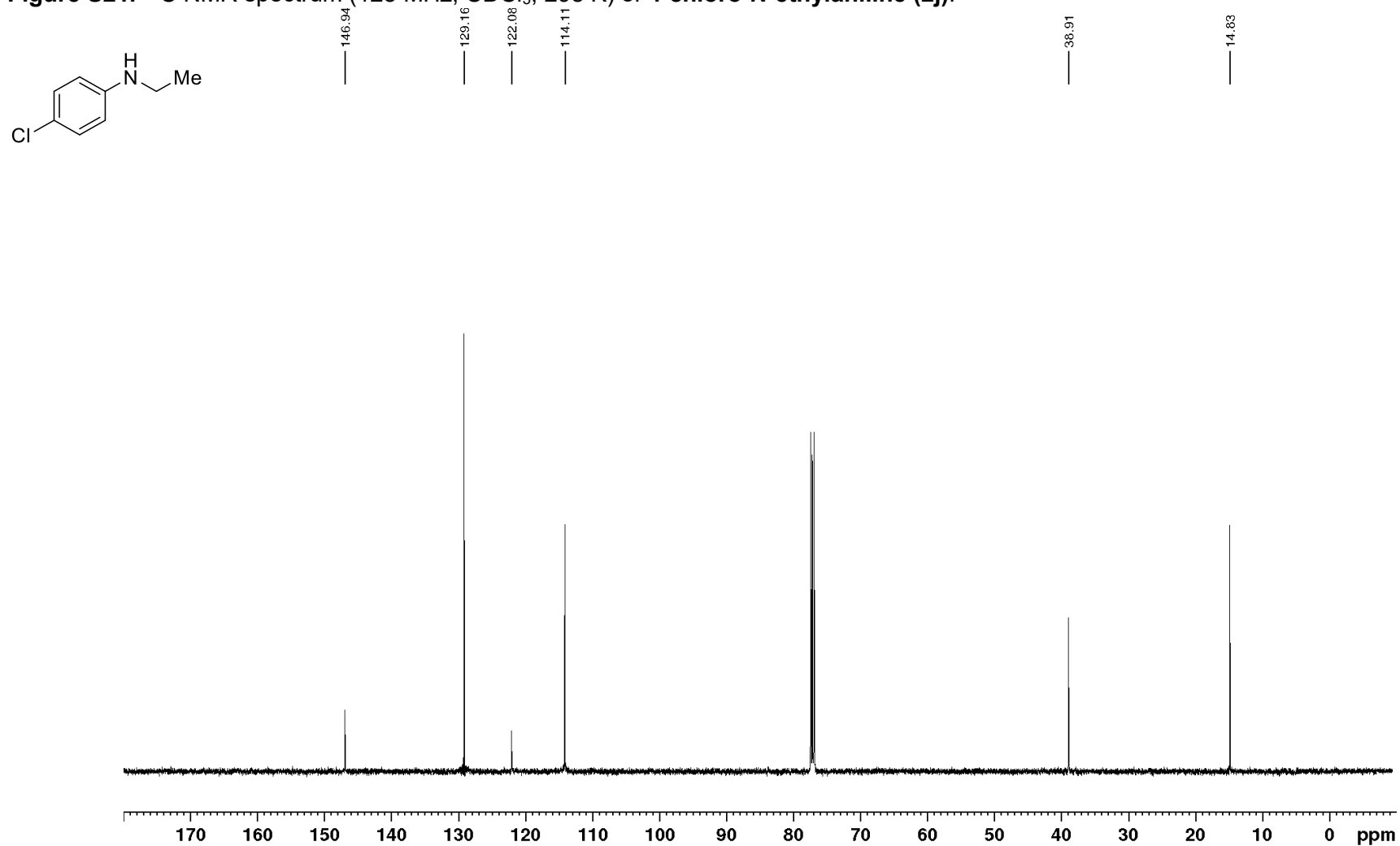
Figure S21. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 4-chloro-*N*-ethylaniline (2j).

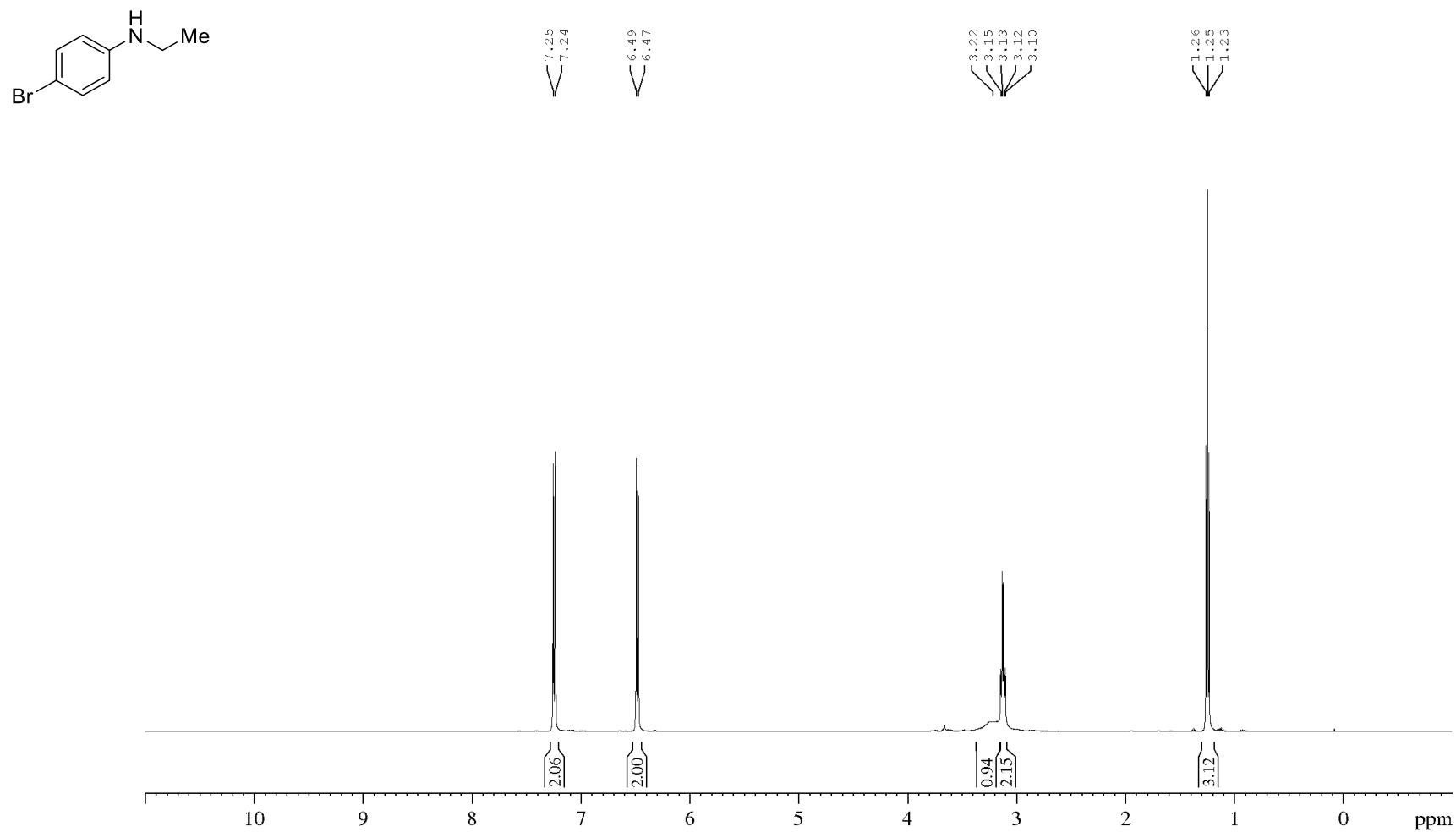
Figure S22. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **4-bromo-*N*-ethylaniline (2k)**.

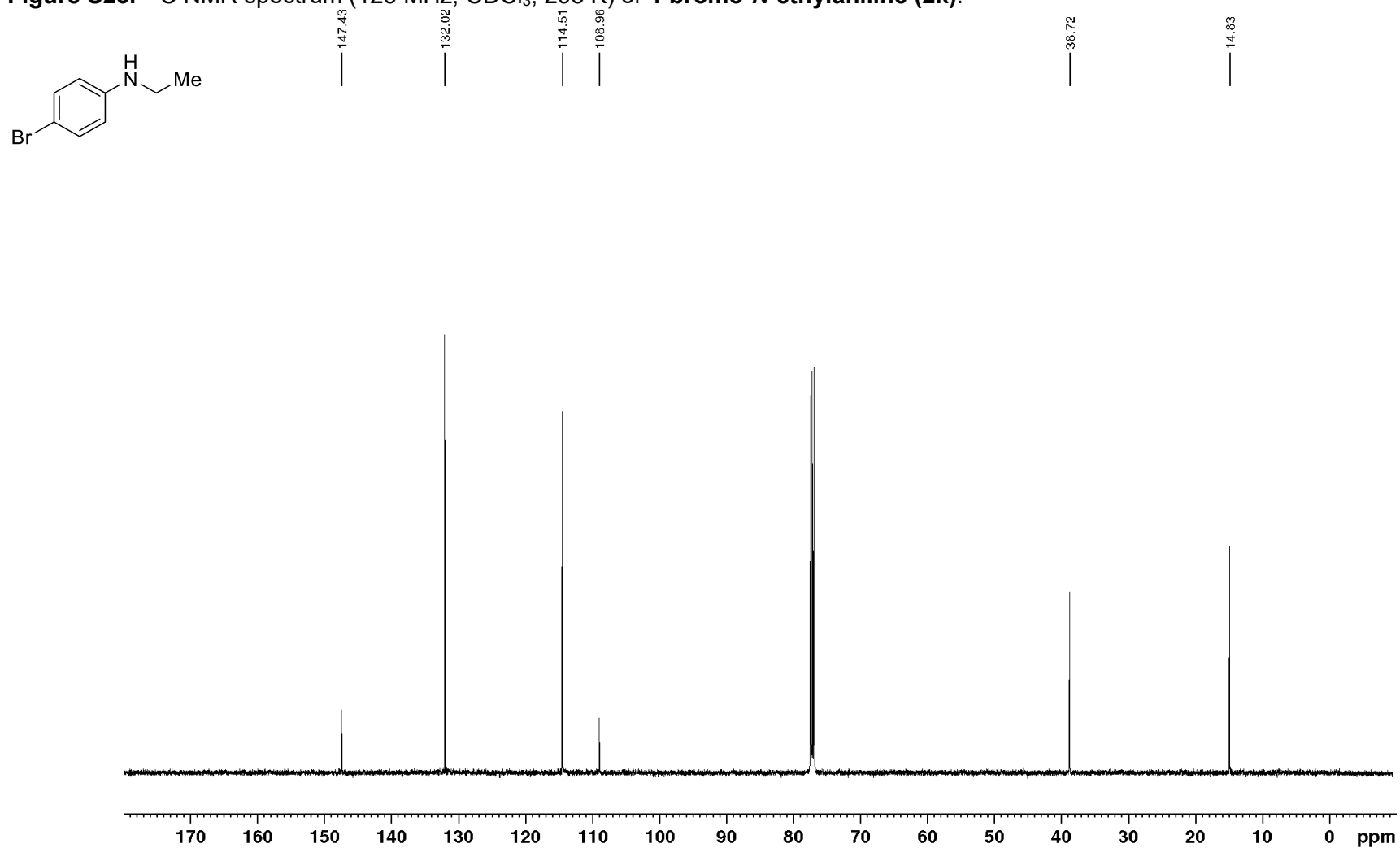
Figure S23. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 4-bromo-*N*-ethylaniline (2k).

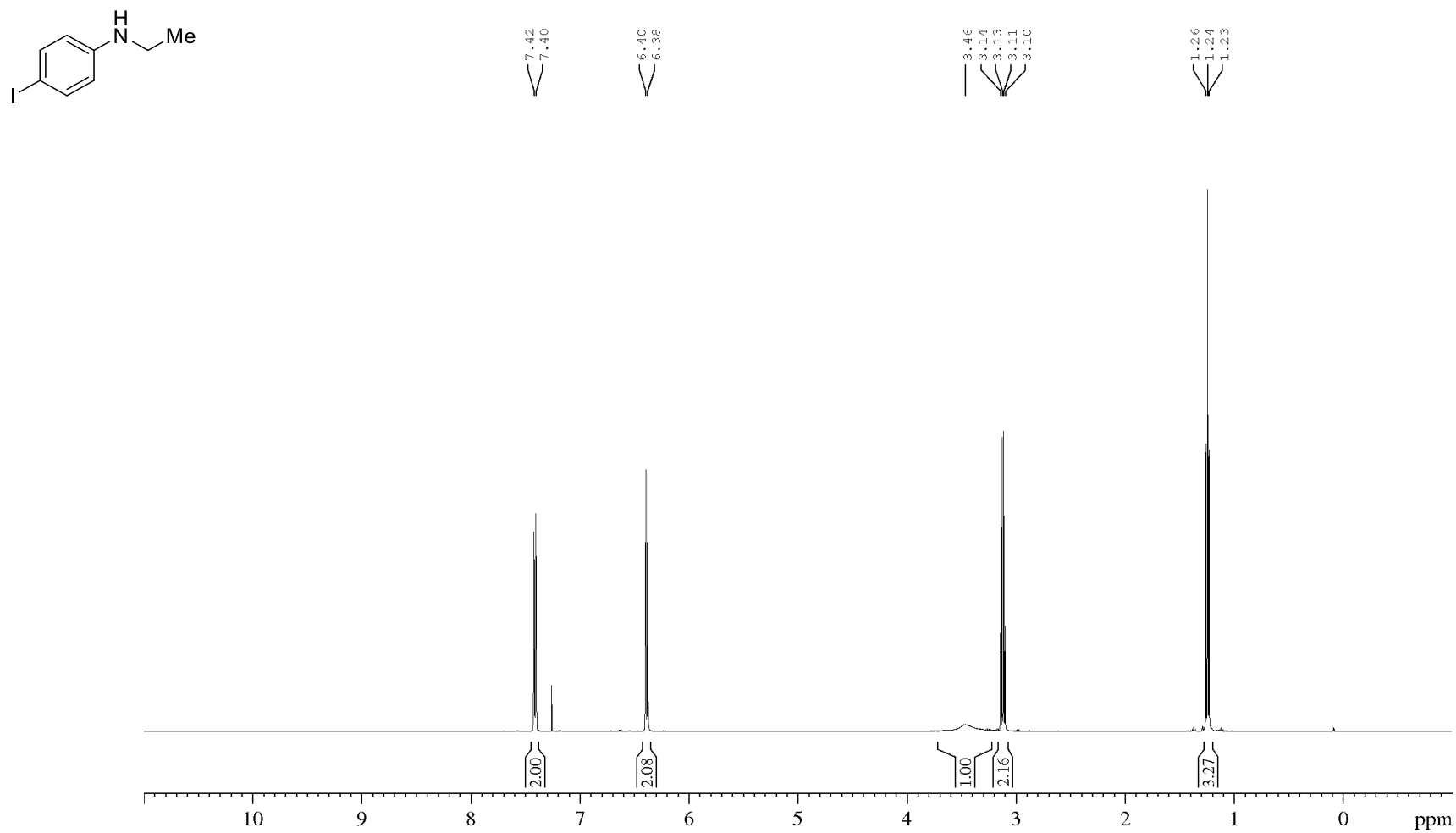
Figure S24. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethyl-4-iodoaniline (2l)**.

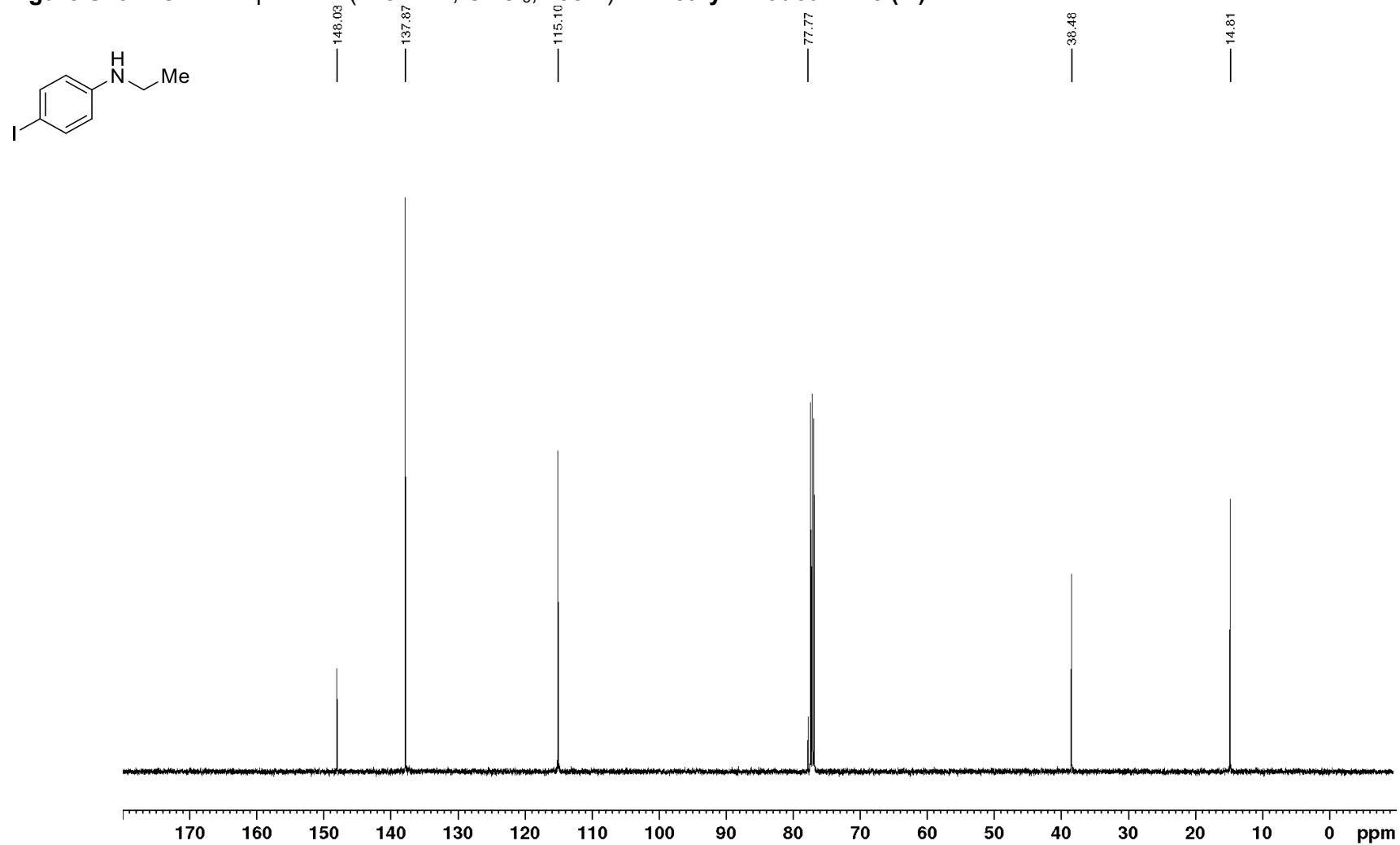
Figure S25. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-4-iodoaniline (**2l**).

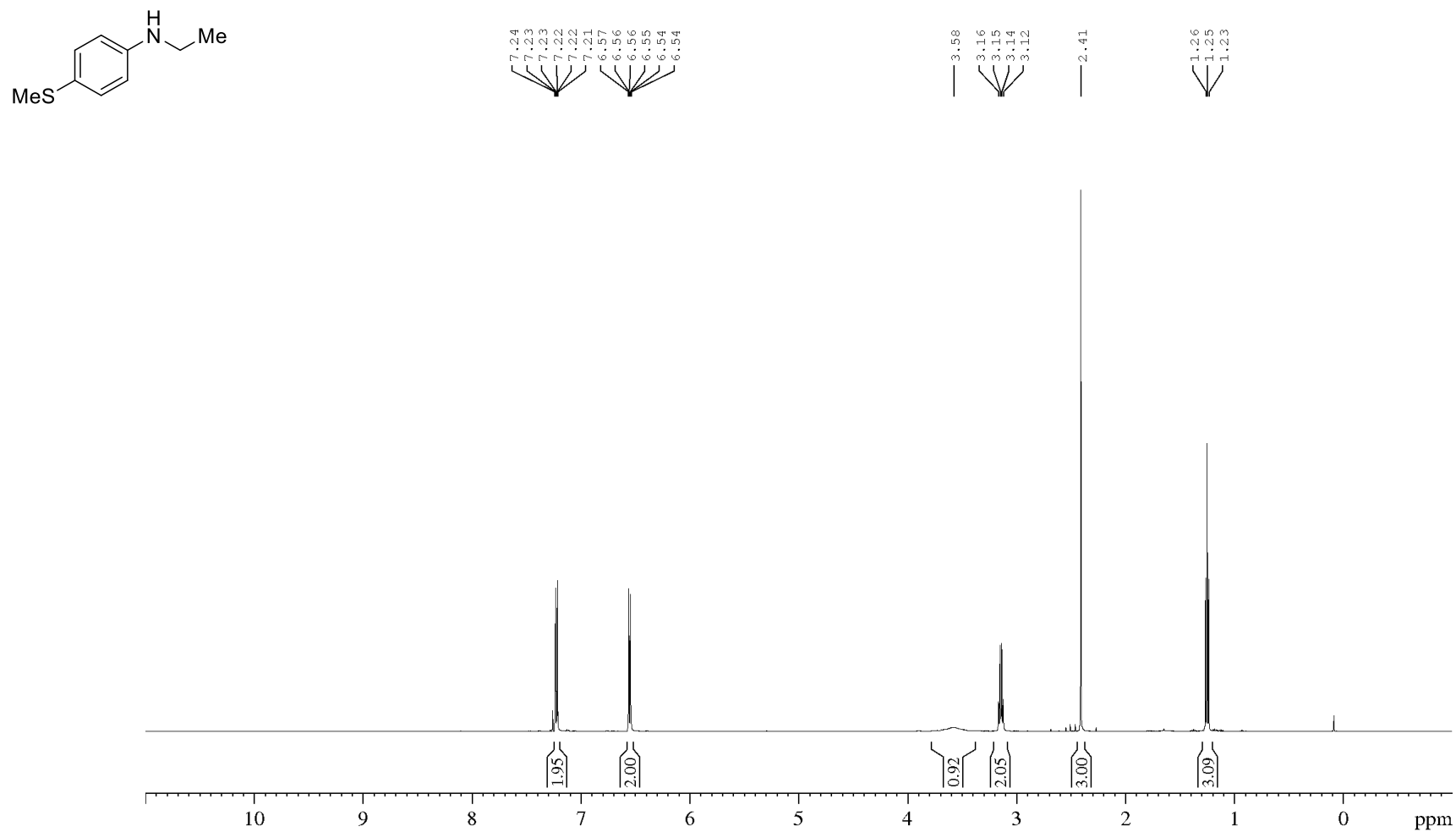
Figure S26. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-ethyl-4-(methylthio)aniline (**2n**).

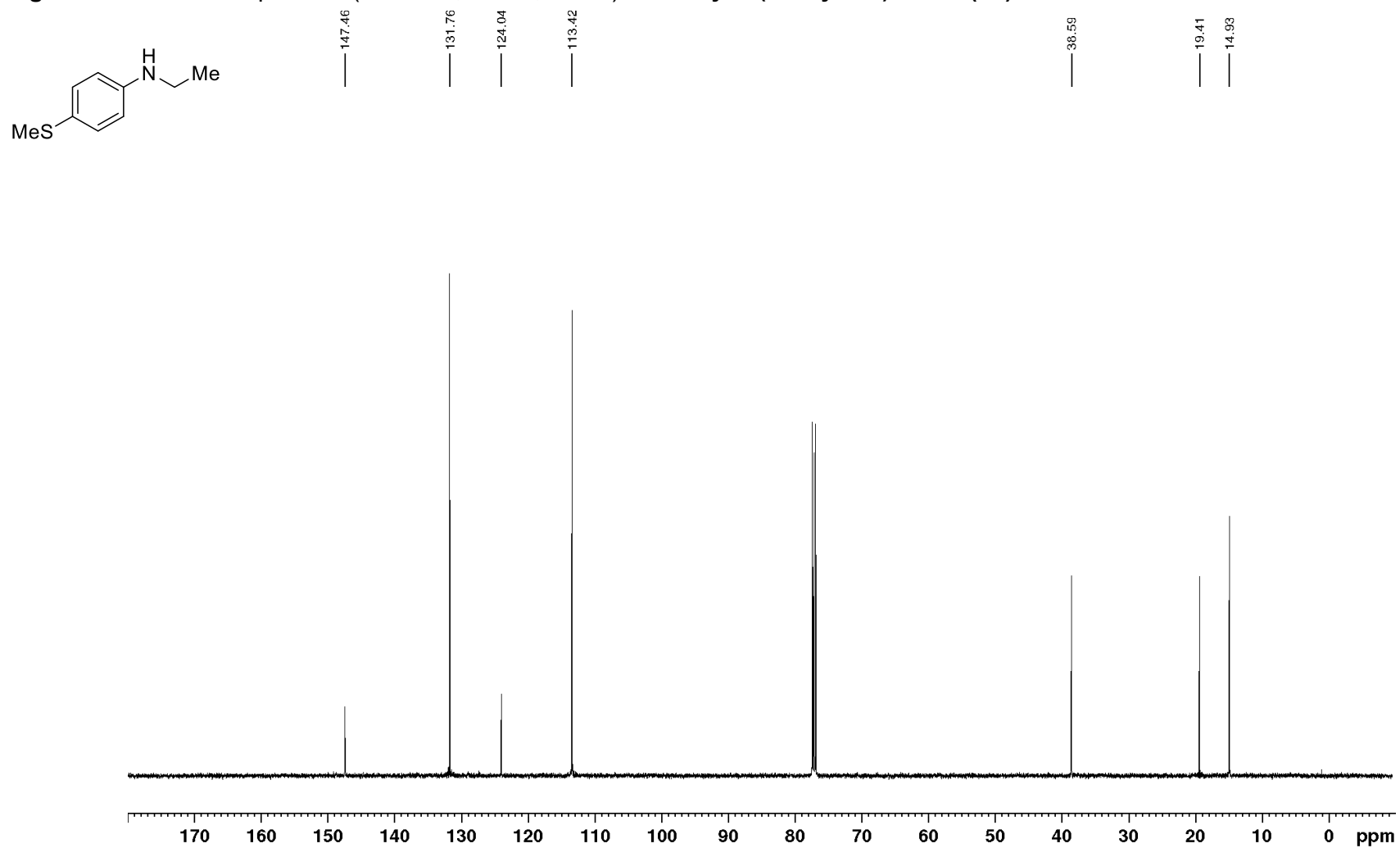
Figure S27. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-4-(methylthio)aniline (**2n**)

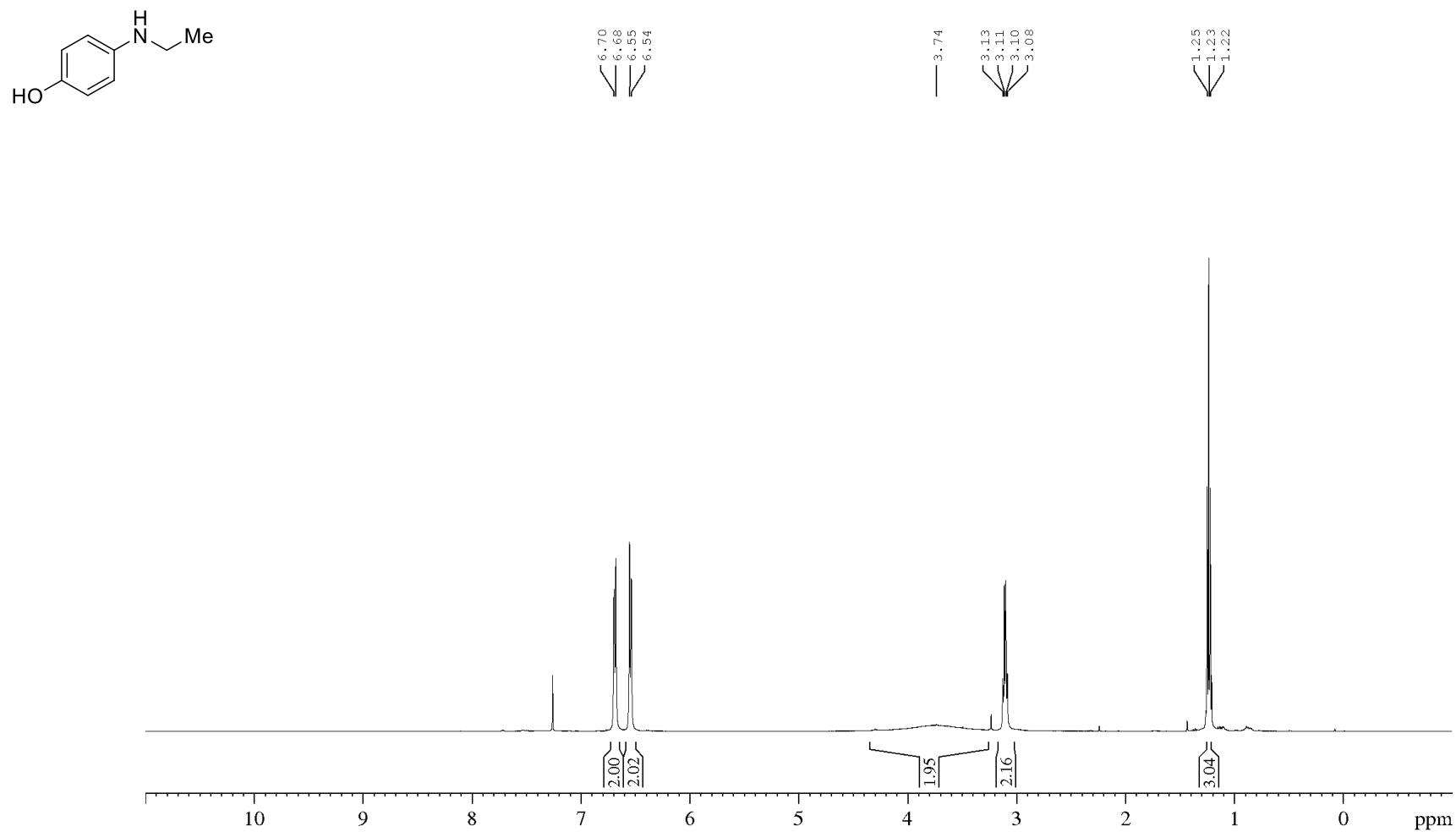
Figure S28. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **4-(ethylamino)phenol (2o)**.

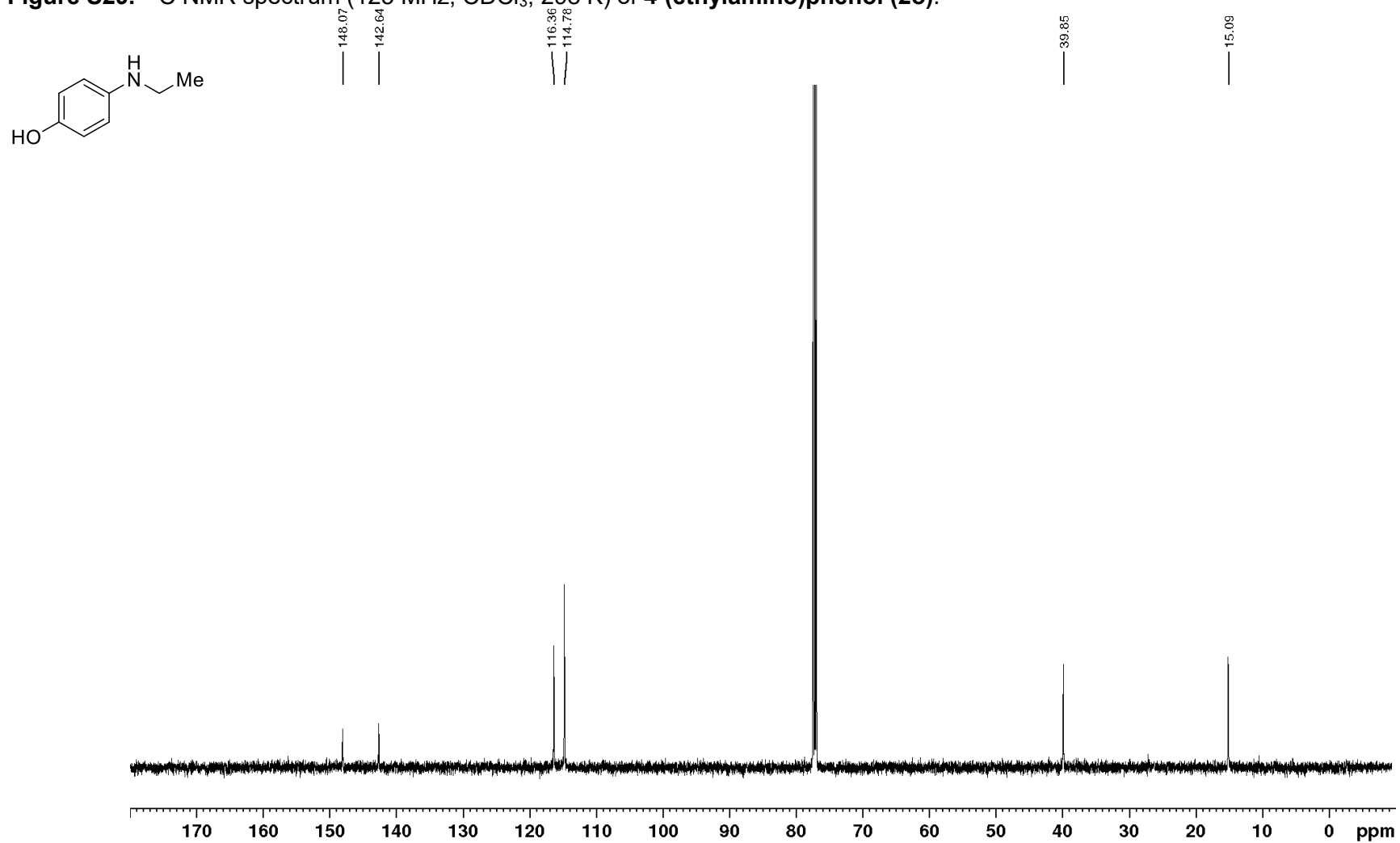
Figure S29. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 4-(ethylamino)phenol (2o).

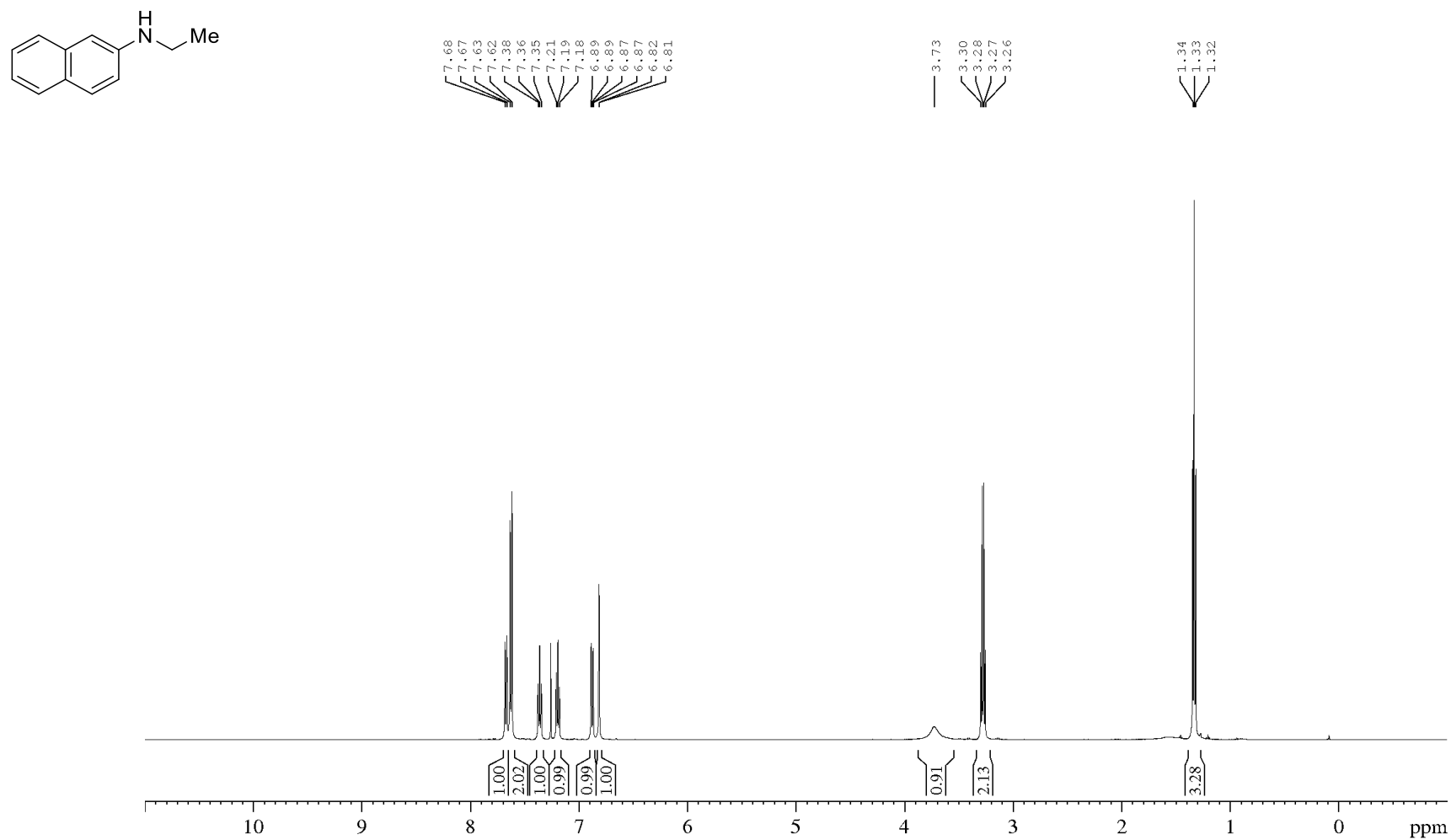
Figure S30. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethylnaphthalen-2-amine (2q)**.

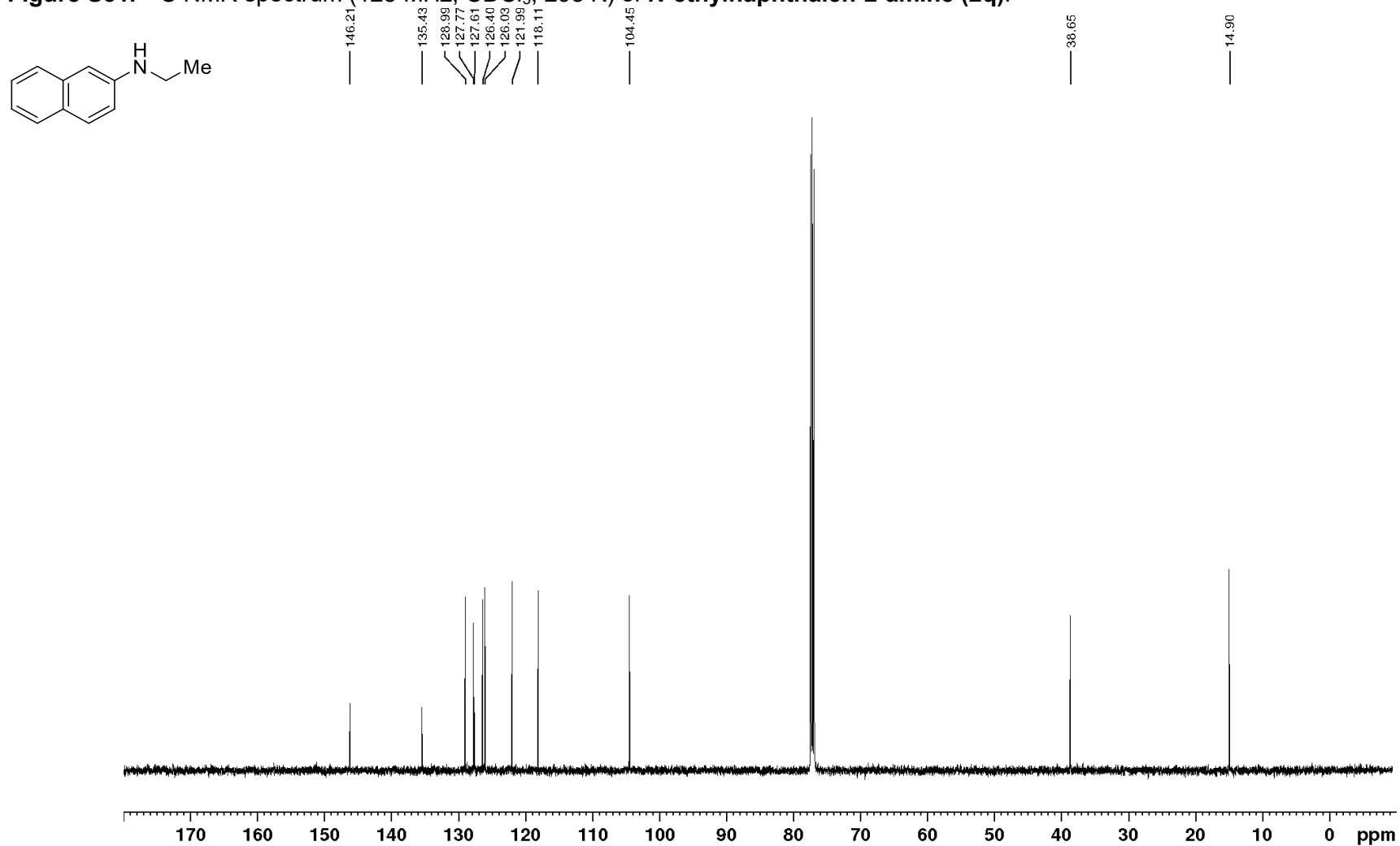
Figure S31. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethylnaphthalen-2-amine (2q).

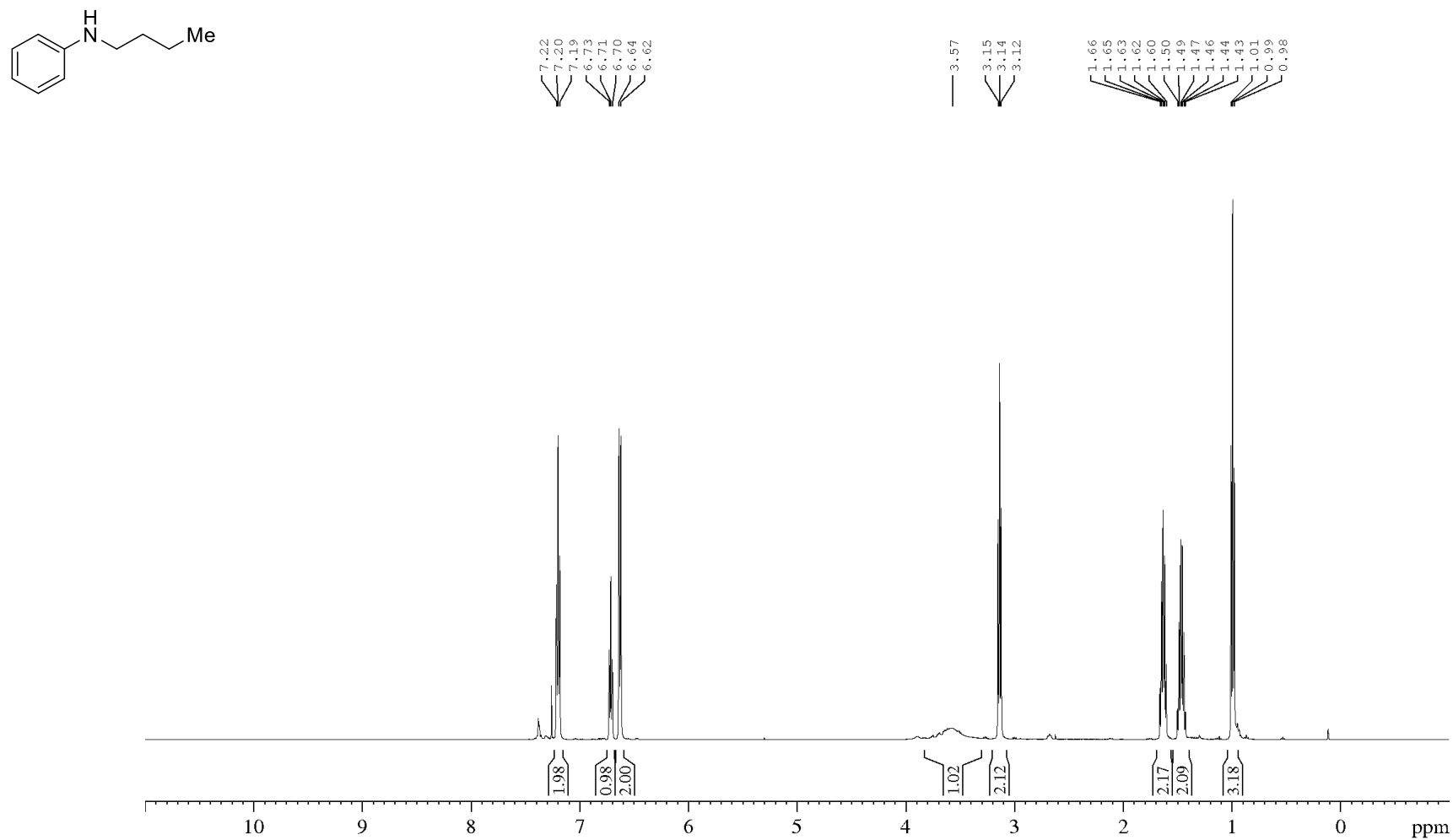
Figure S32. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-butylaniline (**2r**).

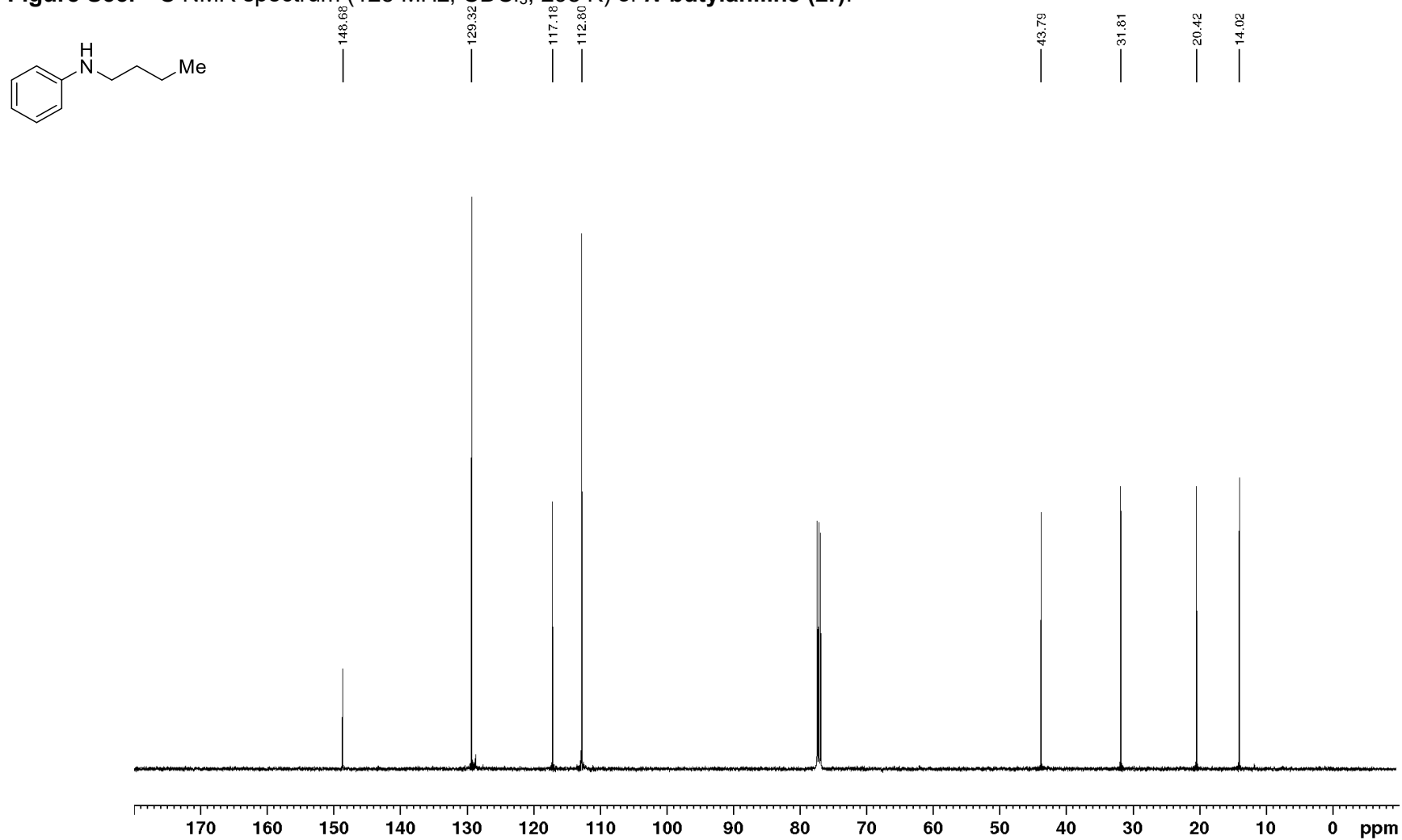
Figure S33. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-butylaniline (**2r**).

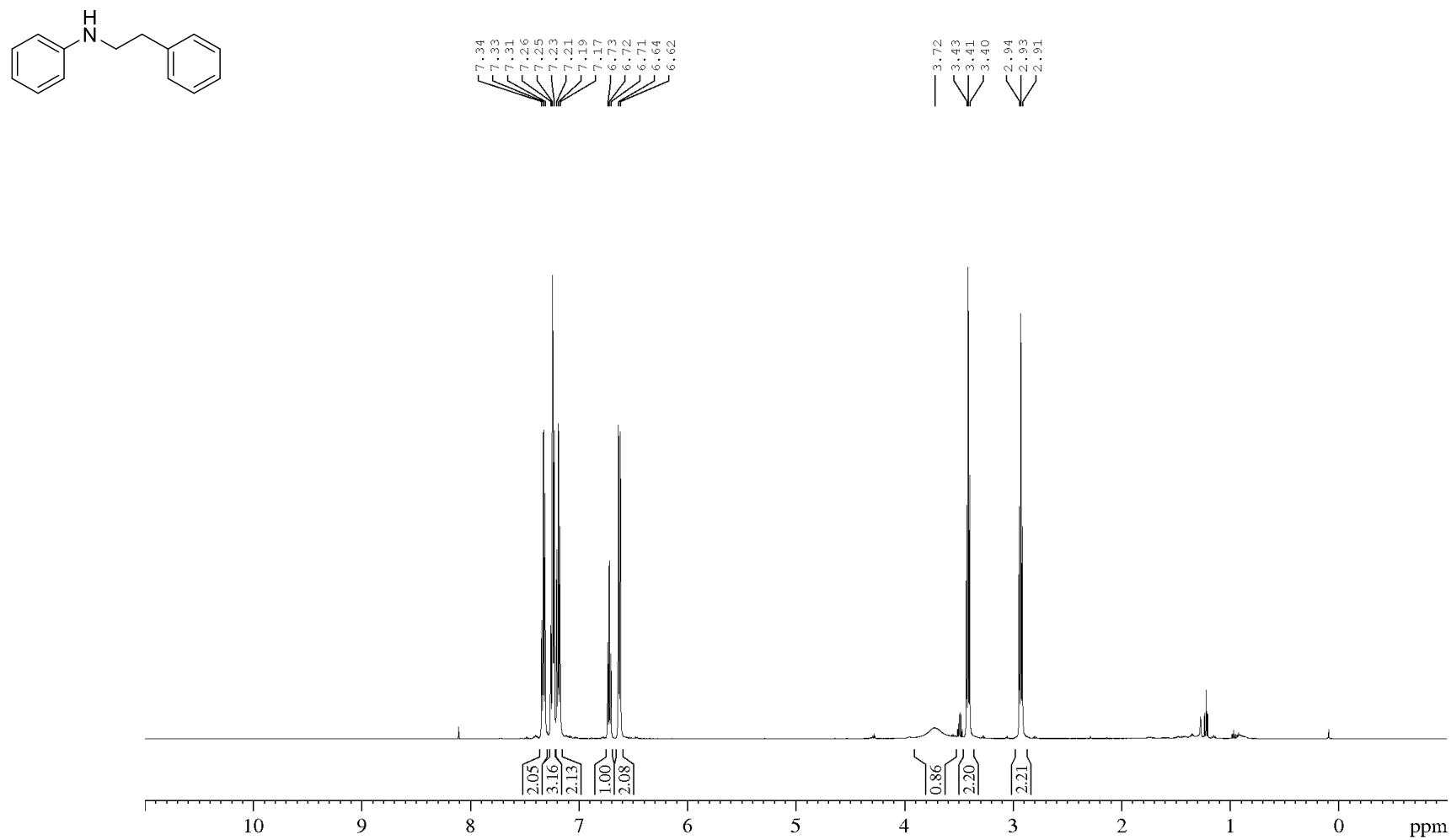
Figure S34. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-phenethylamine (2s)**.

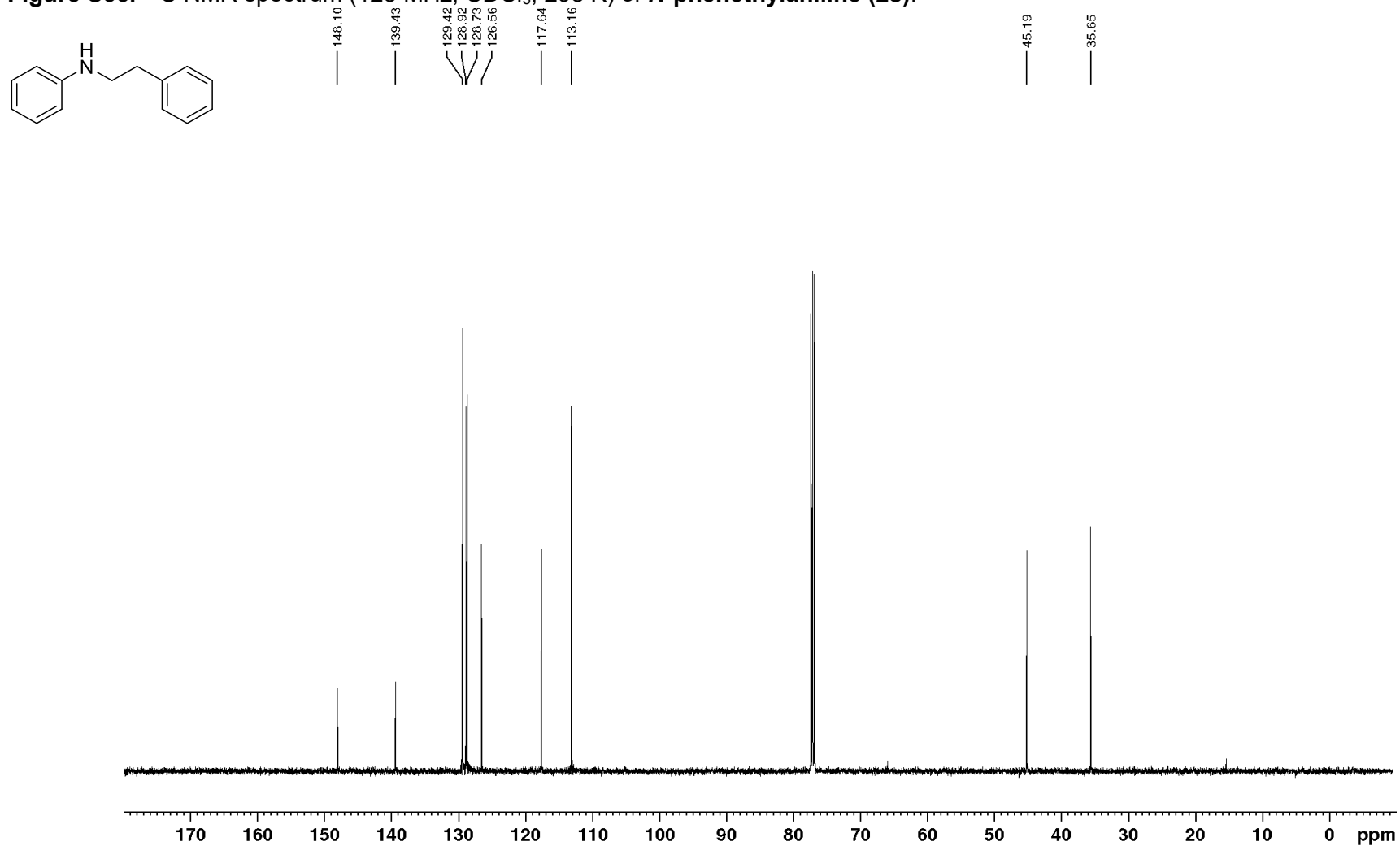
Figure S35. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-phenethylamine (2s).

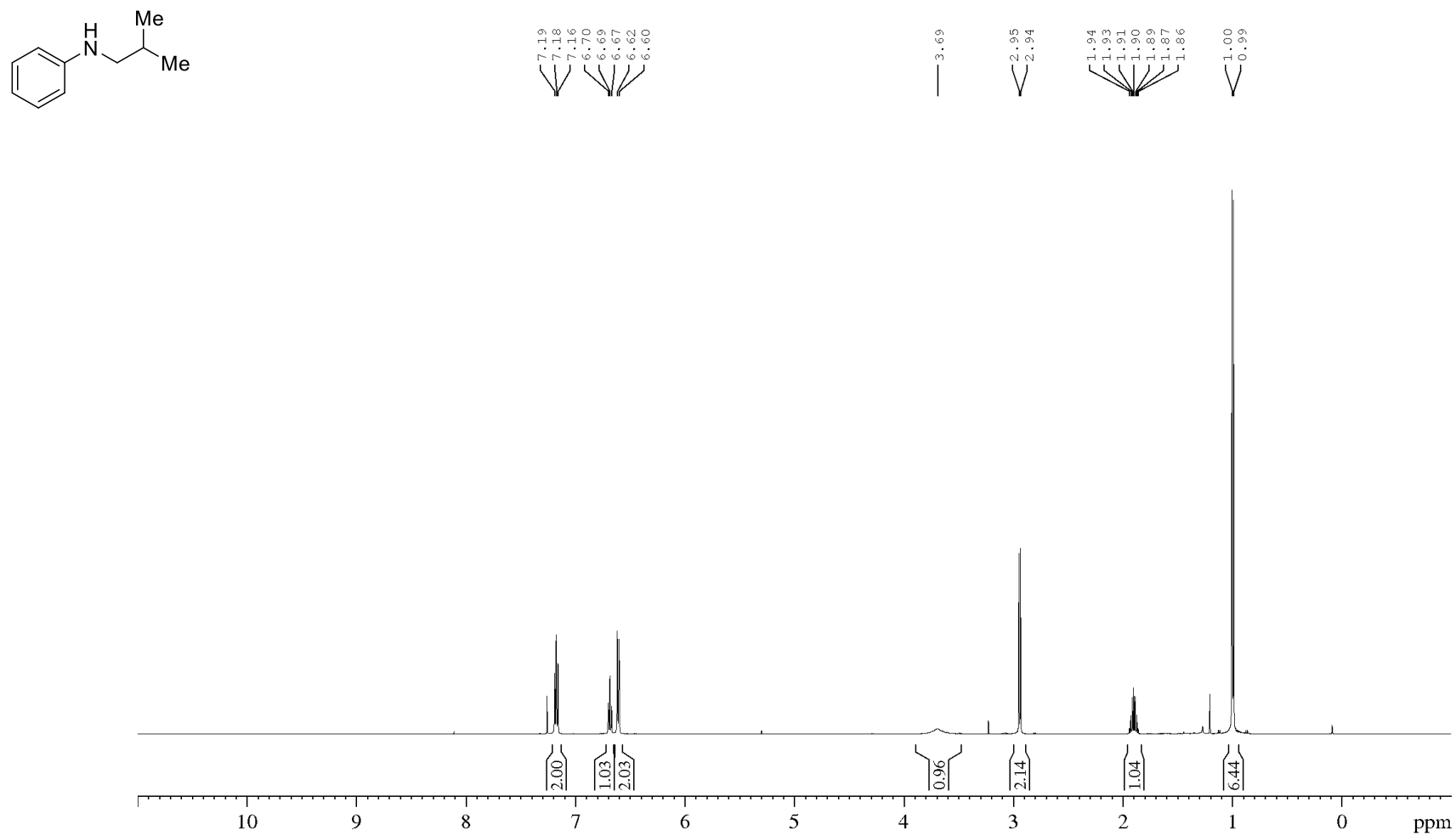
Figure S36. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-isobutylaniline (S2a)**.

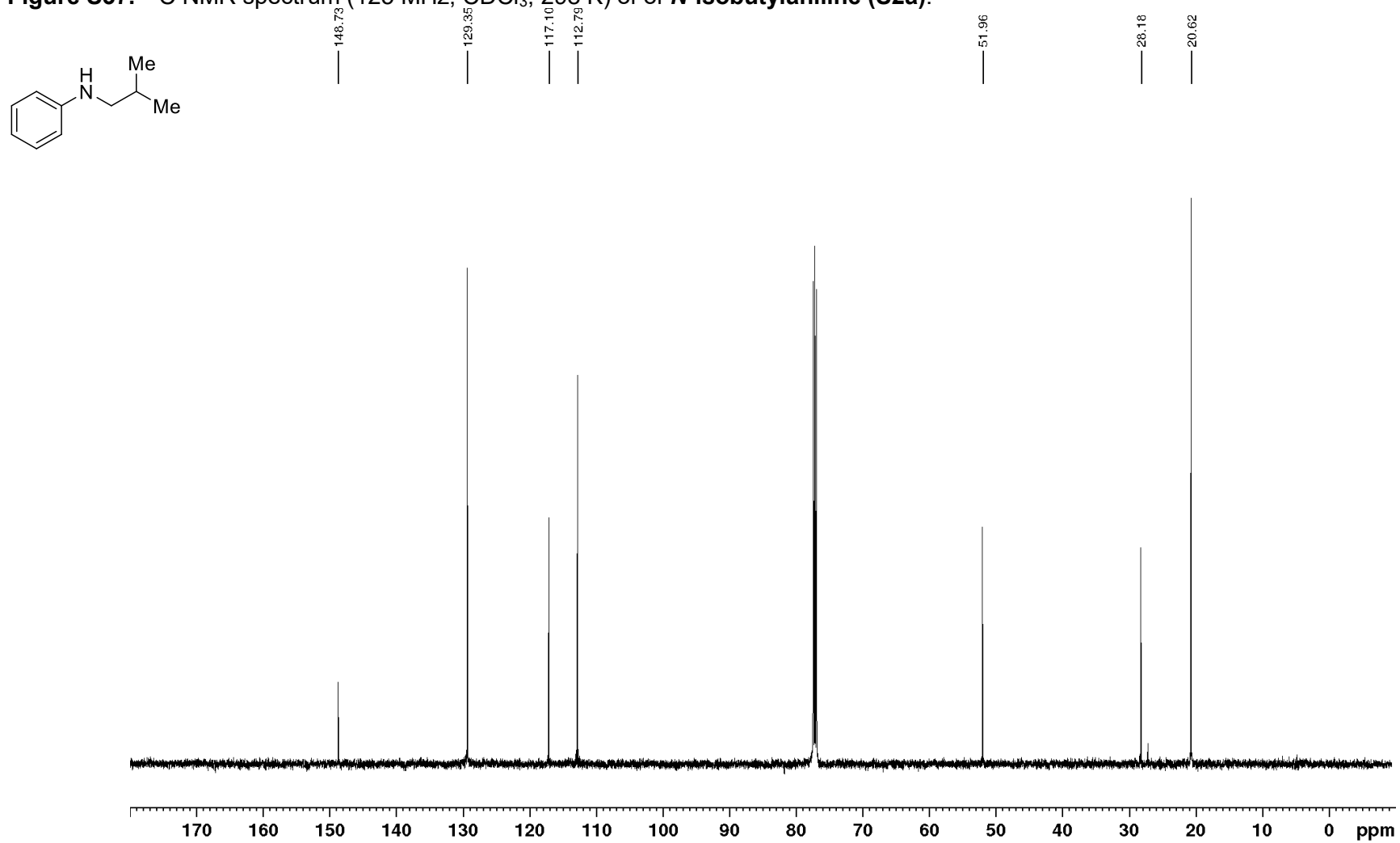
Figure S37. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-isobutylaniline (S2a).

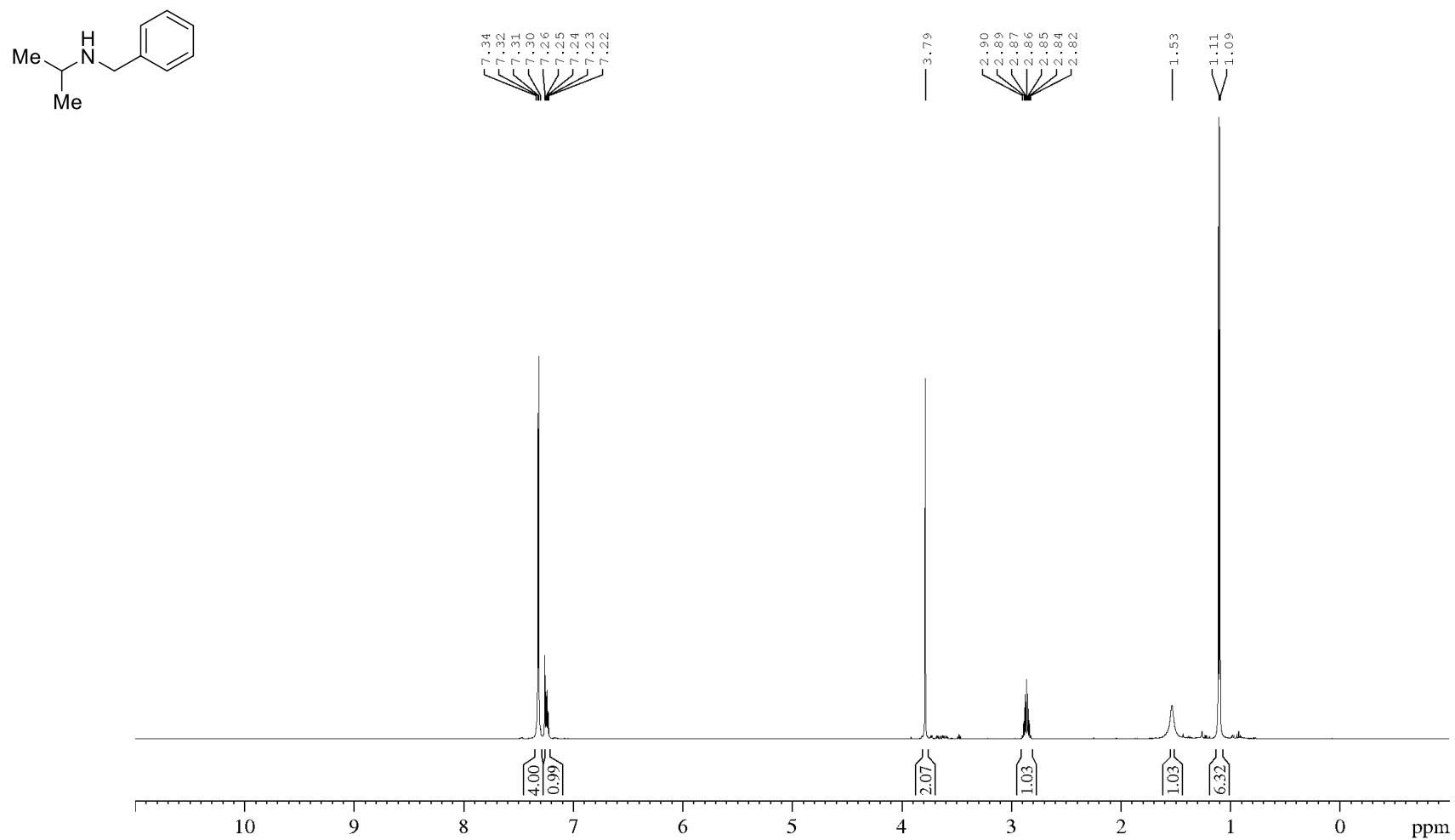
Figure S38. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-benzylpropan-2-amine (**S2a'**).

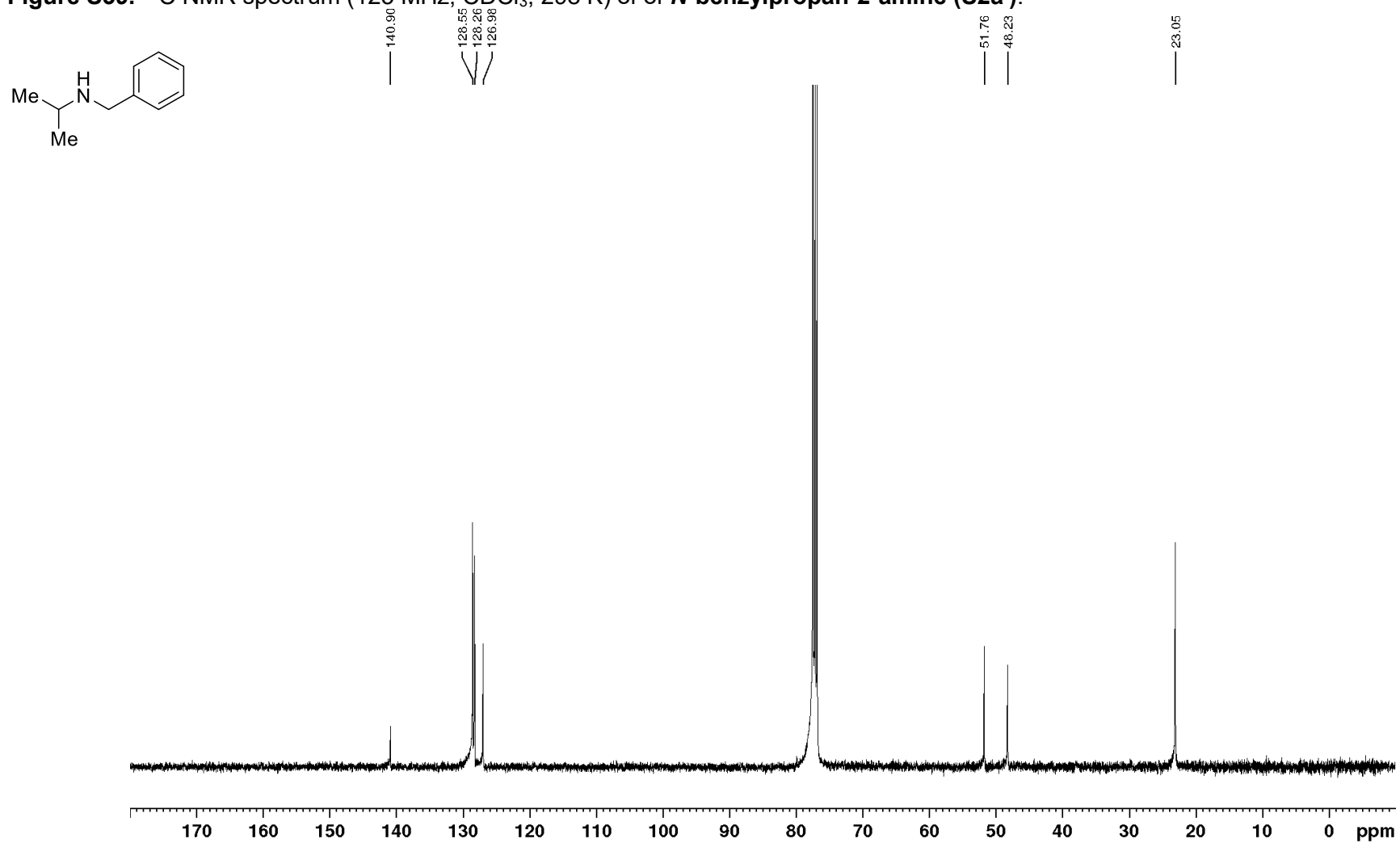
Figure S39. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-benzylpropan-2-amine (**S2a'**).

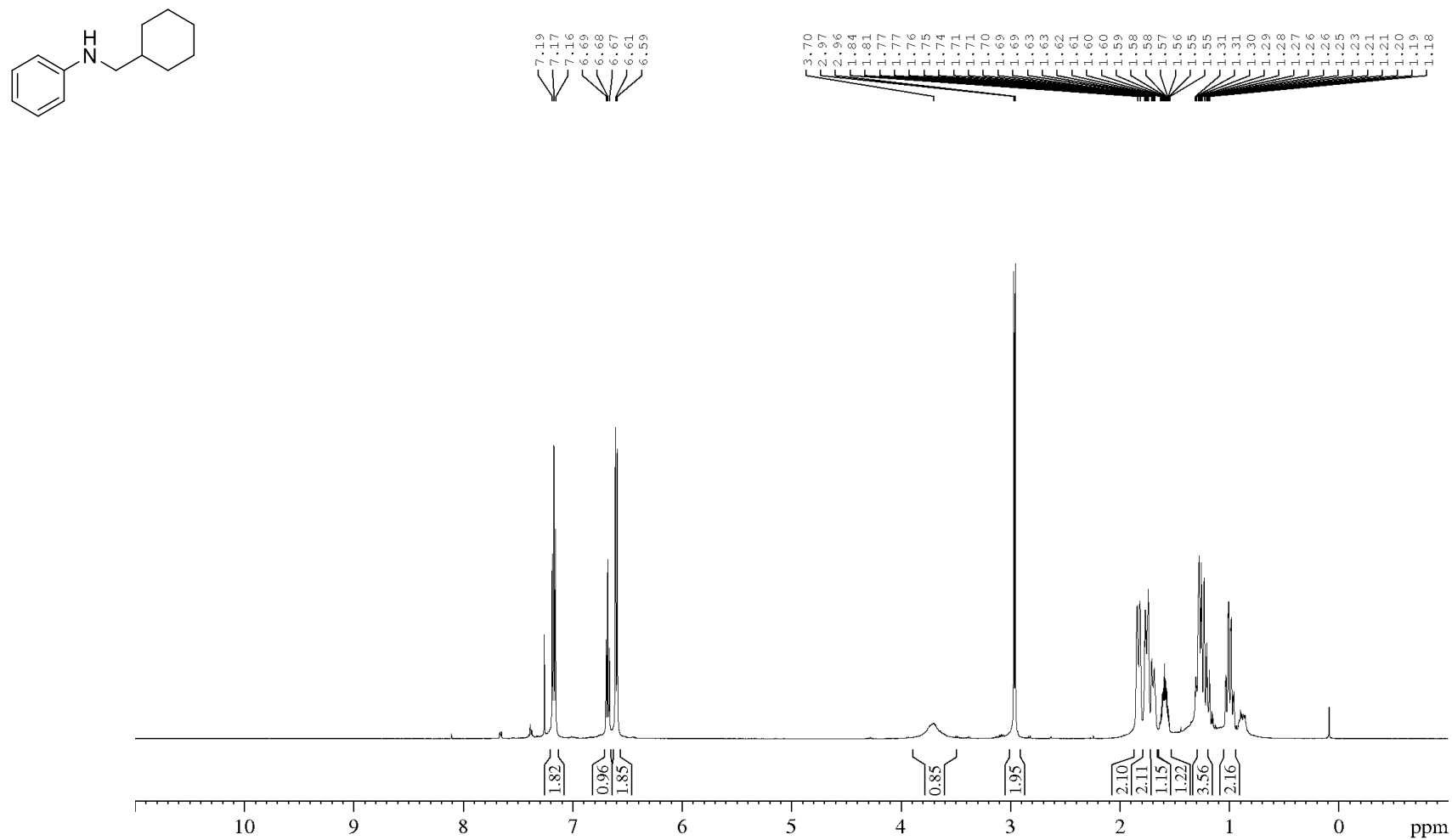
Figure S40. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-(cyclohexylmethyl)aniline (**S2b**).

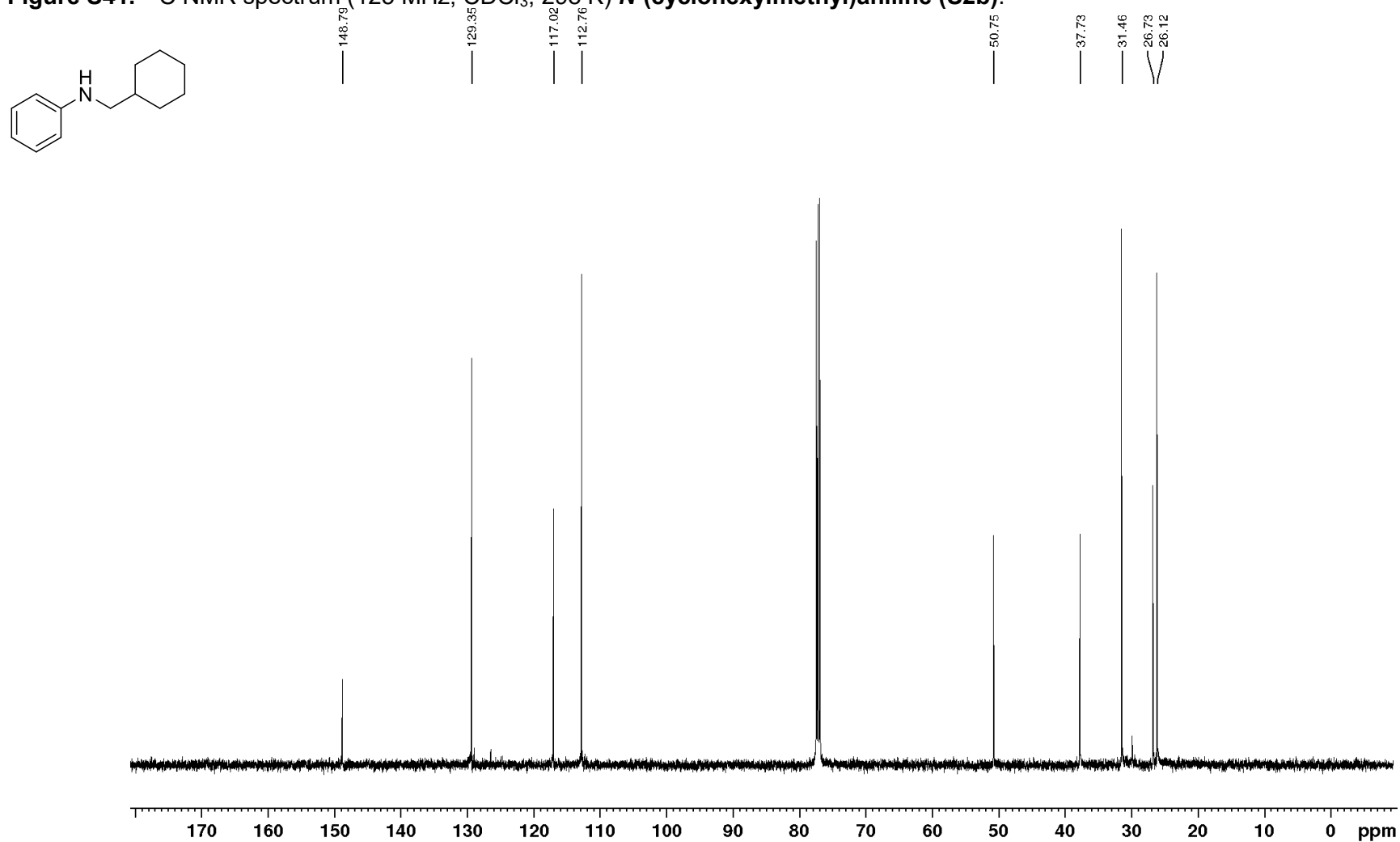
Figure S41. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) *N*-(cyclohexylmethyl)aniline (**S2b**).

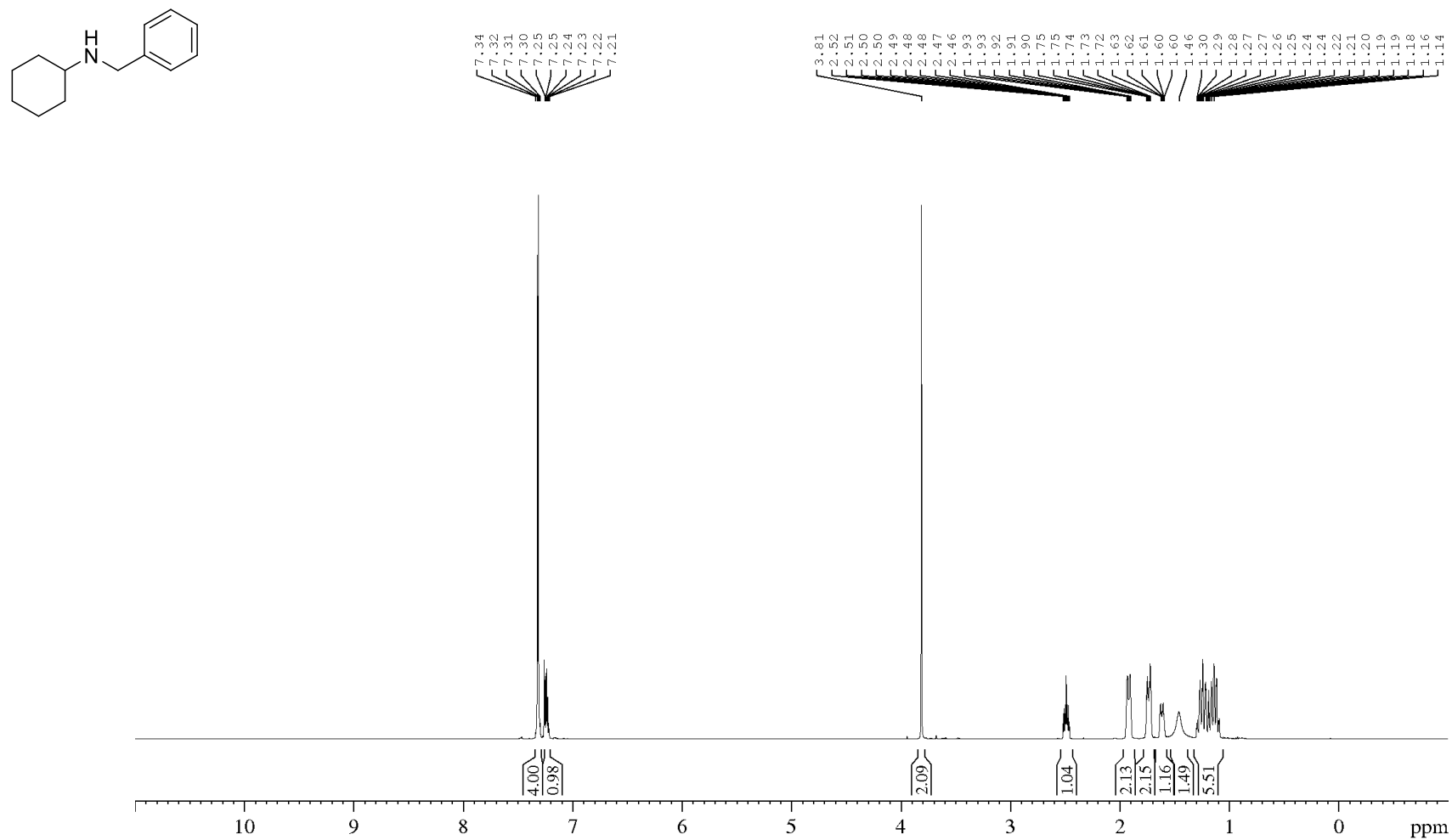
Figure S42. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-benzylcyclohexanamine (**S2b'**).

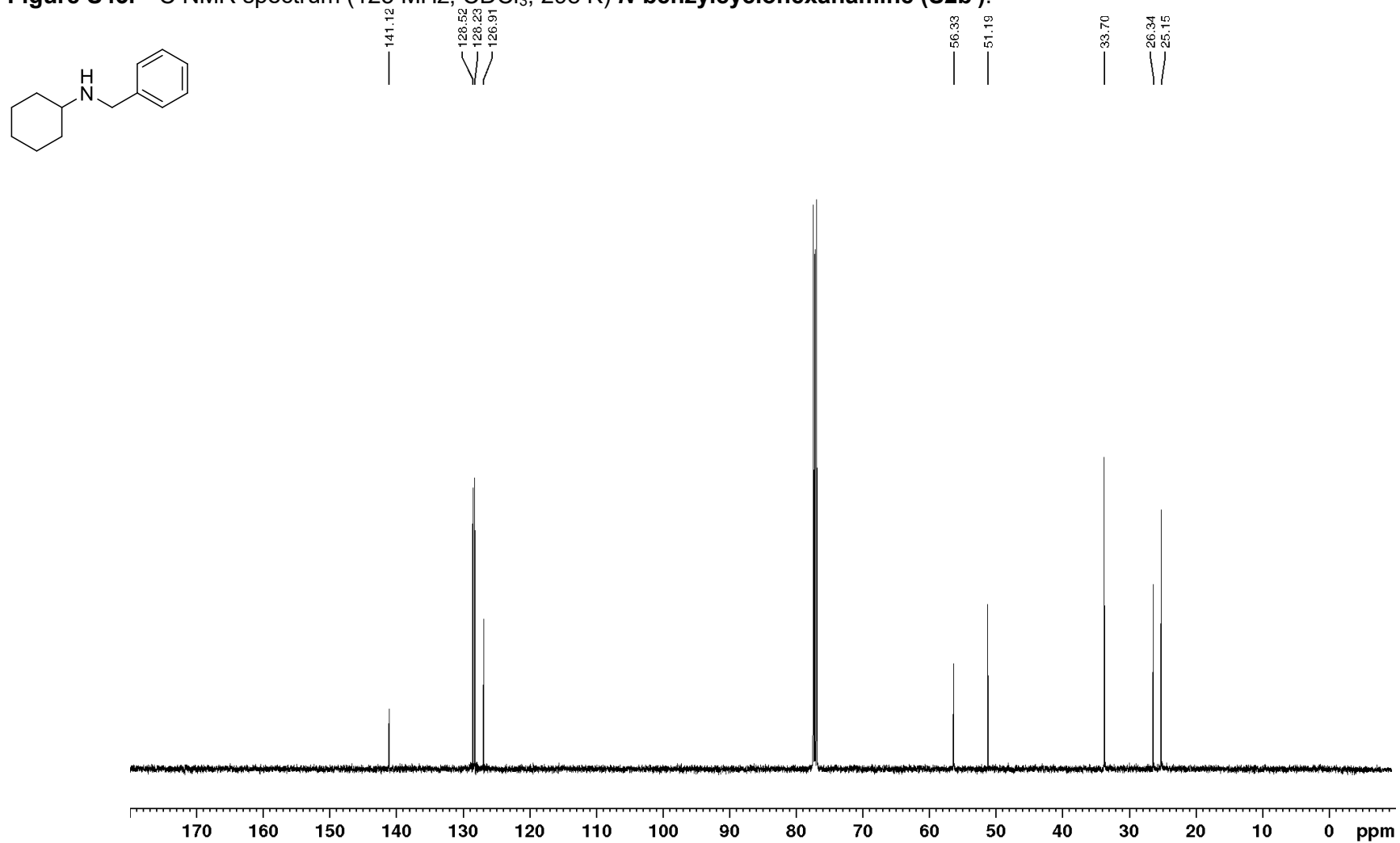
Figure S43. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) *N*-benzylcyclohexanamine (**S2b'**).

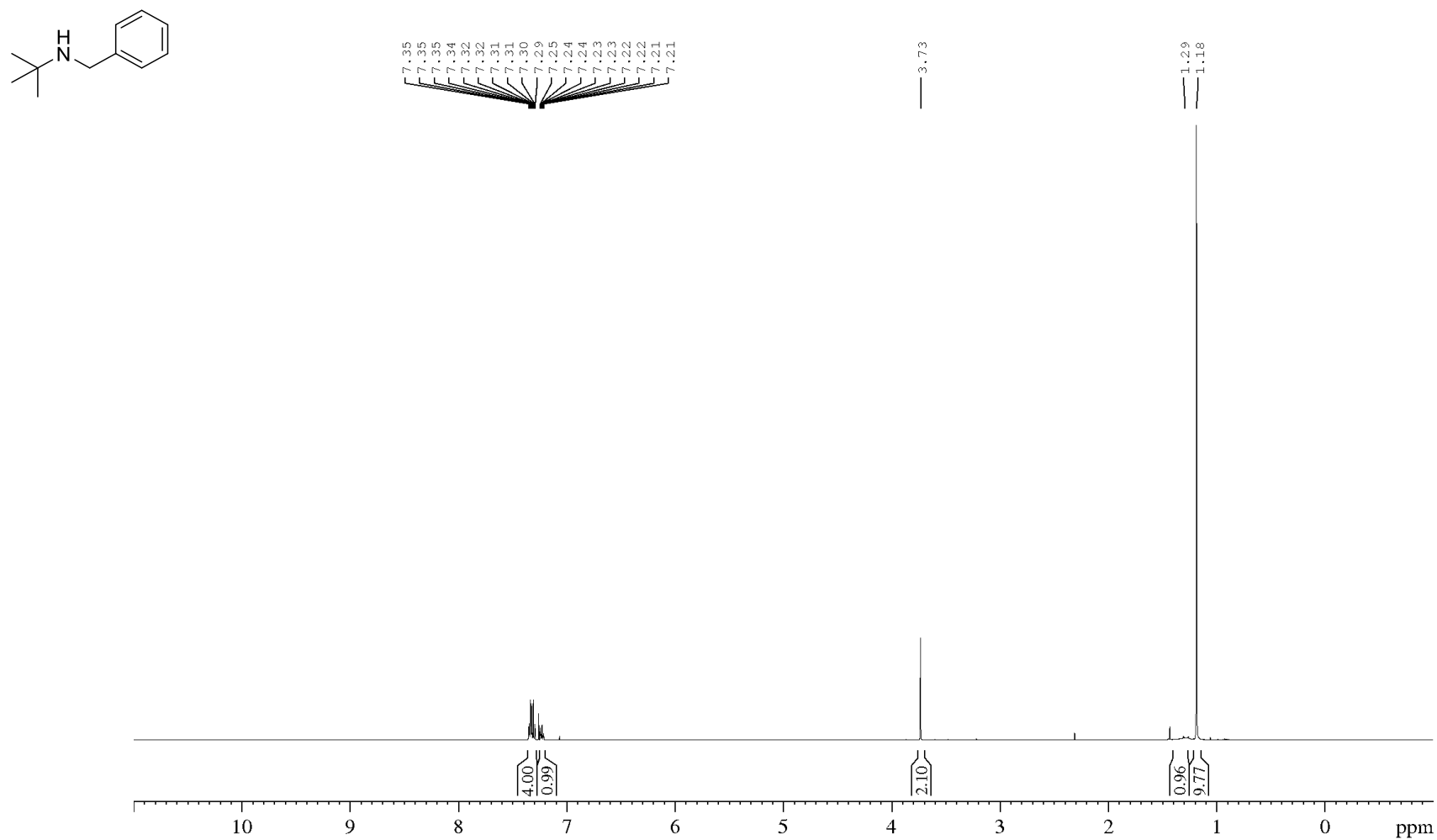
Figure S44. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-benzyl-2-methylpropan-2-amine (S2c')**.

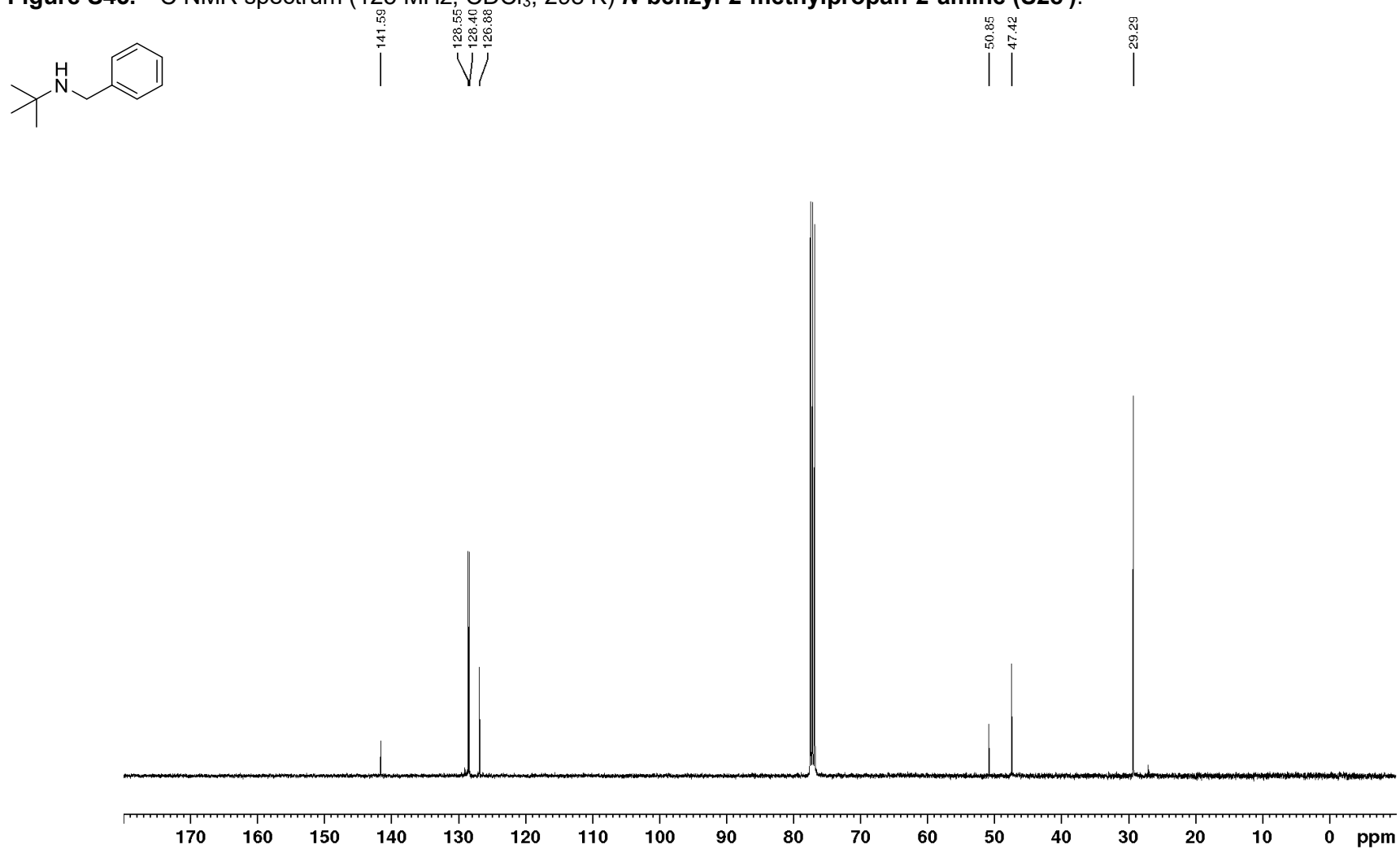
Figure S45. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) *N*-benzyl-2-methylpropan-2-amine (S2c').

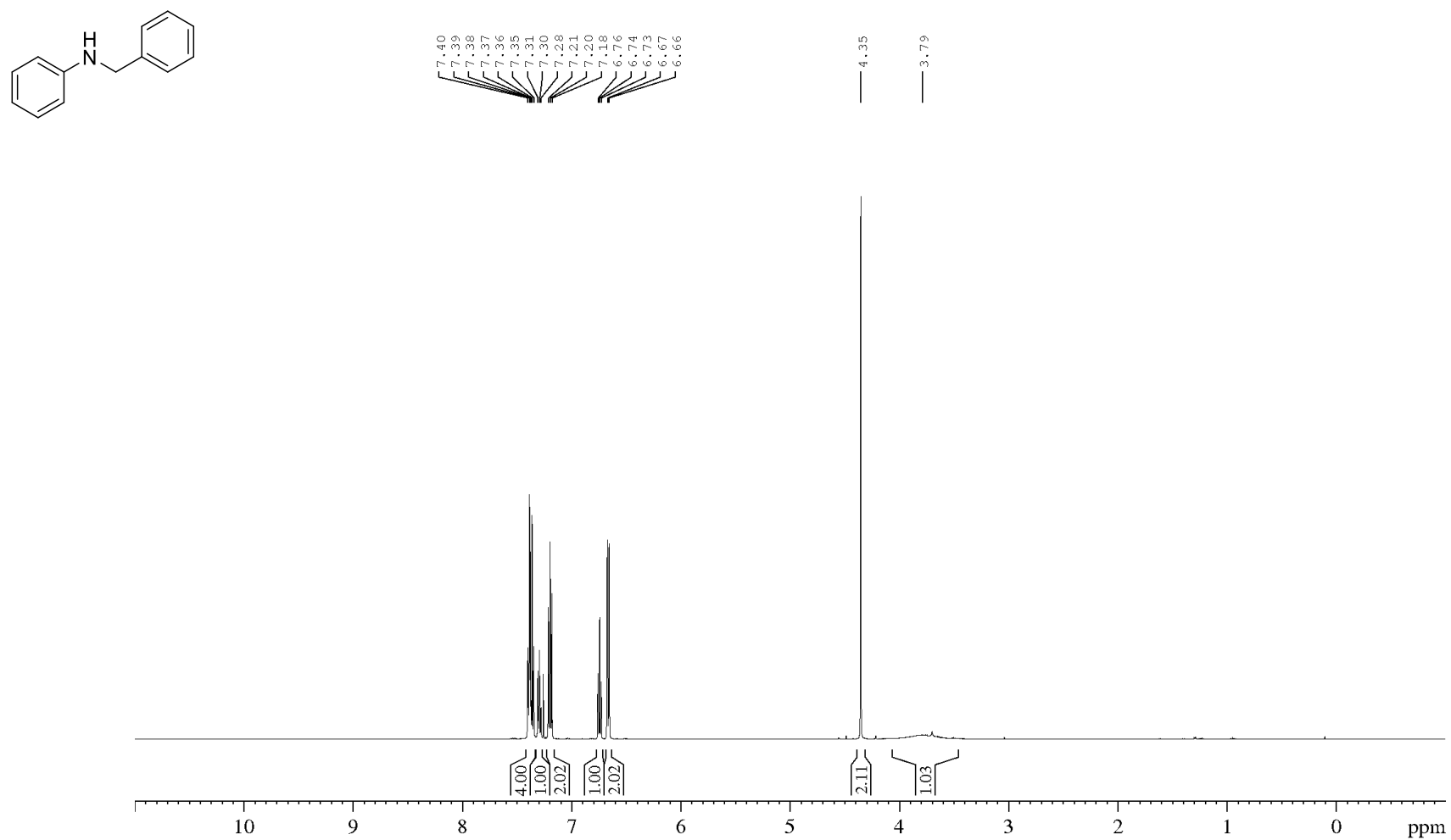
Figure S46. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-benzylaniline (2t)**.

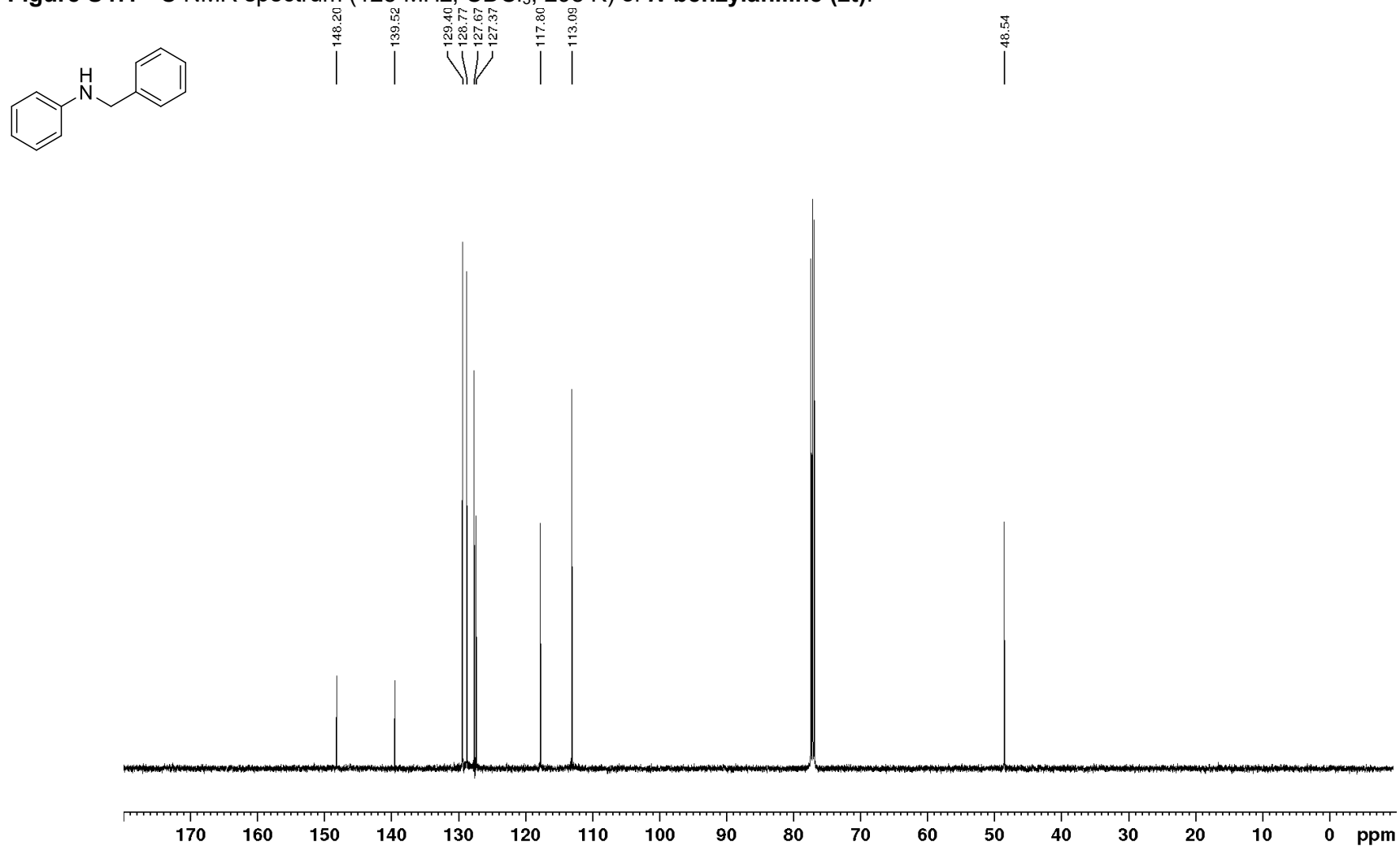
Figure S47. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-benzylaniline (2t).

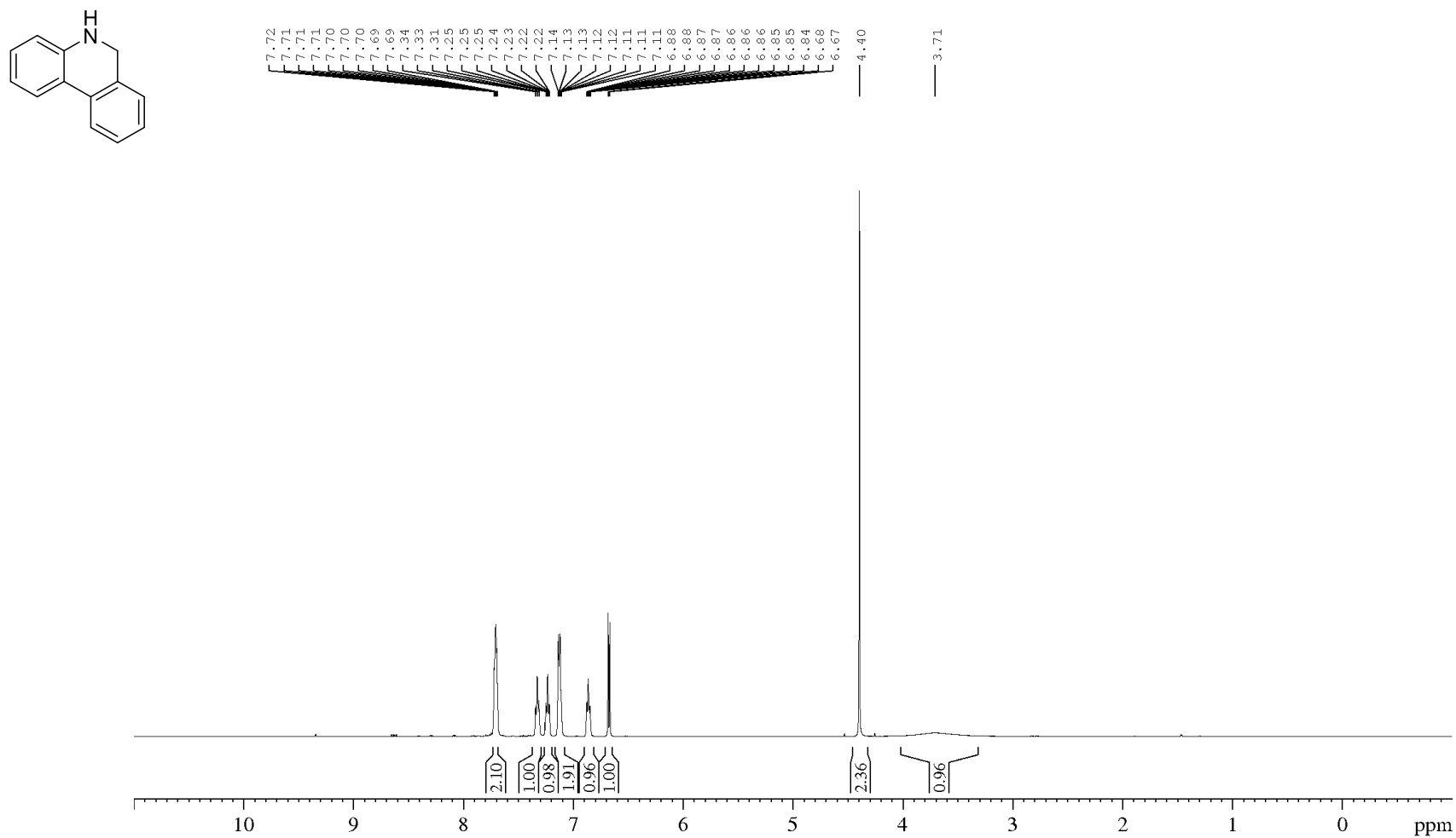
Figure S48. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **5,6-dihydrophenanthridine (2u)**.

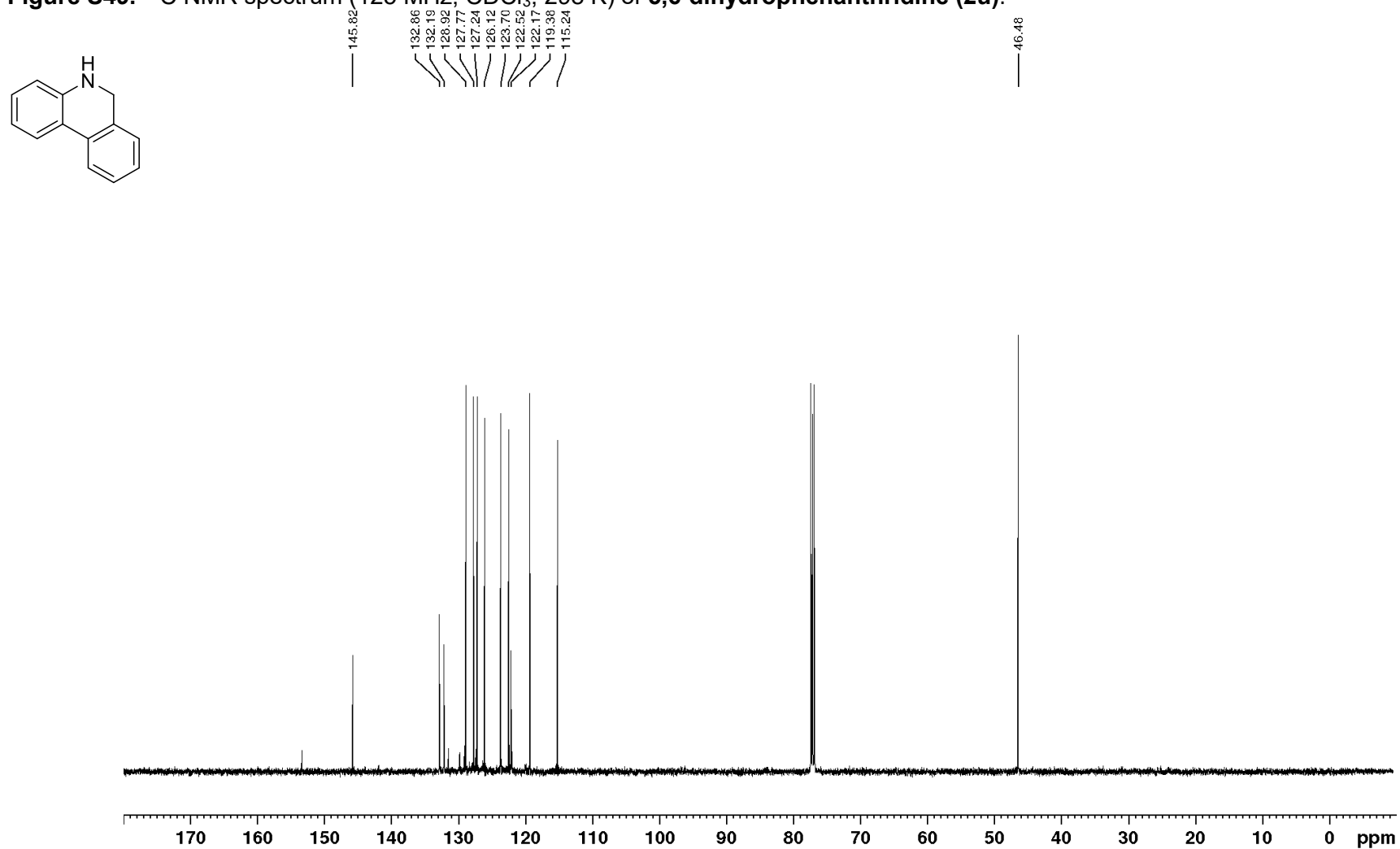
Figure S49. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 5,6-dihydrophenanthridine (2u).

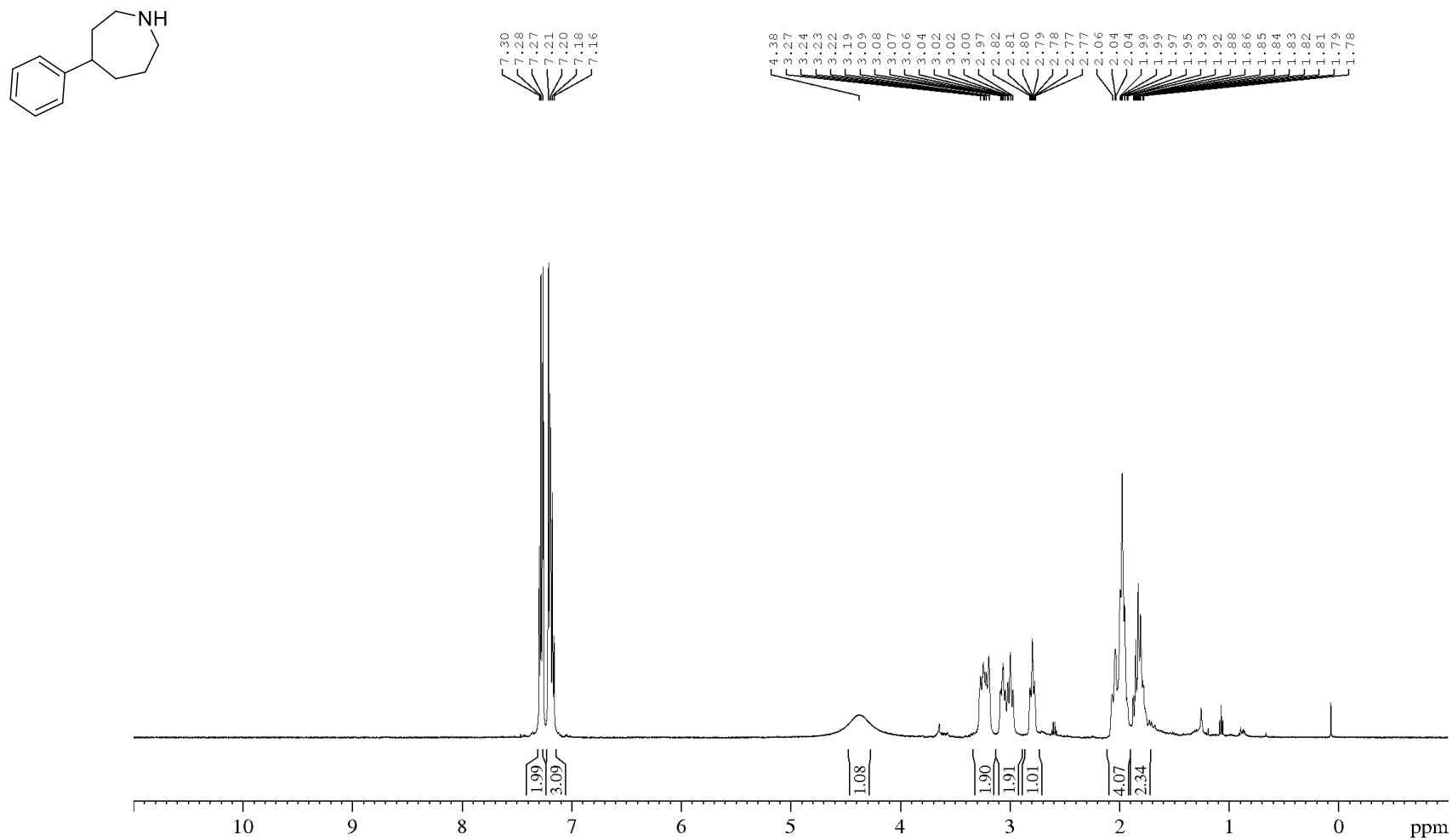
Figure S50. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **4-phenylazepane (2w)**.

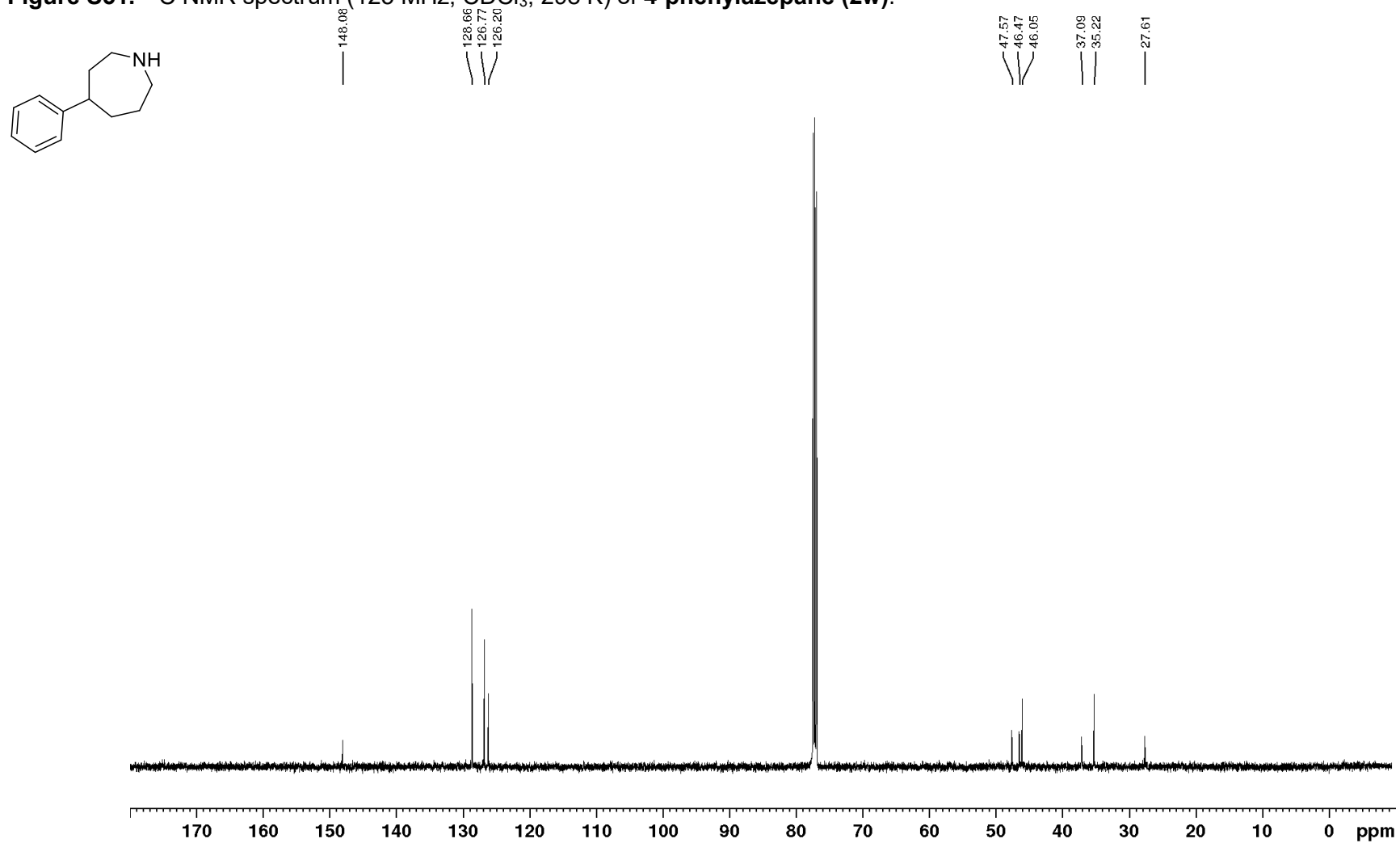
Figure S51. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 4-phenylazepane (**2w**).

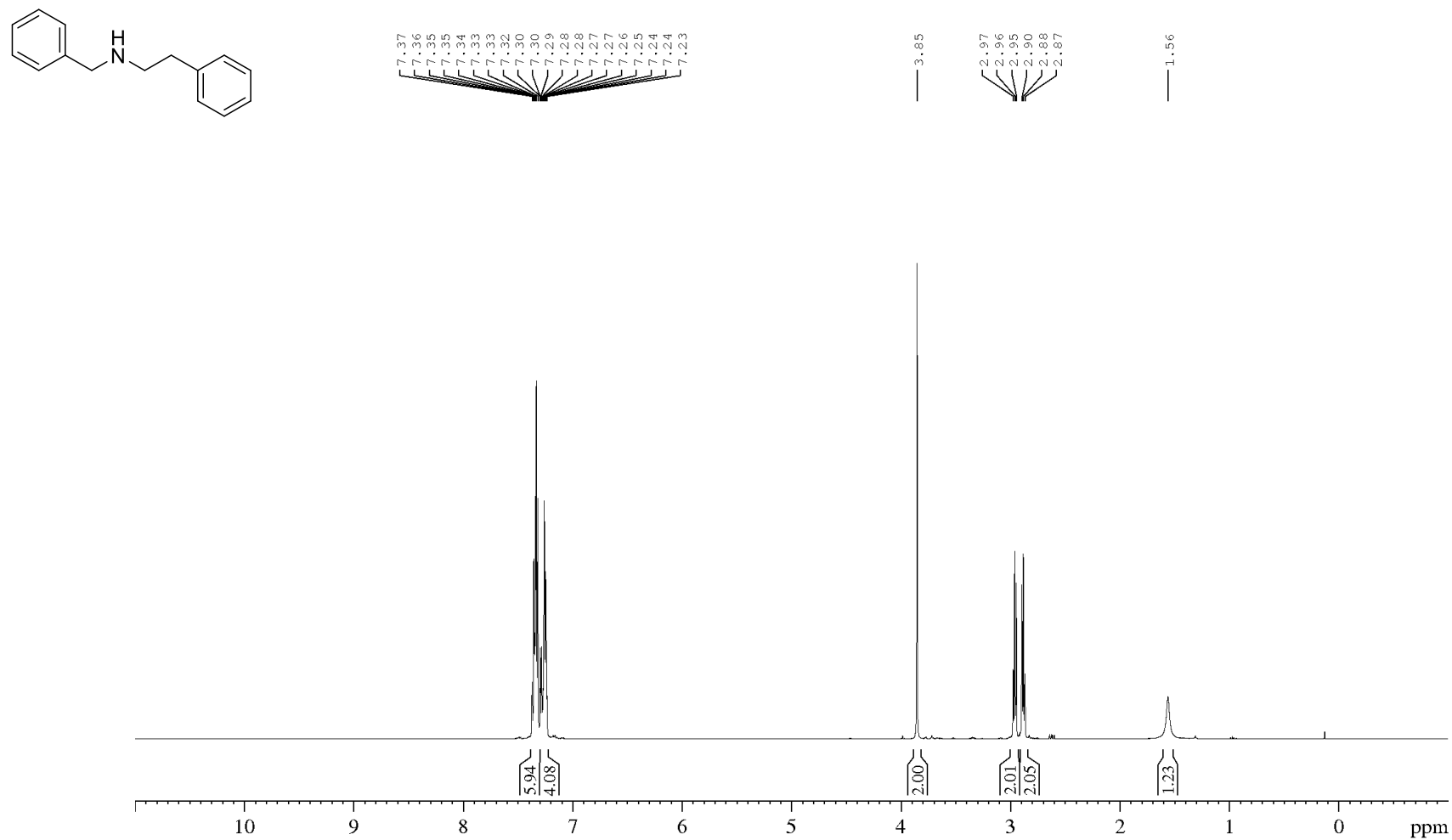
Figure S52. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-benzyl-2-phenylethan-1-amine (**2x**).

Figure S53. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-benzyl-2-phenylethan-1-amine (**2x**).

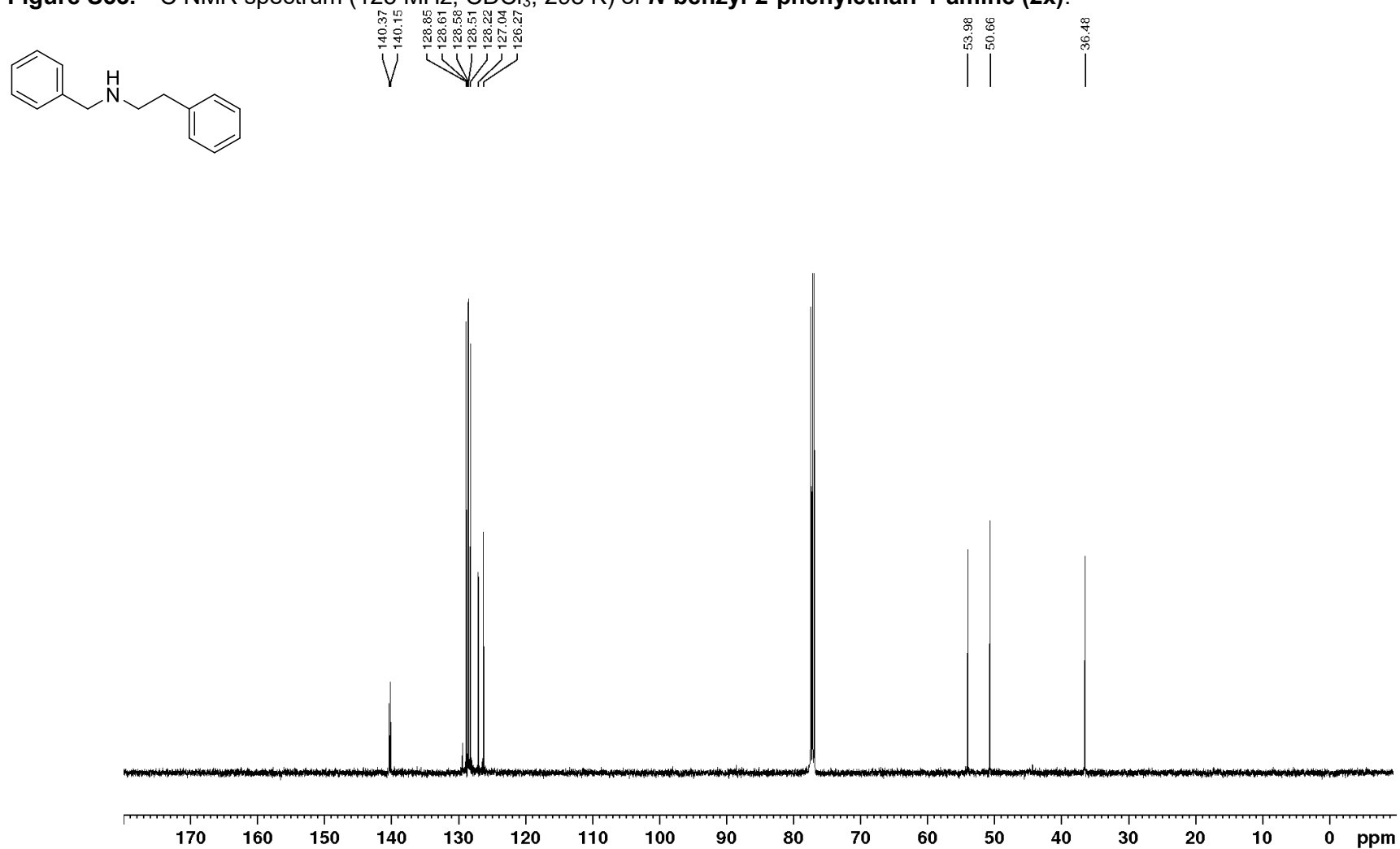


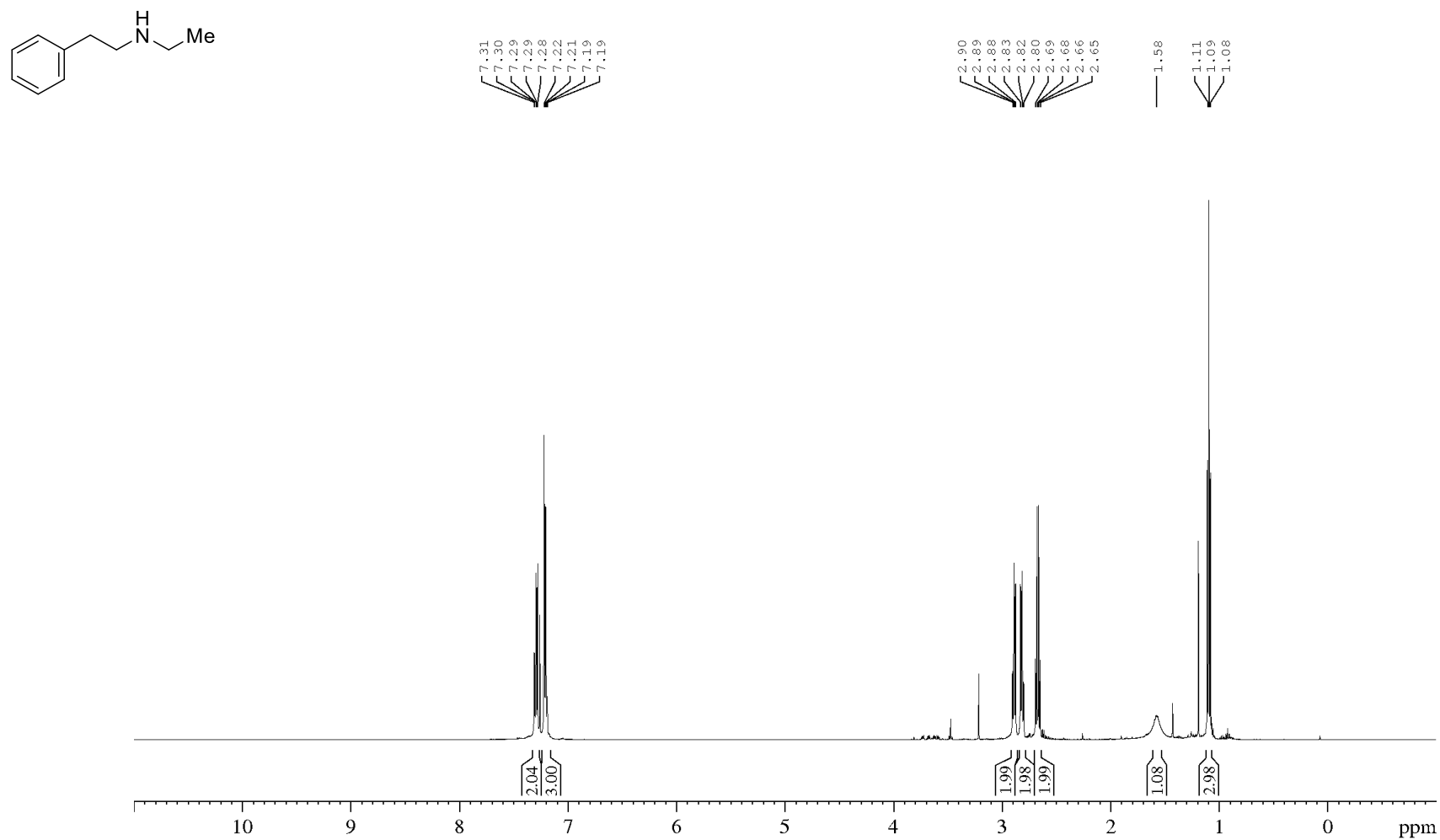
Figure S54. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of ***N*-ethyl-2-phenylethan-1-amine (2y)**.

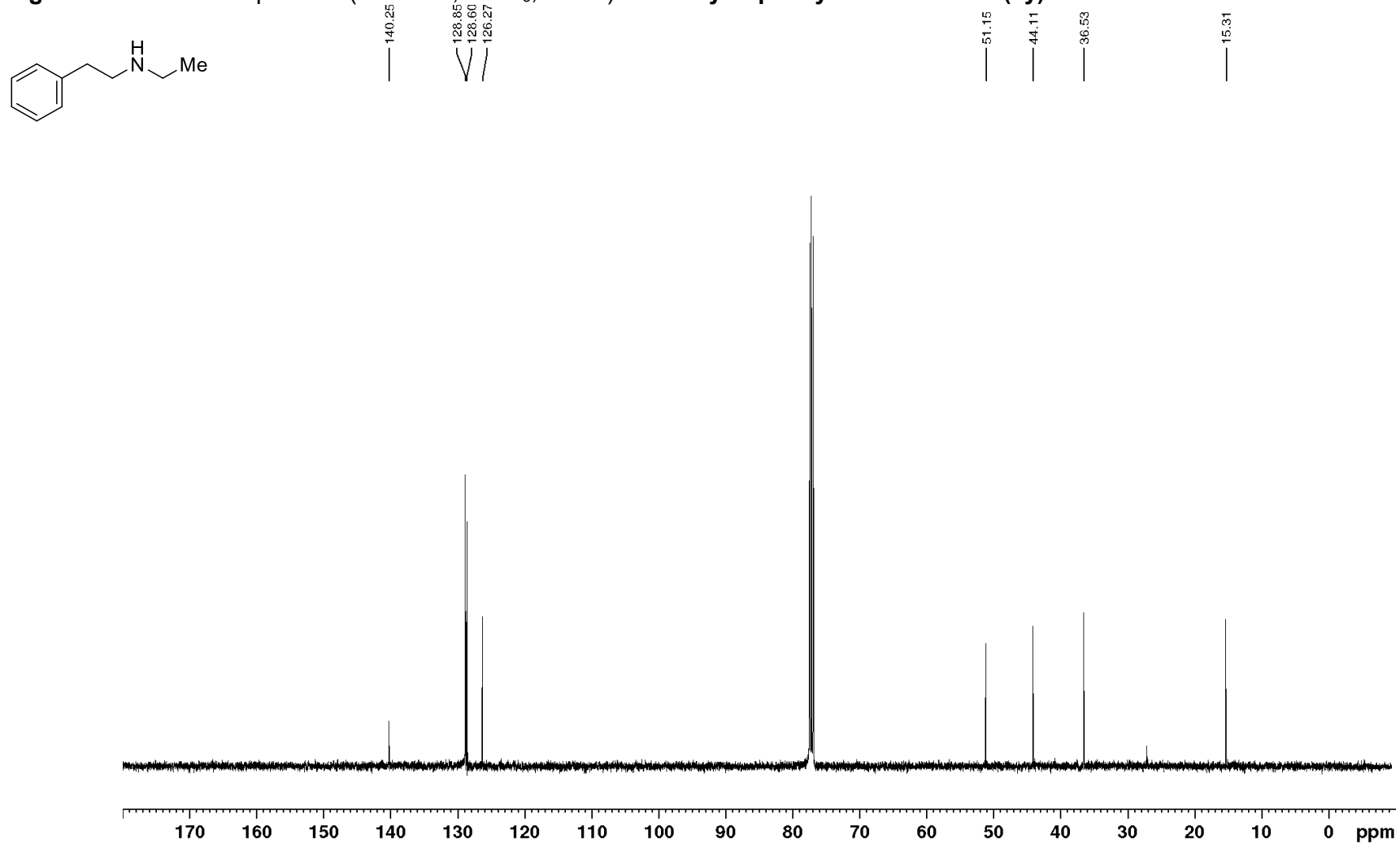
Figure S55. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-ethyl-2-phenylethan-1-amine (**2y**).

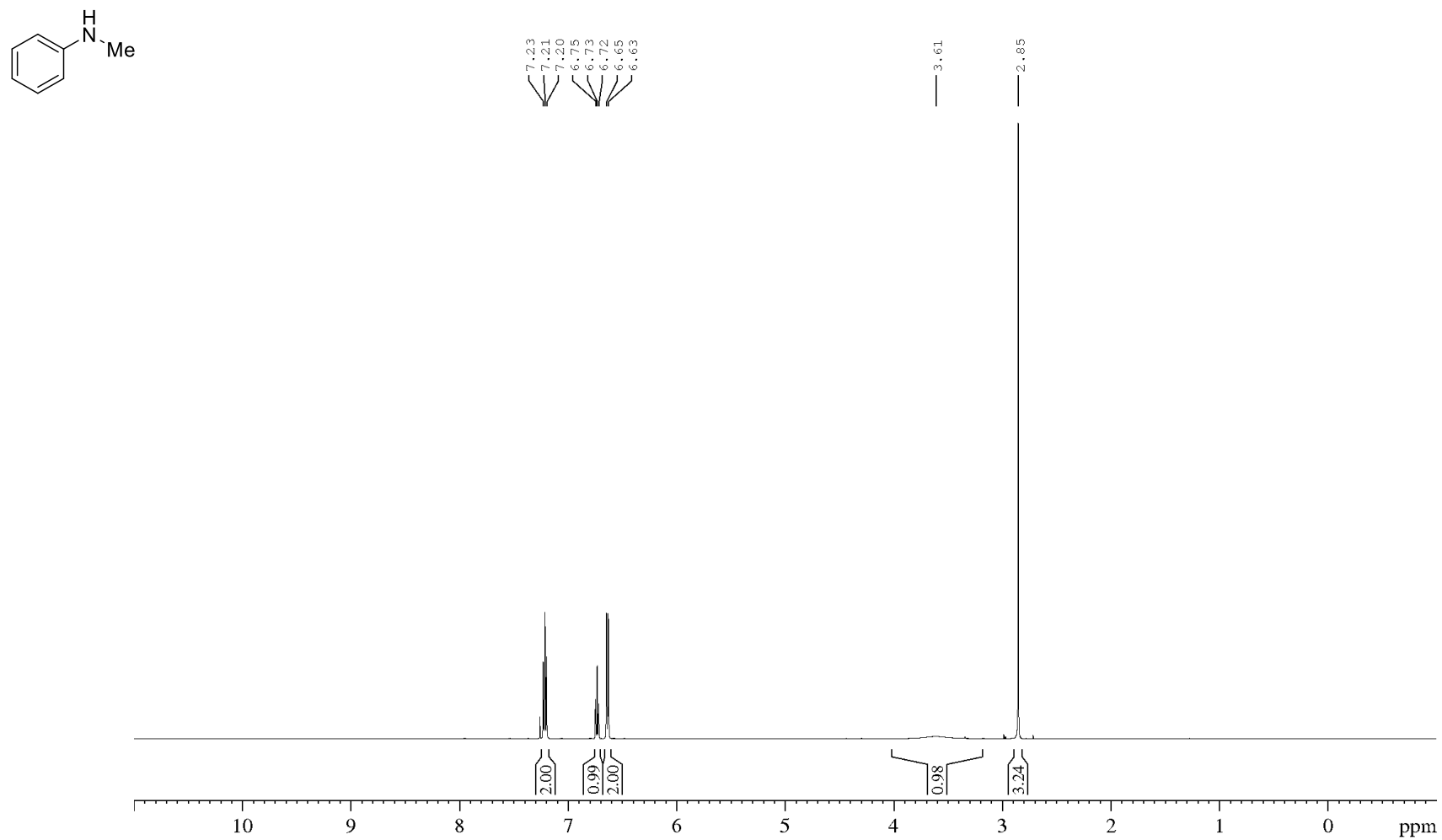
Figure S56. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*-methylaniline (**2z**).

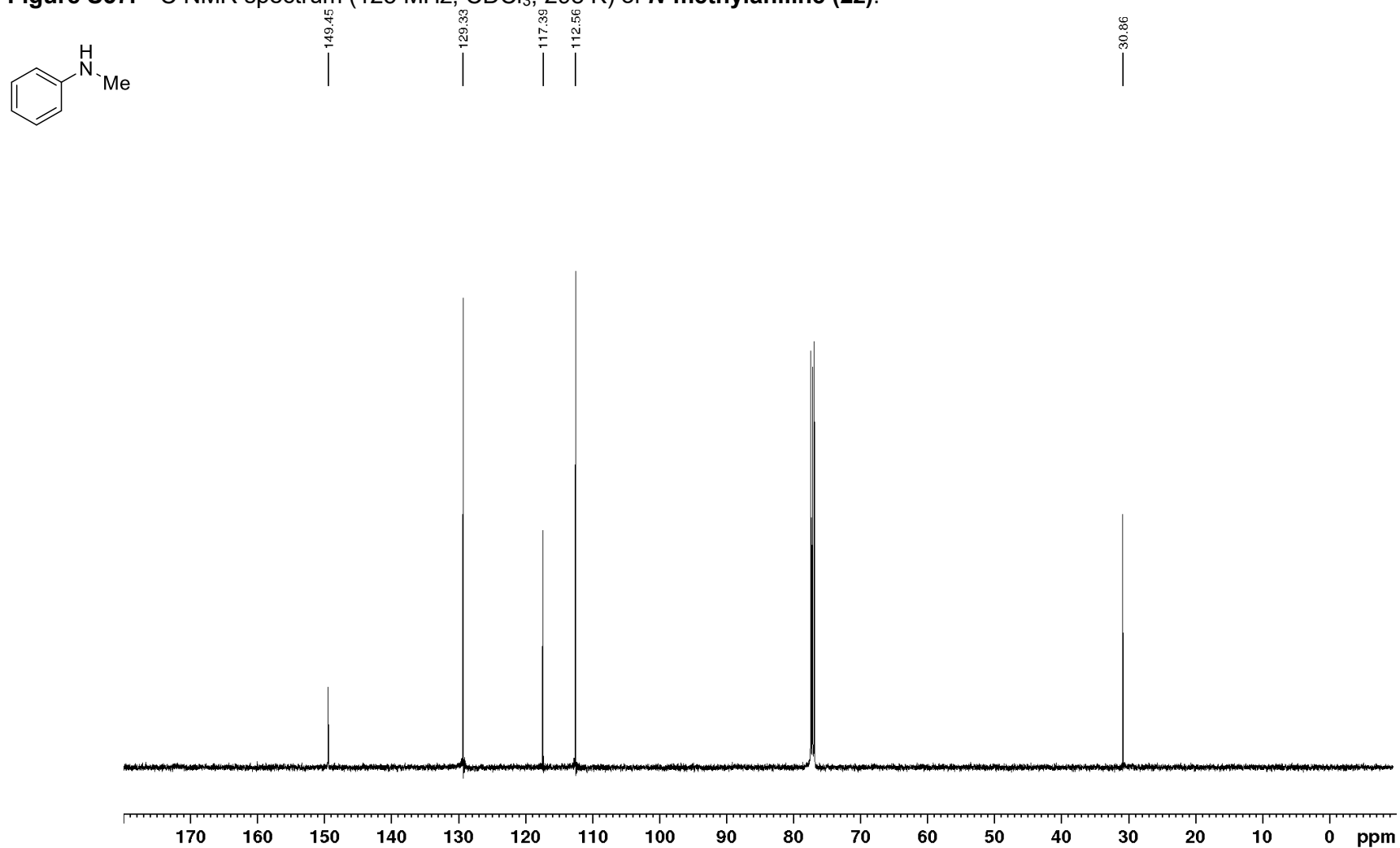
Figure S57. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of *N*-methylaniline (**2z**).

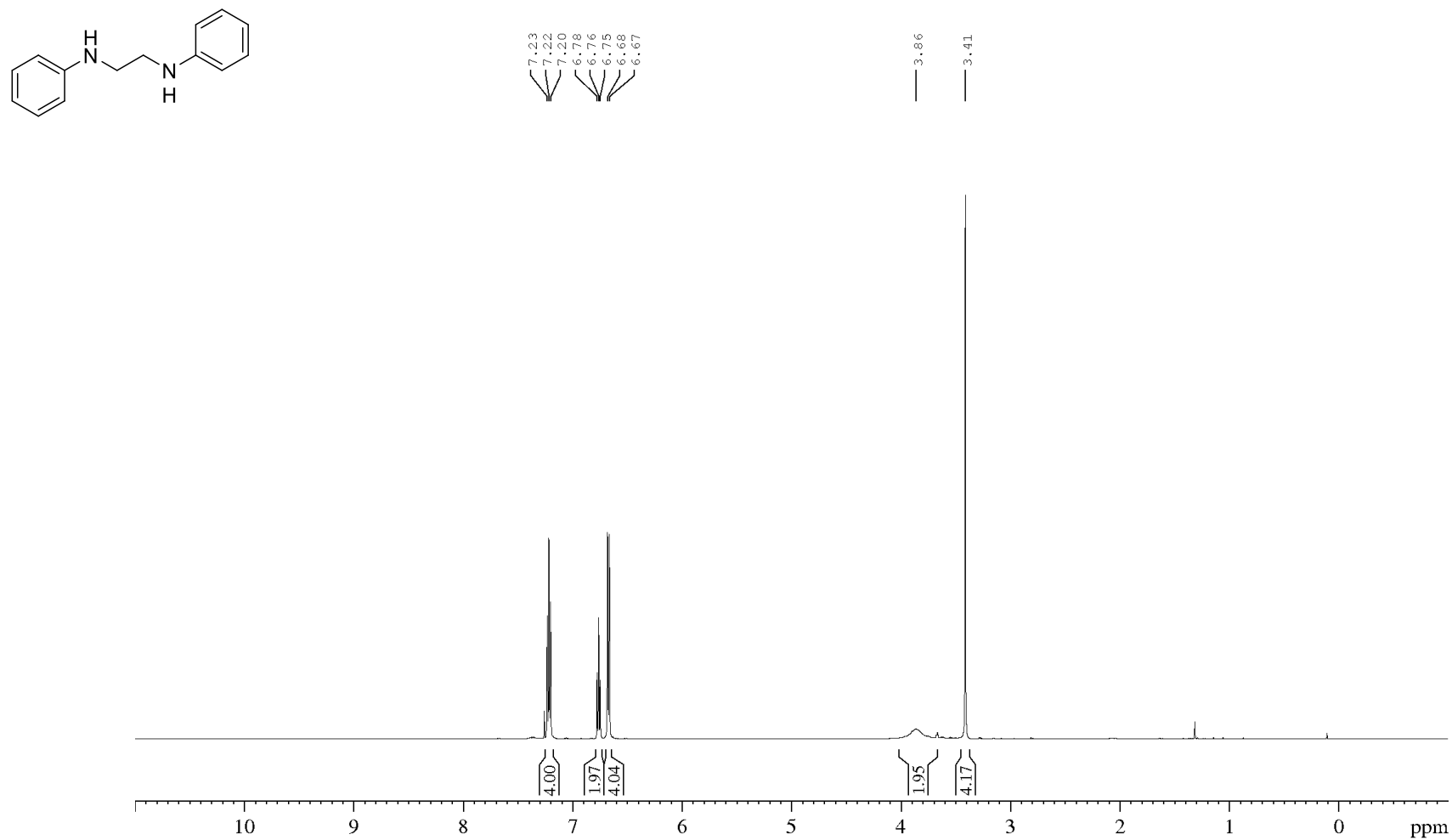
Figure S58. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *N*¹,*N*²-diphenylethane-1,2-diamine (**5**).

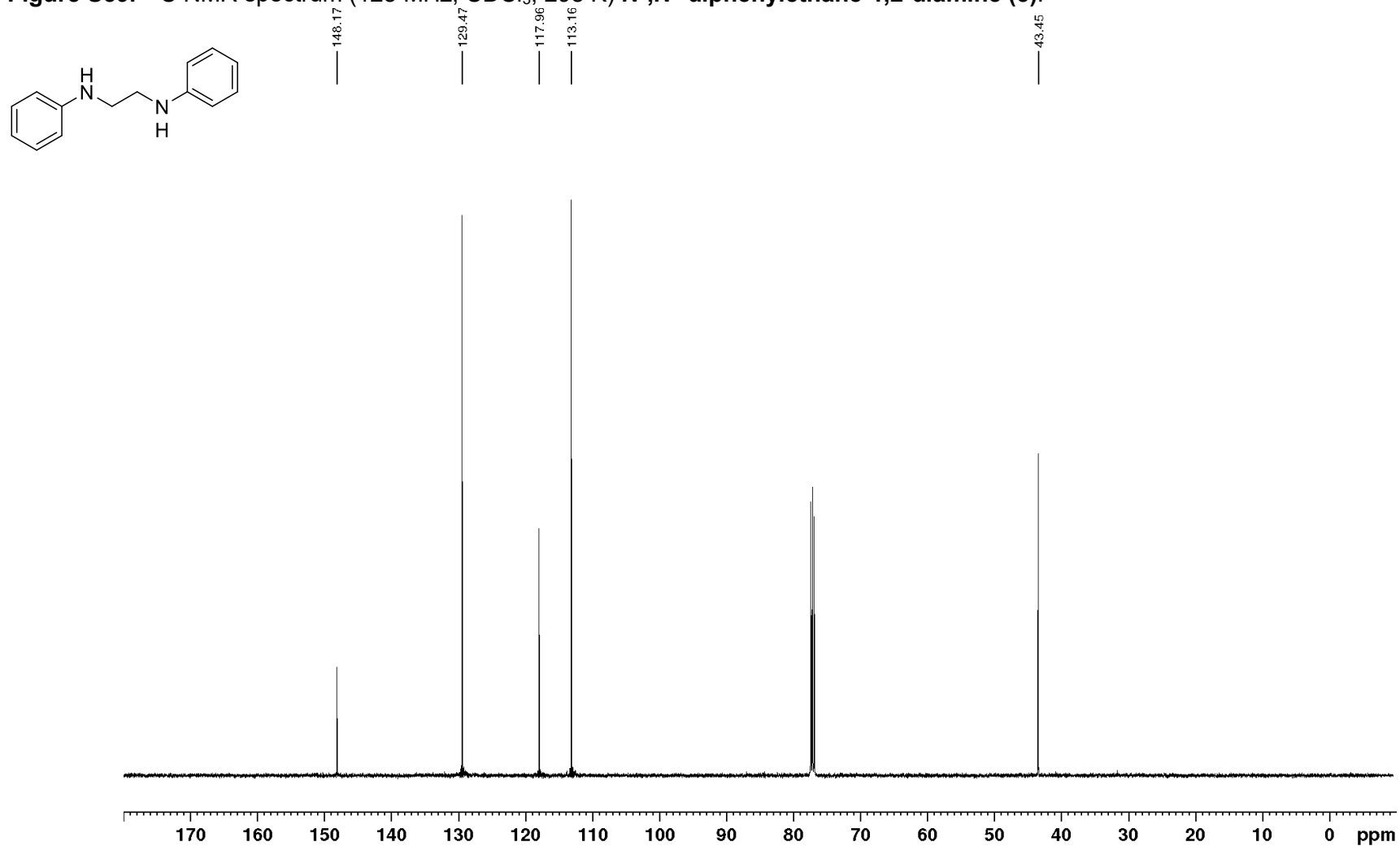
Figure S59. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) N^1,N^2 -diphenylethane-1,2-diamine (**5**).

Figure S60. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **2,3,4,5-tetrahydro-1H-benzo[*b*]azepine-2,2- d_2 (2d- d_2).**

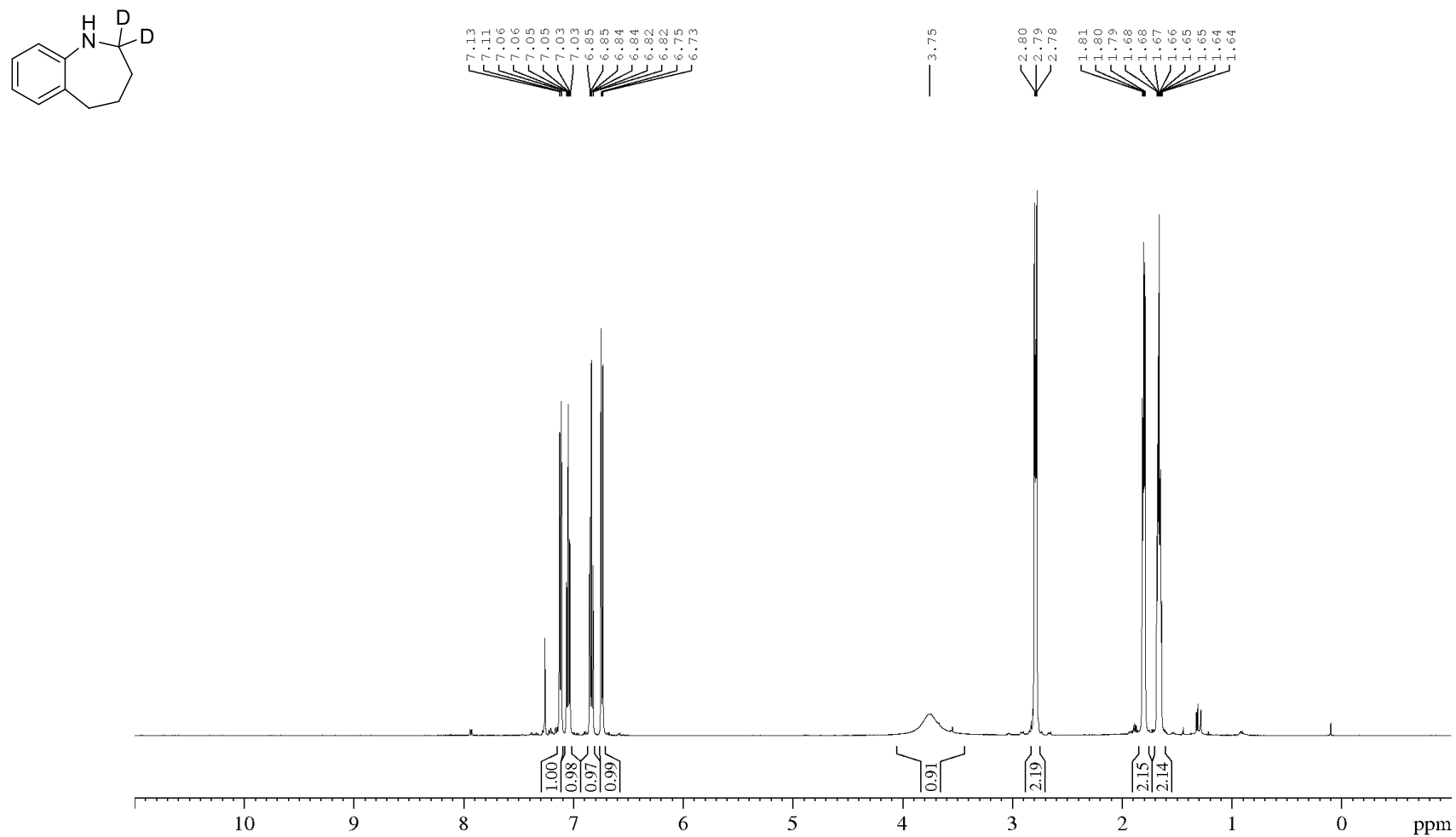


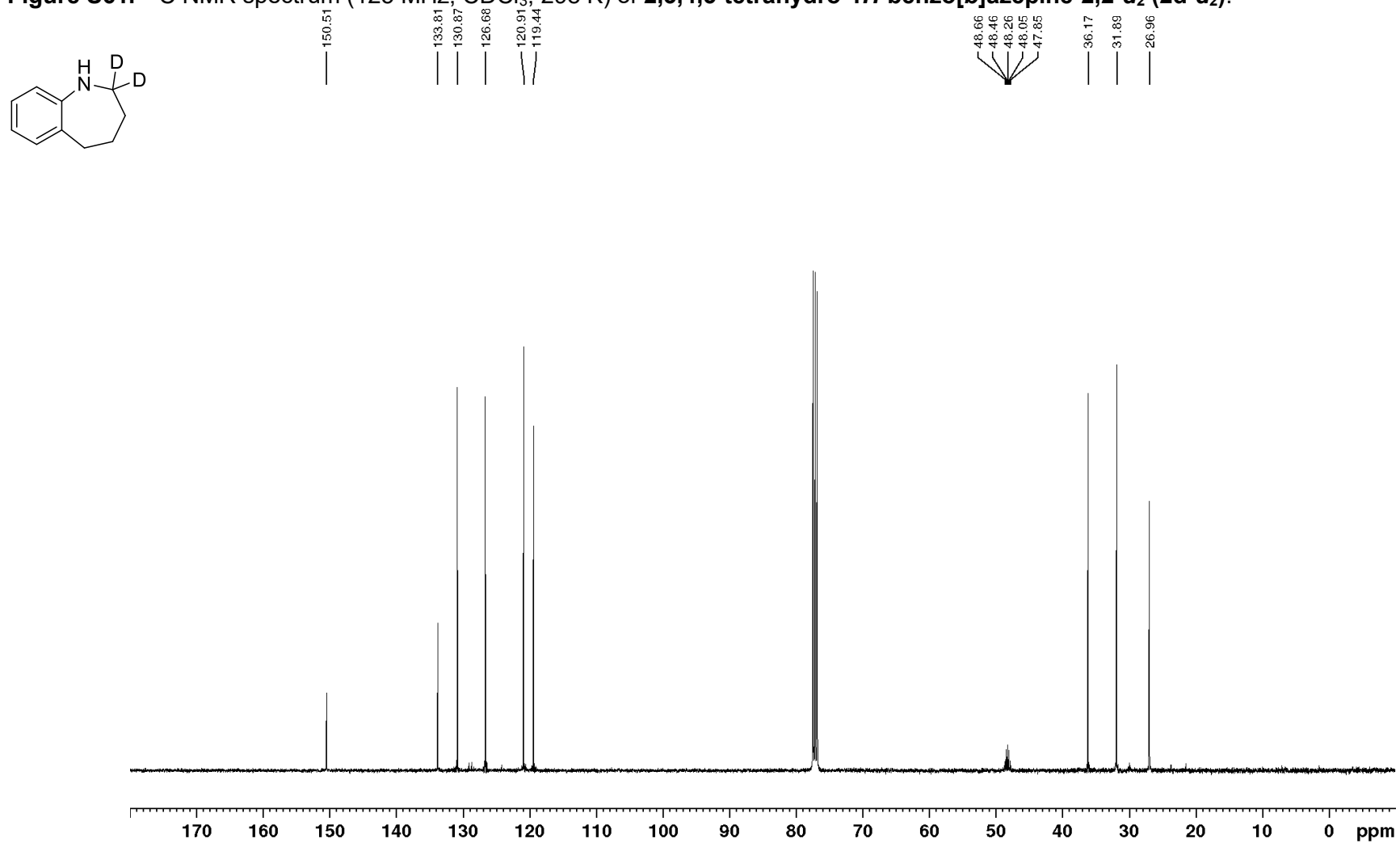
Figure S61. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 2,3,4,5-tetrahydro-1*H*-benzo[*b*]azepine-2,2- d_2 (2d- d_2).

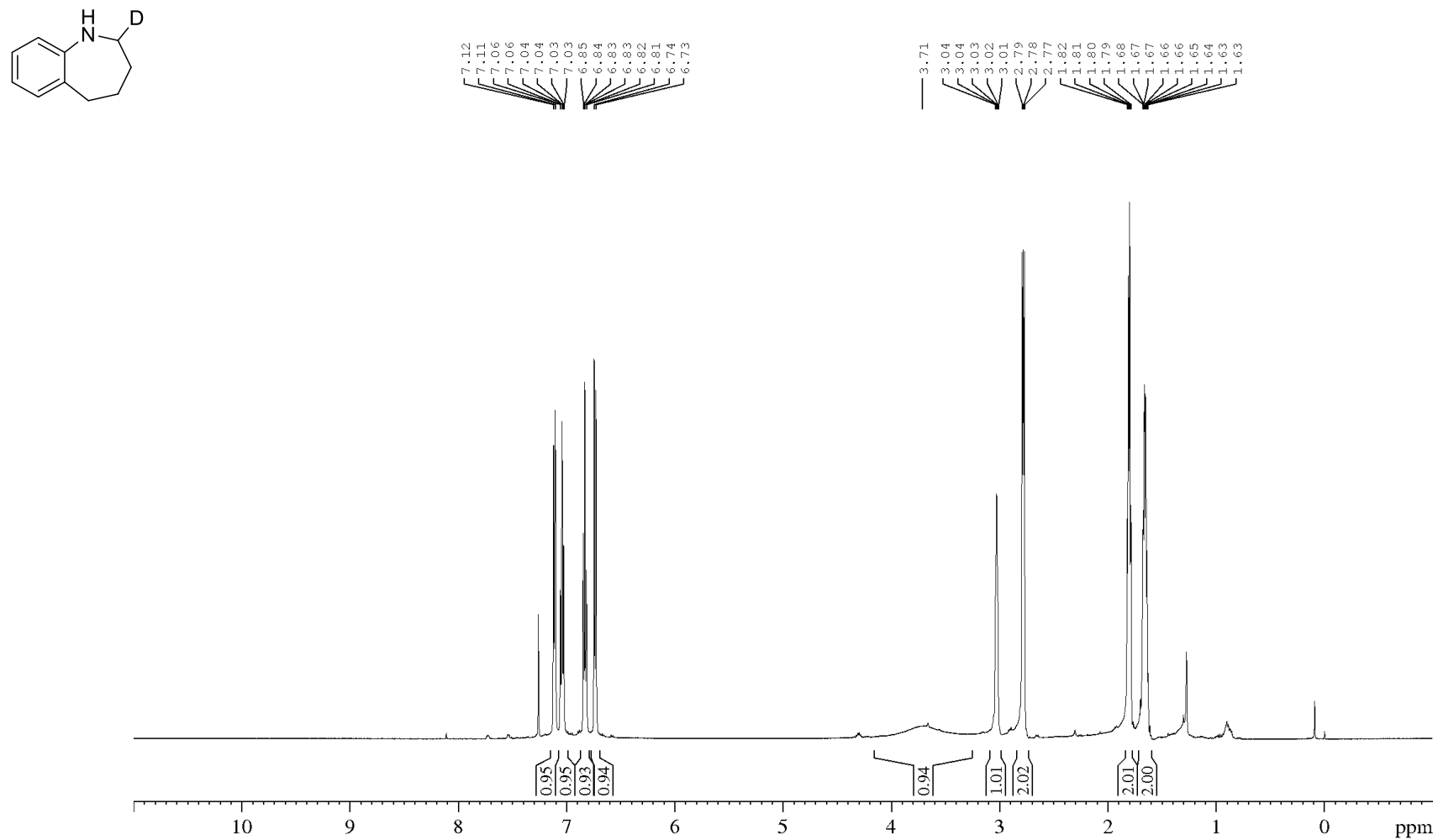
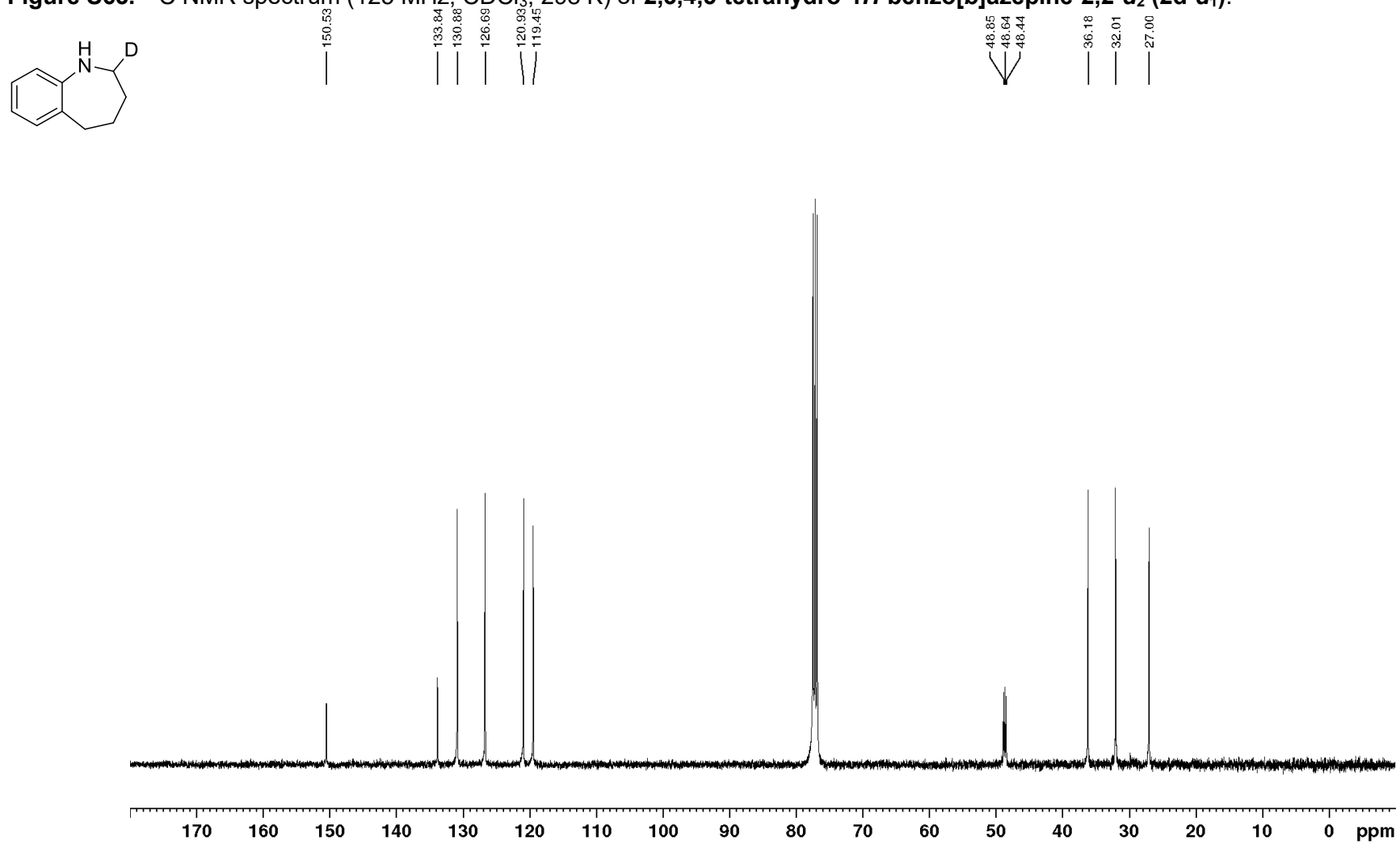
Figure S62. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **2,3,4,5-tetrahydro-1H-benzo[*b*]azepine-2-*d* (2d-*d*₁)**.

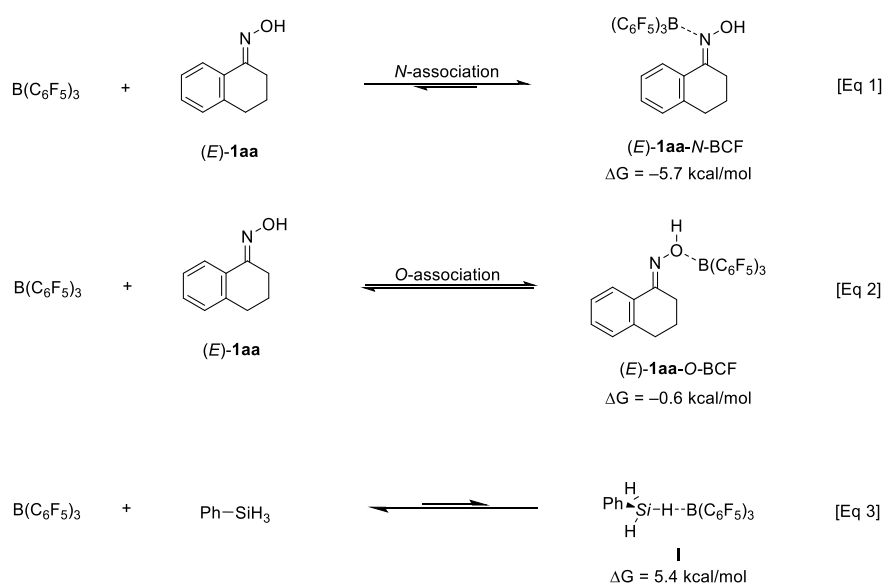
Figure S63. ^{13}C NMR spectrum (125 MHz, CDCl_3 , 298 K) of 2,3,4,5-tetrahydro-1*H*-benzo[*b*]azepine-2,2- d_2 (2d- d_1).

6 Computational Data

All density functional theory (DFT) calculations were performed with the Gaussian 16 package.^[38] The 3D structures of the optimized species were generated using CYLview.^[39] Geometry optimization and vibrational frequency calculations of all stationary points were carried out at M06-2X^[40]/6-311G(d,p) level of theory. To get more accurate energies, single-point energies were computed at M06-2X/cc-PVTZ level for all the species along the reaction pathway. Solvent effects in toluene were treated with the polarizable continuum model (PCM) in both geometry optimization and single-point calculation.^[41]

Activation free energy barriers here are defined as the free energy difference between the transition state and the lowest-energy stationary point before it along the reaction pathway.

6.1 Results of the DFT Calculations



Scheme S1. Calculated relative Gibbs free energies of $\text{B}(\text{C}_6\text{F}_5)_3$ -(E)-1aa Lewis adducts and $\text{B}(\text{C}_6\text{F}_5)_3$ -hydrosilane complex (in kcal/mol, BCF = $\text{B}(\text{C}_6\text{F}_5)_3$).

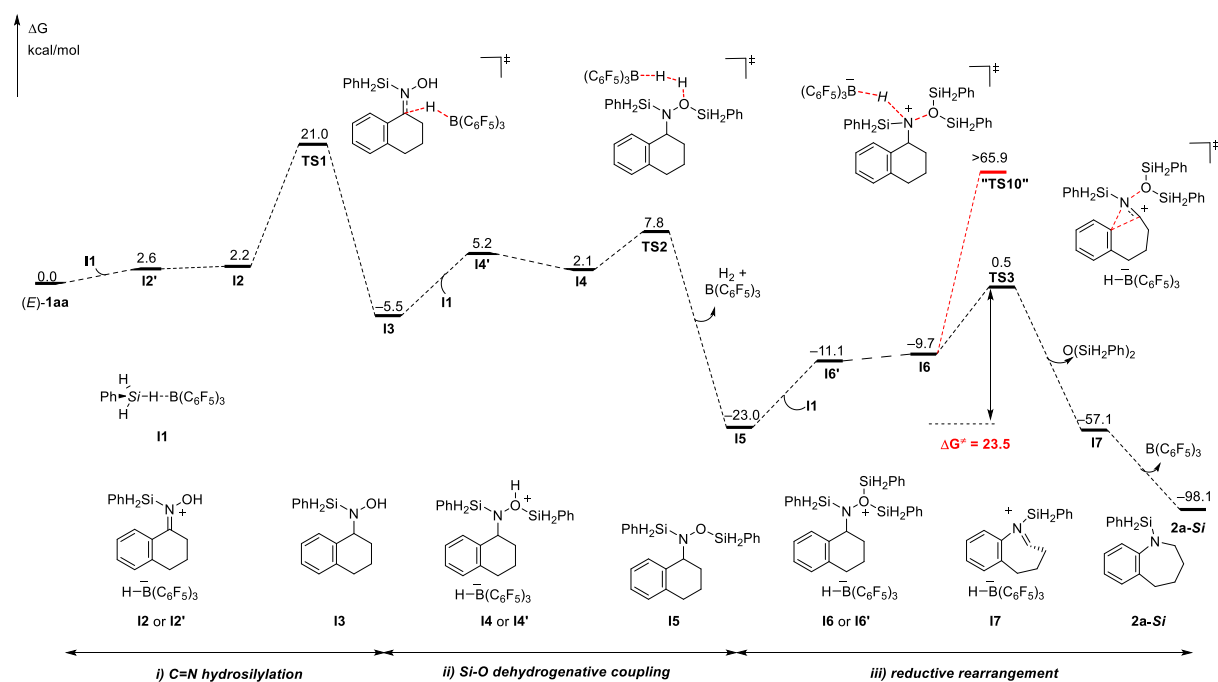


Figure S64. Gibbs free energy profile in black dashed line for the B(C₆F₅)₃-catalyzed reductive rearrangement of oxime (E)-1aa with PhSiH₃ via Path A: proceeding through a C=N hydrosilylation/Si-O dehydrogenative coupling/reductive rearrangement sequence (potential for formation of the primary amine via reductive deoxygenation of **I6** in red dashed line).

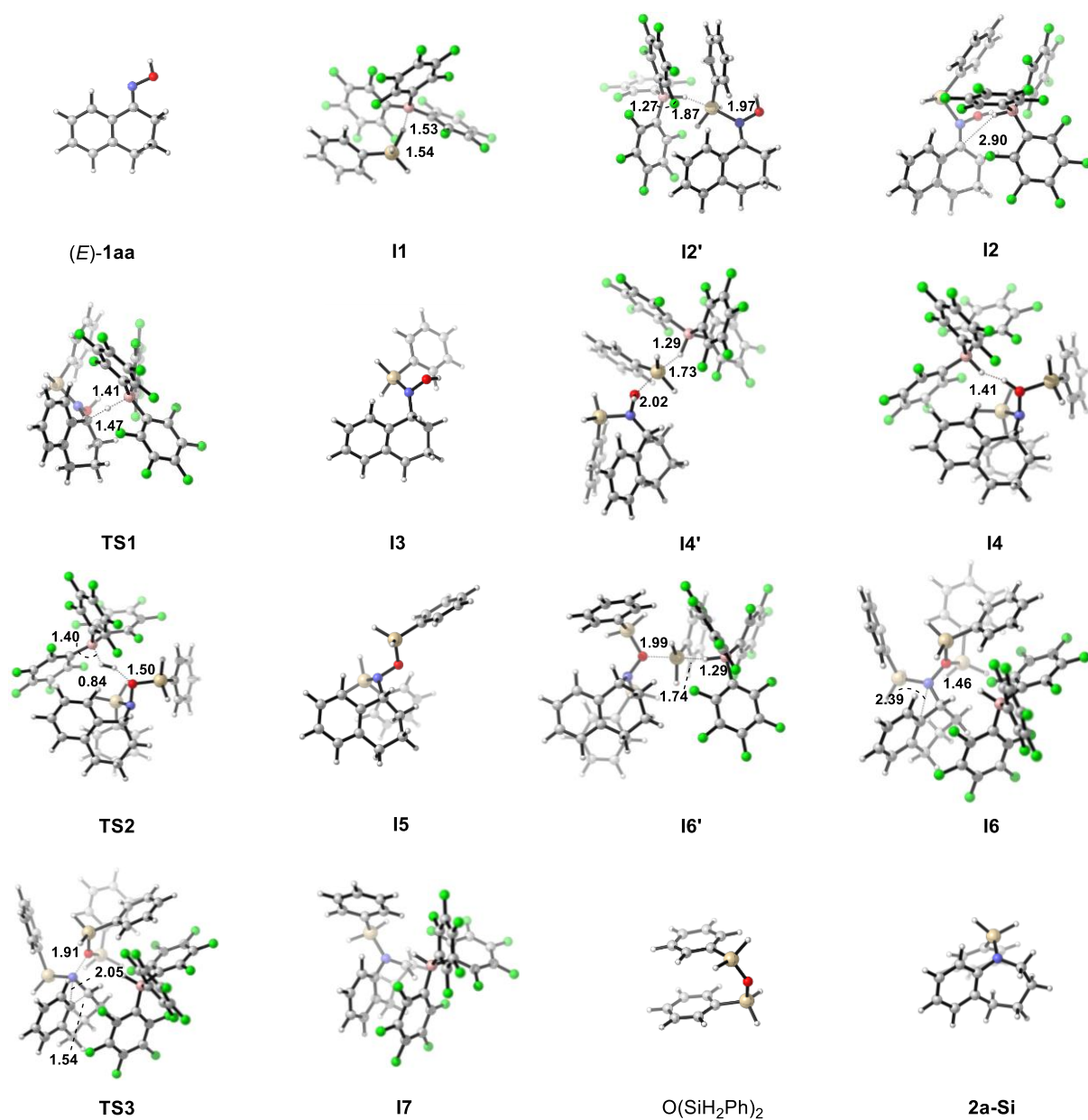


Figure S65. Optimized 3D structures of the intermediates and transition states involved in Path A. Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

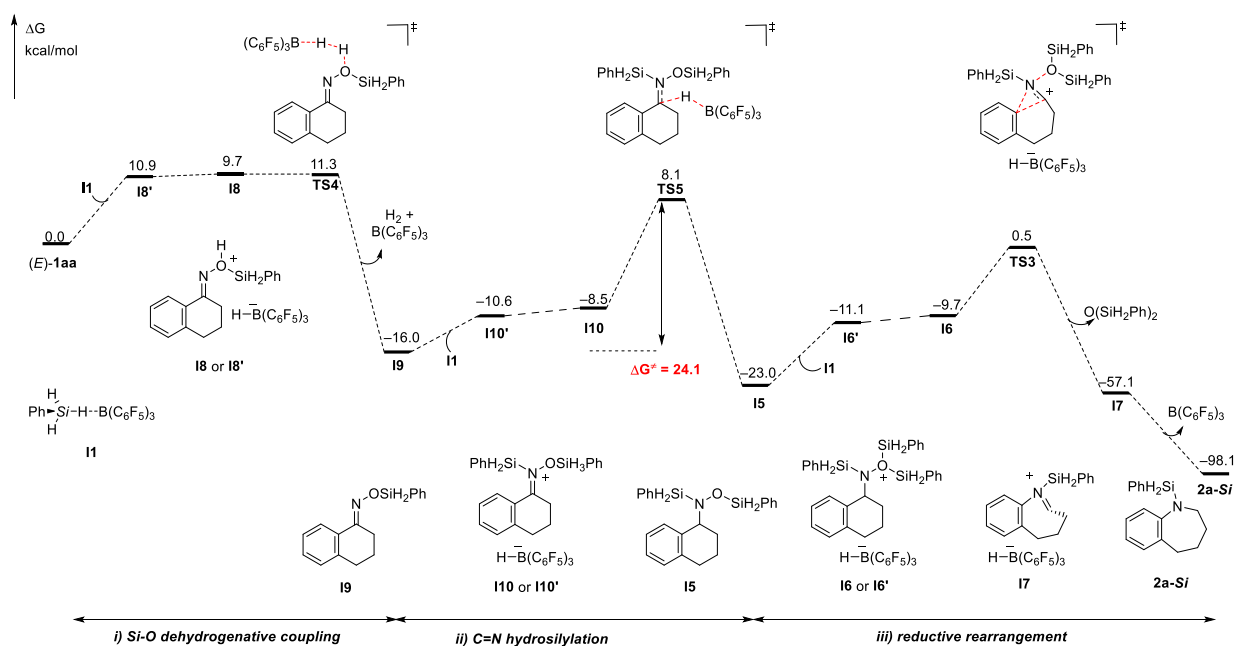


Figure S66. Gibbs free energy profile for the B(C₆F₅)₃-catalyzed reductive rearrangement of oxime (E)-1aa with PhSiH₃ via path B: proceeding through a Si–O dehydrogenative coupling/C=N hydrosilylation/reductive rearrangement sequence.

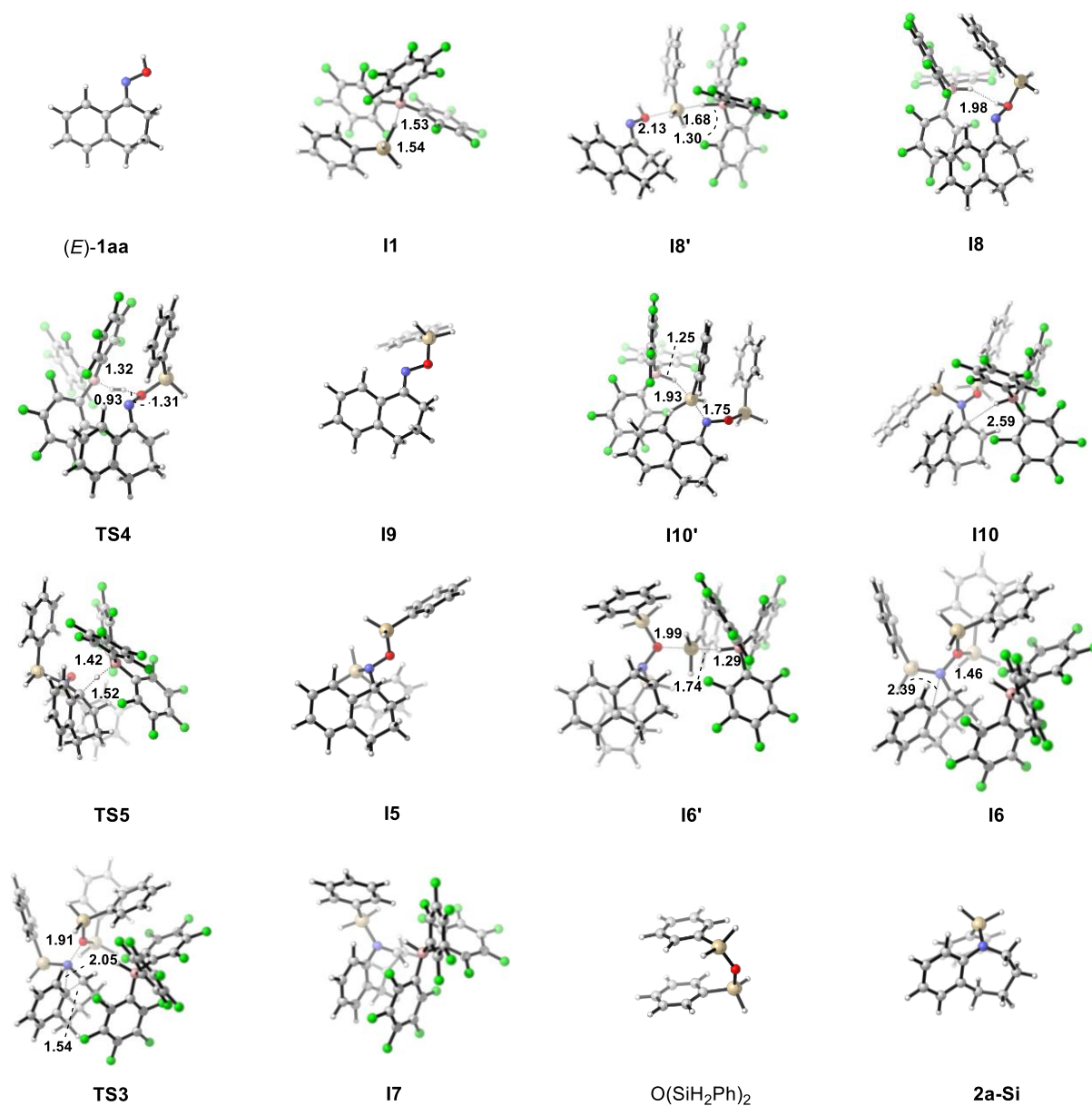


Figure S67. Optimized 3D structures of the intermediates and transition states involved in Path B. Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

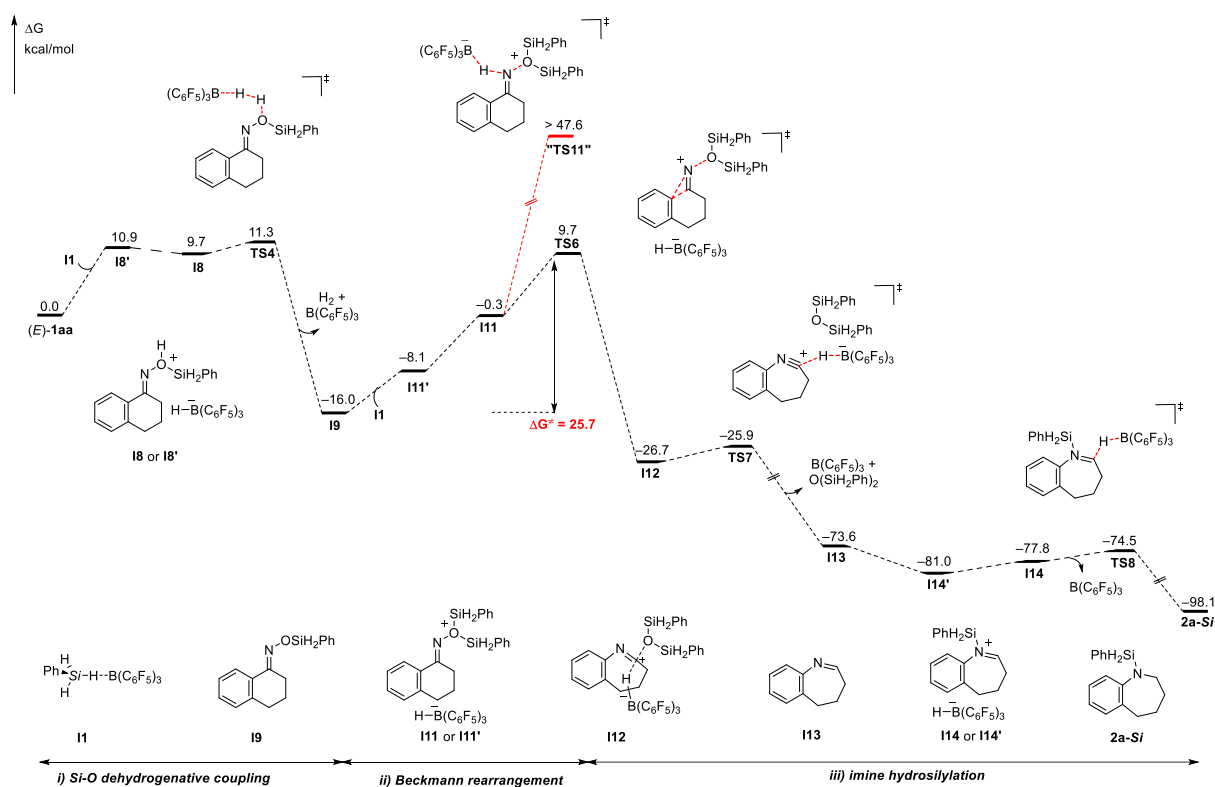


Figure S68. Gibbs free energy profile in black dashed line for the B(C₆F₅)₃-catalyzed reductive rearrangement of oxime (E)-1aa with PhSiH₃ via path C: proceeding through a Si–O dehydrogenative coupling/Beckmann rearrangement/imine hydrosilylation sequence (potential formation of the primary amine via reductive deoxygenation of intermediate **I11** (in red dashed line).

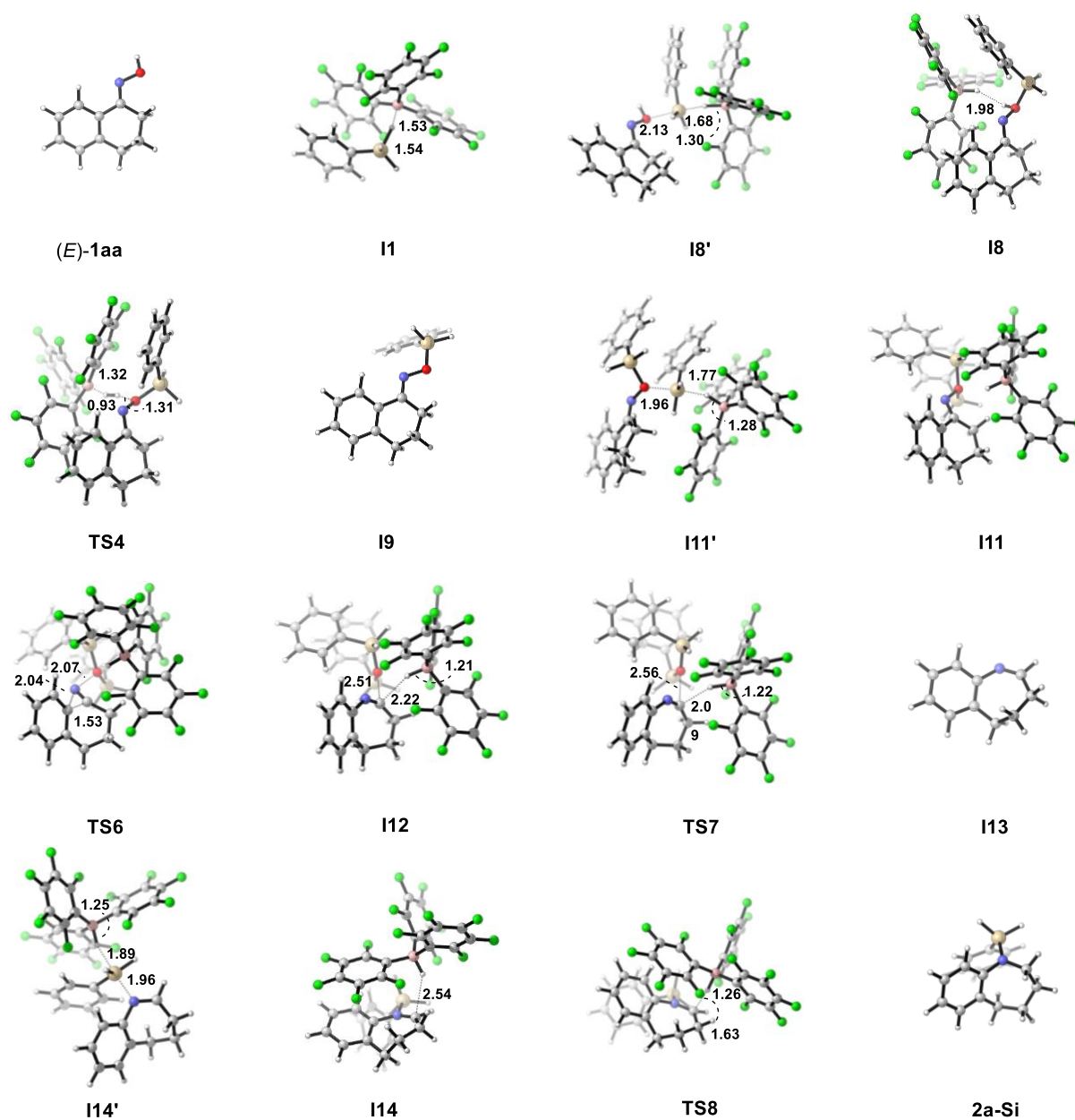


Figure S69. Optimized 3D structures of the intermediates and transition states involved in Path C. Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

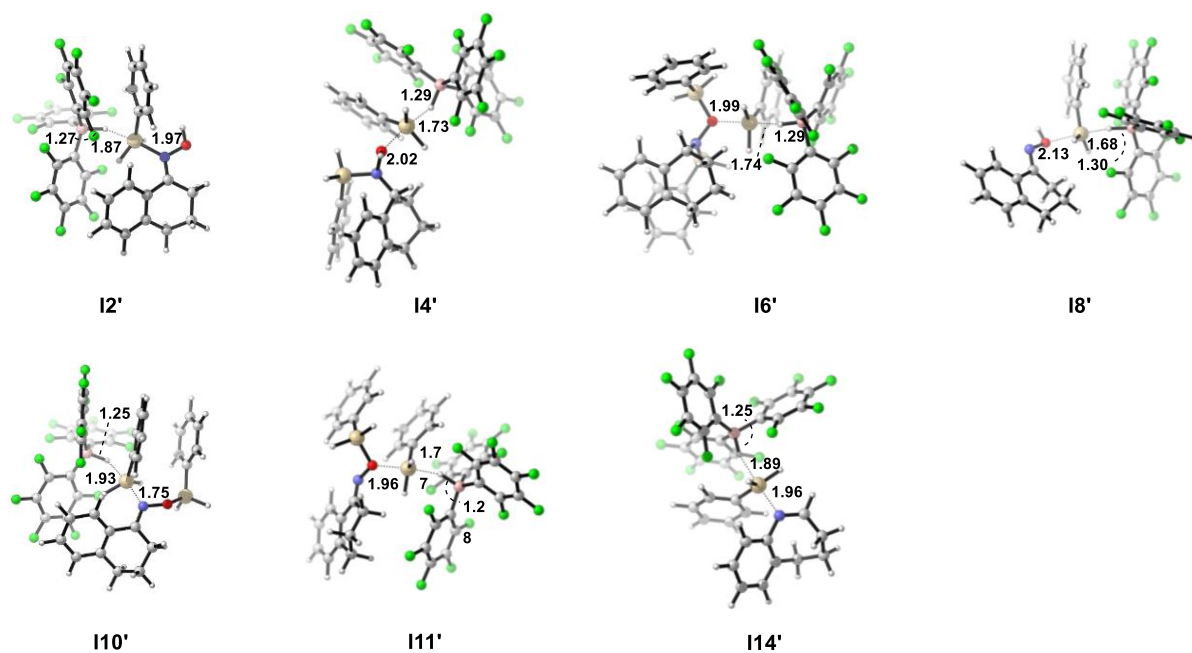


Figure S70. Optimized 3D structures of the transition complex involved in the cleavage of Si-H in borane-PhSiH₃ complex. Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

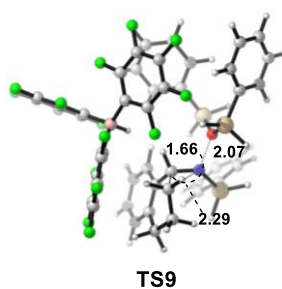


Figure S71. Optimized 3D structures of alkyl migration/N-O cleavage transition states. Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

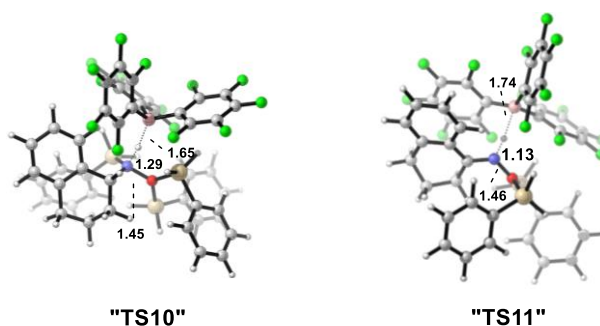


Figure S72. Optimized 3D structures of the deoxygenation pathway of ion-pair I6 (left) and bisssilyloxonium ion I11 (right). Distances are in Å. Color code: H, white; B, pink; C, gray; N, blue; F, green; Si, brown.

The formation of the primary amine **3a** pathway proceeding through the deoxygenation reaction of ion-pair **I6** or bisilyloxonium ion **I11** was also investigated. Through extensive scans for the hydride transfer from the borohydride to the nitrogen atom in **I6** or **I11**, it was found that there is no transition state to connect **I6** or **I11** with the related deoxygenation intermediates. Structures “**TS10**” and “**TS11**” (Figure S72) are *NOT* the transition states but structures obtained with a fixed N–H bond at 1.29 and 1.13 Å, respectively. The activation free energies of these two processes are estimated at more than 65 kcal/mol and 47 kcal/mol, respectively (Figures S64 and S68). The involvement of high-energy species in the formation of the primary amine **3a** can account for the high selectivity in favor of the secondary amine **2a** under the experimental conditions.

Table S2. M06-2X/6-311G(d,p) computed free energies in toluene (G, in a.u.), M06-2X/cc-pVTZ calculated single point energies in toluene (E_{sol} , in a.u.), and corrected free energies (G_{c} , in a.u.) for all stationary points involved.

Species	G	E_{sol}	G_{c}
Path A			
B(C ₆ F ₅) ₃	-2208.06178	-2208.419742	-2208.321559
PhSiH ₃	-517.37922	-517.59268	-517.43489
(E)- 1aa	-522.78555	-522.901447	-522.81706
I1	-2730.84405	-2731.33547	-2731.12995
I2'	-3248.23114	-3248.95954	-3248.56942
I2	-3248.23239	-3248.96120	-3248.56995
TS1	-3248.20447	-3248.93229	-3248.54002
I3	-1040.17528	-1040.52911	-1040.26074
I4'	-3771.01414	-3771.88241	-3771.38232
I4	-3771.02009	-3771.88901	-3771.38730
TS2	-3771.00975	-3771.87485	-3771.37815
I5	-1561.81637	-1562.28979	-1561.93545
I6'	-4292.65745	-4293.64859	-4293.05502
I6	-4292.65623	-4293.64889	-4293.05281
TS3	-4292.63887	-4293.62925	-4293.03662
O(SiH ₂ Ph) ₂	-1119.70732	-1119.96249	-1119.78344
I7	-3173.01639	-3173.73253	-3173.34503
2a-Si	-965.01197	-965.35550	-965.08868
Path B			
I8'	-3248.217268	-3248.942922	-3248.556202
I8	-3248.222371	-3248.948944	-3248.557987
TS4	-3248.219404	-3248.941883	-3248.555479
H ₂	-1.16977	-1.16895	-1.17024
I9	-1039.01847	-1039.35174	-1039.10727
I10'	-3769.86685	-3770.72012	-3770.23722
I10	-3769.86284	-3770.71359	-3770.23385
TS5	-3769.83947	-3770.68909	-3770.20756

I5	-1561.81637	-1562.289787	-1561.935445
I6'	-4292.65745	-4293.64859	-4293.05502
I6	-4292.65623	-4293.64889	-4293.05281
TS3	-4292.63887	-4293.62925	-4293.03662
O(SiH ₂ Ph) ₂	-1119.70732	-1119.96249	-1119.78344
I7	-3173.01639	-3173.73253	-3173.34503
<i>Path C</i>			
I8'	-3248.217268	-3248.942922	-3248.556202
I8	-3248.222371	-3248.948944	-3248.557987
TS4	-3248.219404	-3248.941883	-3248.555479
H ₂	-1.16977	-1.16895	-1.17024
I9	-1039.01847	-1039.35174	-1039.10727
I11'	-3769.86422	-3770.71180	-3770.23325
I11	-3769.85036	-3770.70079	-3770.22086
TS6	-3769.83368	-3770.67919	-3770.20492
I12	-3769.88929	-3770.73666	-3770.26287
TS7	-3769.88759	-3770.73704	-3770.26159
I13	-442.18588	-442.38756	-442.23270
I14'	-3173.05172	-3173.76891	-3173.38307
I14	-3173.04716	-3173.76277	-3173.37797
TS8	-3173.04332	-3173.75842	-3173.37275
2a-Si	-965.01197	-965.35550	-965.08868
<i>Alkyl migration pathway</i>			
TS9	-4292.62348	-4293.21884	-4293.61415
I15	-3173.06644	-3173.45554	-3173.78615
2a'-Si	-965.00816	-965.27489	-965.35184

6.2 Cartesian Coordinates of the Optimized Stationary Point

Path A				F	4.39902000	-0.01719200	-0.10217200
				F	3.11386500	-1.93650500	1.30947400
B(C ₆ F ₅) ₃				F	0.45374700	-1.95843700	1.42800300
				F	-0.49680700	-2.50115600	-1.13195100
B	-1.30095700	-0.01760100	0.15408100	F	-1.84505000	-4.79450800	-1.02514300
C	-2.08400400	1.33895400	0.15983300	F	-4.14910800	-4.95622100	0.38683000
C	-3.33684300	1.47621500	-0.43951700	F	-5.10731700	-2.78467400	1.68954100
C	-1.57274400	2.48823800	0.76422500	F	-3.79767800	-0.46944100	1.57835700
C	-4.03680600	2.66828300	-0.45222000				
C	-2.25380500	3.69107300	0.78733300	PhSiH ₃			
C	-3.49141500	3.77981100	0.17027000				
C	0.26389800	-0.01757900	0.08437900	Si	6.99051300	2.23041600	-4.71187400
C	0.97559900	0.95547200	-0.61891100	H	7.25082500	3.61488000	-5.17196400
C	1.03616200	-0.99008300	0.72125300	H	6.73121600	1.38473400	-5.89973300
C	2.35570700	0.96545500	-0.69956800	C	8.45665200	1.54519400	-3.76277300
C	2.41793500	-0.99983600	0.67709200	C	8.53926800	1.68040700	-2.37175200
C	3.07892100	-0.01714700	-0.04251500	C	9.50691500	0.90091500	-4.42797600
C	-2.08273900	-1.37342400	0.21790700	C	9.63736400	1.19587500	-1.66840600
C	-1.62635400	-2.52515500	-0.42487400	H	7.73580200	2.16582900	-1.82649500
C	-3.28067000	-1.50754600	0.92149300	C	10.60687100	0.41479500	-3.72919600
C	-2.30825400	-3.72713200	-0.38658800	H	9.46710100	0.77114500	-5.50512400
C	-3.97870600	-2.69854900	0.99646200	C	10.67331100	0.56297600	-2.34744700
C	-3.48933400	-3.81251800	0.33329100	H	9.68287700	1.30866600	-0.59155900
F	-4.15169100	4.92451800	0.17541400	H	11.40941600	-0.08236000	-4.26131700
F	-5.22002100	2.75801900	-1.04687200	H	11.52836400	0.18268800	-1.80104600
F	-3.90880700	0.43999500	-1.05247800	H	5.79992000	2.24459200	-3.83122200
F	-1.73677600	4.75603600	1.38736900				
F	-0.38690700	2.46047100	1.37221400	(E)-1aa			
F	0.33192100	1.92417800	-1.26989200				
F	2.99139400	1.90202600	-1.39262100	C	-4.08822500	-3.19674700	-0.71371800

C	-2.72566100	-3.28080400	-0.03033200	C	12.19057900	3.36994700	-3.66345200
C	-2.05876700	-1.92651700	-0.01670300	C	8.55521200	4.61317000	-7.46632900
C	-2.83208300	-0.76310000	0.10721100	C	8.27470200	5.60875700	-8.39420200
C	-4.30415300	-0.87715900	0.25840400	C	8.67750400	3.32993500	-7.98340000
C	-4.98528700	-2.20155300	0.01703300	C	8.12218200	5.34703800	-9.74804000
H	-0.07630100	-2.70895800	-0.23573000	C	8.52103600	3.02369500	-9.32018700
H	-3.94828700	-2.87477900	-1.75008400	C	8.24155800	4.04895300	-10.21113600
H	-2.85939200	-3.63435300	0.99946300	C	7.88734100	6.13095300	-5.33183200
C	-0.67321900	-1.80871500	-0.13404700	C	6.51592600	6.21600400	-5.53762100
C	-2.20567200	0.48878600	0.10433700	C	8.46637400	7.19475700	-4.65409700
H	-5.91267500	-2.01895200	-0.52809200	C	5.74751900	7.27655900	-5.09432700
C	-0.82908100	0.58890800	-0.00924200	C	7.73373800	8.28133400	-4.20487200
C	-0.05710400	-0.56562400	-0.12786900	C	6.36748300	8.32039800	-4.42650600
H	-2.81796100	1.37700800	0.19403800	F	8.95953600	2.31481800	-7.14997300
H	-0.35623800	1.56356300	-0.01173800	F	8.63904800	1.77498000	-9.75798900
H	1.01981400	-0.49405100	-0.22368000	F	8.09330400	3.78520100	-11.50106800
H	-5.28170000	-2.60518100	0.99272700	F	7.86303500	6.33122300	-10.60201500
H	-4.56909200	-4.17641900	-0.73780500	F	8.15743600	6.88452300	-8.01740400
H	-2.07752000	-4.00199600	-0.53245600	F	8.95559900	4.79049200	-3.06635000
N	-4.93539800	0.17077700	0.62393200	F	11.04052700	3.86328100	-1.67393500
O	-6.29764000	-0.06479100	0.74641100	F	13.19622500	2.85264400	-2.97284900
H	-6.64216200	0.78975100	1.01739300	F	13.29394500	2.90115300	-5.68132800
I1				F	11.27162900	3.89318400	-7.08728800
				F	9.78035500	7.20987900	-4.41471000
				F	8.32712100	9.28364200	-3.56492000
				F	5.65356500	9.35233300	-3.99883600
Si	7.09575100	2.59139600	-4.74629800	F	4.43559000	7.30805500	-5.30454500
B	8.71460600	4.89479400	-5.90396700	F	5.88198500	5.22559000	-6.18387000
C	10.01861300	4.40643800	-5.13822700	H	7.75900900	3.80805300	-5.41016300
C	11.15898400	3.90427000	-5.75681200	H	6.52917100	1.85619500	-5.88961400
C	10.03244100	4.37385700	-3.74528300	C	8.41563000	1.71619100	-3.77946300
C	12.23195900	3.38821800	-5.04622500	C	8.43816800	1.84931300	-2.38382700
C	11.08509800	3.87838600	-3.00171000				

C	9.44365500	0.99499900	-4.40465400	C	5.92611000	7.27272000	-3.70556400
C	9.46520200	1.28768800	-1.63368100	F	7.90817800	2.56573900	-7.92500600
H	7.65797100	2.40861200	-1.87855200	F	7.98789200	3.15812700	-10.52918400
C	10.47588600	0.44457700	-3.65443400	F	8.87618000	5.58512300	-11.36083600
H	9.44637300	0.86676600	-5.48025200	F	9.69240900	7.42643300	-9.54057000
C	10.49101000	0.59660400	-2.27003100	F	9.62165900	6.84335900	-6.91283200
H	9.47517200	1.40634100	-0.55729400	F	9.02379500	3.97235400	-2.90411900
H	11.27197100	-0.09881500	-4.14981800	F	11.20107900	3.04423700	-1.68387000
H	11.30285800	0.17633700	-1.68844400	F	13.49275700	2.63149600	-3.09055800
H	6.07724300	3.19259600	-3.86569300	F	13.56262900	3.21191600	-5.74412500
I2'				F	11.40996200	4.10753400	-6.99181200
				F	9.45232300	6.62141200	-3.78932600
				F	7.73103400	8.24667200	-2.56521100
				F	5.07238500	8.07012000	-3.06527500
Si	7.03750100	2.20467000	-4.53923000	F	4.14631600	6.21095200	-4.81894700
B	8.67839600	4.41849400	-5.72093400	F	5.86279000	4.58086100	-6.07657800
C	10.10094300	4.10426600	-5.00682300	H	8.05815400	3.31826300	-5.63555200
C	11.30040400	3.89566900	-5.67307100	H	6.34292900	1.77821000	-5.76371000
C	10.14200700	3.82696500	-3.64497900	C	8.57463900	1.21587100	-4.15009300
C	12.44609200	3.42079300	-5.04639400	C	8.87174200	0.79992600	-2.84601200
C	11.25125200	3.34181800	-2.98241400	C	9.50960800	0.96285300	-5.16388700
C	12.41914900	3.13099800	-3.69650100	C	10.07981000	0.17226600	-2.55581000
C	8.73885800	4.69868400	-7.31111900	H	8.16625400	0.97786300	-2.03966600
C	9.18994700	5.92177400	-7.78500700	C	10.71354400	0.33228400	-4.87686800
C	8.34351100	3.78930200	-8.27602800	H	9.30260300	1.28797200	-6.17965900
C	9.24626400	6.24021600	-9.12984500	C	11.00355200	-0.05410500	-3.56997600
C	8.38061900	4.06548400	-9.63483100	H	10.30420400	-0.12438800	-1.53864000
C	8.83304500	5.30088200	-10.06181300	H	11.43241100	0.15530900	-5.66826000
C	7.73533000	5.52361600	-4.99403500	H	11.95157400	-0.52758800	-3.34335500
C	6.36690300	5.50054400	-5.23434700	H	6.69288400	3.46794000	-3.91698900
C	8.15723900	6.49379600	-4.09719100	C	2.51049700	1.60048200	-1.72717500
C	5.45655000	6.32741600	-4.60005400	C	2.44249300	3.01656800	-2.30994800
C	7.28285300	7.35676000	-3.45155400				

C	3.72531300	3.73115800	-1.97311300	C	7.68279400	0.48822000	0.65748100
C	4.93216000	3.01816500	-2.05506400	C	8.27002300	0.01087700	1.82086700
C	4.87478100	1.65581400	-2.59811500	C	8.09791800	1.74561900	0.26661000
C	3.65091700	0.81201700	-2.37272500	C	9.23350100	0.70621000	2.52943300
H	2.84090800	5.62343100	-1.49404700	C	9.06402200	2.48156500	0.93550400
H	2.66379800	1.67016600	-0.64751300	C	9.63664100	1.95483800	2.07810800
H	2.30649900	2.96603100	-3.39638900	C	5.24879800	-0.48307700	0.87005800
C	3.76171800	5.05342300	-1.53725600	C	4.51025400	0.65902000	1.15415000
C	6.13170100	3.59634900	-1.61856900	C	4.81955300	-1.63278800	1.51618300
H	3.93869000	-0.06442900	-1.78513000	C	3.41446300	0.68005100	1.99947600
C	6.14701100	4.90528200	-1.16975900	C	3.72415100	-1.65944000	2.36930900
C	4.96114200	5.63878400	-1.14826900	C	3.01505400	-0.49652500	2.61110800
H	7.05111900	3.02298600	-1.63502900	F	7.56111300	2.33854800	-0.82462700
H	7.07769600	5.35480300	-0.84582600	F	9.43810100	3.68342100	0.48708900
H	4.97176100	6.66968900	-0.81464900	F	10.56436000	2.63999100	2.74222100
H	3.35153200	0.42669800	-3.35338500	F	9.78059200	0.19897200	3.63323500
H	1.57395800	1.06744200	-1.89354200	F	7.91314000	-1.19350200	2.28390000
H	1.59435700	3.56814100	-1.90323100	F	4.87606200	-1.94563300	-1.73942300
N	5.85164800	1.20607300	-3.31672900	F	5.47992500	-4.23416400	-2.99324000
O	5.70751400	-0.11786800	-3.69081800	F	7.97883700	-5.29886300	-2.76491700
H	6.60485500	-0.40667500	-3.91795300	F	9.84603800	-4.01733000	-1.26714800
I2				F	9.28067900	-1.76640400	-0.02013200
				F	5.45875600	-2.79522300	1.33941900
				F	3.34782500	-2.79275300	2.95988400
				F	1.96333800	-0.50515600	3.42629800
Si	6.90888600	2.18592000	-3.84114700	F	2.74018900	1.81066600	2.22875300
B	6.53470900	-0.34624900	-0.12927700	F	4.84949000	1.83357100	0.58039900
C	7.02439000	-1.75822200	-0.77913300	H	6.17167000	0.35886300	-1.04191500
C	8.27947000	-2.34202000	-0.70033400	H	6.37429100	2.16434300	-5.21257900
C	6.12079700	-2.45376200	-1.57180900	C	8.11890100	0.81532300	-3.53132300
C	8.60705000	-3.52753900	-1.34513100	C	9.25847500	1.01961500	-2.74272200
C	6.39856600	-3.63134900	-2.23849300	C	7.94607300	-0.43075500	-4.15422600
C	7.66540300	-4.17822000	-2.11777000				

C	10.18079100	-0.00318100	-2.55116300				
H	9.42699600	1.97847700	-2.26552300	TS1			
C	8.87562100	-1.44678400	-3.97432800				
H	7.07860800	-0.60915100	-4.78078000	Si	-2.25410700	-1.67154900	-2.46675500
C	9.98952800	-1.23539000	-3.16590800	B	0.49114300	0.44403600	0.64483600
H	11.04477400	0.16070800	-1.91892200	C	-0.98267900	1.11612000	0.76151500
H	8.72927200	-2.40568500	-4.45817400	C	-1.97365000	0.74466000	1.66875900
H	10.70316300	-2.03591800	-3.00692000	C	-1.34420000	2.19096700	-0.05099100
H	7.39530100	3.50950000	-3.44268300	C	-3.23336000	1.32893400	1.71382700
C	2.11135000	2.23189200	-1.14895400	C	-2.58940100	2.79322800	-0.04982800
C	1.87711500	3.56645600	-1.85296900	C	-3.55209400	2.34867900	0.84144200
C	3.13912700	4.38238200	-1.75348900	C	0.71859800	-0.90231800	1.50267600
C	4.39900200	3.75542000	-1.85437400	C	1.77597500	-1.15594300	2.36907400
C	4.40069000	2.33449100	-2.21332700	C	-0.19562700	-1.94053800	1.39931000
C	3.21241400	1.47550500	-1.87654300	C	1.92589900	-2.35788400	3.04944600
H	2.12756100	6.23846800	-1.43211300	C	-0.08667000	-3.15386500	2.04412900
H	2.39673700	2.41450600	-0.11061100	C	0.99522300	-3.36629300	2.88320900
H	1.61348700	3.39050200	-2.90256400	C	1.73842600	1.45665500	0.60820000
C	3.09272300	5.75015800	-1.50103600	C	2.96838800	0.98701600	0.16224400
C	5.56686700	4.48942700	-1.60605900	C	1.72443700	2.79025600	0.99533200
H	3.57337900	0.61278800	-1.30603100	C	4.09778900	1.77283100	0.04690800
C	5.49524000	5.84408700	-1.33329500	C	2.83849600	3.61354100	0.90691900
C	4.25687800	6.48041700	-1.30506100	C	4.02969000	3.10516900	0.42219800
H	6.52258600	3.99403300	-1.56532200	F	-1.26260300	-1.78828500	0.58735400
H	6.40119000	6.39885800	-1.12597300	F	-0.98674900	-4.11640600	1.84497600
H	4.19785200	7.54173100	-1.09586500	F	1.13569300	-4.52365300	3.51670700
H	2.84320800	1.06666300	-2.82371200	F	2.96074900	-2.54542400	3.86402700
H	1.20613600	1.62398100	-1.14683800	F	2.71685100	-0.23786100	2.60895500
H	1.05301100	4.11781900	-1.39973200	F	-0.45531900	2.70377200	-0.91615600
N	5.35856500	1.78214400	-2.90006600	F	-2.87012400	3.78292600	-0.89426900
O	5.13181400	0.45426900	-3.26361100	F	-4.75856200	2.89756900	0.85584100
H	5.45957600	-0.07701000	-2.50831600	F	-4.13591600	0.90863000	2.59504200

F	-1.76851500	-0.20119200	2.58940700	C	1.47243600	-4.02354200	-1.50780000
F	0.61902500	3.35309100	1.49629500	C	2.54424800	-4.14252900	-2.38379100
F	2.77090100	4.88702100	1.28740400	H	-0.04996900	-2.75180400	-0.75718900
F	5.09986500	3.88394600	0.32164600	H	1.16023400	-4.86136700	-0.89619900
F	5.23511800	1.26949800	-0.42876900	H	3.08834200	-5.07596900	-2.46195400
F	3.08570600	-0.30270200	-0.18781000	H	0.53440300	1.06636000	-3.61296900
H	0.53625800	-0.06683100	-0.66970800	H	2.86761600	1.46999700	-3.73915000
H	-2.60100500	-1.66897800	-3.89997100	H	3.70337900	-0.84416800	-4.27781500
C	-3.67128800	-1.00722100	-1.44268200	N	-0.91851600	-0.47479600	-2.33822100
C	-4.04436400	-1.62899600	-0.24265000	O	-1.51417200	0.74522800	-2.71982900
C	-4.41809700	0.09963500	-1.87648300	H	-1.97771500	1.06682000	-1.93304500
C	-5.11056100	-1.14735500	0.50930500				
H	-3.49477800	-2.49183500	0.11588300	I3			
C	-5.48090300	0.58639100	-1.12204000				
H	-4.17609100	0.58210000	-2.81875000	Si	0.96043500	-0.68511800	-0.84239800
C	-5.82485700	-0.03537800	0.07430100	H	-1.53472000	-1.04323000	1.89106100
H	-5.37747000	-1.63342000	1.43983900	H	1.06794400	-1.97284900	-1.57274300
H	-6.03762200	1.44992000	-1.46612700	C	2.69133900	-0.09846900	-0.44475400
H	-6.64610500	0.34817300	0.66800300	C	2.91274900	0.82248400	0.58655500
H	-1.83244500	-2.99636100	-1.99749000	C	3.79394800	-0.55593200	-1.17384700
C	2.56530700	0.61140300	-3.13628100	C	4.19463900	1.27614400	0.87730900
C	2.68194200	-0.67826000	-3.93258700	H	2.07167800	1.18142700	1.17202000
C	2.24595600	-1.83344200	-3.07260200	C	5.07835000	-0.10168100	-0.89000000
C	1.17048500	-1.70725900	-2.17426800	H	3.65230300	-1.28167400	-1.96884300
C	0.42452200	-0.39837200	-2.09519300	C	5.27915400	0.81525500	0.13636700
C	1.11441100	0.82536200	-2.71937100	H	4.34955900	1.98776800	1.67997500
H	3.74664300	-3.14029800	-3.84956300	H	5.92169200	-0.46725700	-1.46405700
H	3.23916100	0.56040000	-2.28257900	H	6.27899300	1.16761800	0.36135400
H	2.04357700	-0.61932500	-4.82247500	H	0.19860300	0.28604400	-1.65742800
C	2.91432100	-3.05415200	-3.15992700	C	-3.44350600	-2.10348800	0.13564600
C	0.79563500	-2.81728100	-1.41524200	C	-3.93176200	-0.90979400	-0.68126500
H	1.01862600	1.68105100	-2.05688800	C	-3.21482300	0.37465100	-0.31701800

C	-1.99504900	0.37542800	0.37099200	H	7.02003900	0.29435500	-1.01905600
C	-1.33895000	-0.92610300	0.81661500	C	7.48505900	1.62502100	2.06334300
C	-1.92006400	-2.14563800	0.09823900	H	6.02388400	2.75588200	3.16415900
H	-4.73243100	1.59374800	-1.21247700	H	8.73546500	0.48387600	0.73529600
H	-3.78110100	-2.00550700	1.17354400	H	8.24086600	1.70222800	2.83619700
H	-3.76637900	-1.11415300	-1.74589300	H	3.27357900	2.41449700	-1.17658400
C	-3.78656100	1.59791000	-0.67976100	C	4.37024200	-2.40804900	2.05781100
C	-1.39406700	1.59590600	0.69543300	C	5.85031500	-2.33430300	1.69720400
H	-1.51981000	-3.04942300	0.56109000	C	6.06321100	-2.29999400	0.20193200
C	-1.97089200	2.80192500	0.32802500	C	5.05464100	-1.87248800	-0.66929200
C	-3.17571600	2.80330600	-0.37028000	C	3.68595000	-1.42033000	-0.15855700
H	-0.45597100	1.58434600	1.23738100	C	3.63152300	-1.26846100	1.36574300
H	-1.48582900	3.73607500	0.58500300	H	8.08564100	-2.98708000	0.35283700
H	-3.63829300	3.73829600	-0.66349200	H	3.95734800	-3.37188200	1.74038900
H	-1.58695300	-2.13607000	-0.94777300	H	6.27961800	-1.41904700	2.12678500
H	-3.87029000	-3.02888500	-0.25626600	C	7.30433800	-2.66304200	-0.32719600
H	-5.00792900	-0.76492300	-0.55674500	C	5.30952700	-1.84389400	-2.04295800
N	0.11638200	-0.82310800	0.69558000	H	2.58535600	-1.21730600	1.67378500
O	0.71845800	-1.91249500	1.40376900	C	6.54572000	-2.20381800	-2.55937200
H	1.15776900	-1.48940600	2.14911500	C	7.55475100	-2.61164600	-1.69066300
I4'				H	4.53422700	-1.51801800	-2.73012100
				H	6.72031600	-2.16850900	-3.62769500
				H	8.52609900	-2.89603600	-2.07706600
Si	4.19378500	1.26401700	-1.21919800	H	4.10004300	-0.31957400	1.64152000
H	2.95496400	-2.18528100	-0.44672900	H	4.23865200	-2.33992200	3.13916700
H	4.77097200	1.11260900	-2.57666200	H	6.40364400	-3.17532200	2.12162200
C	5.53042700	1.41781000	0.06911900	N	3.23291500	-0.17228900	-0.79997300
C	5.27059200	2.11619100	1.25615600	O	2.13544600	-0.35057800	-1.69431100
C	6.79389300	0.84130000	-0.10798300	H	2.35440300	-0.95252200	-2.42319700
C	6.23848800	2.21624500	2.24951600	Si	0.33843900	-0.24922000	-0.78137400
H	4.30003500	2.58103200	1.40715700	H	-0.29573100	-0.59977900	-2.05977400
C	7.76426000	0.94154400	0.88339100	C	0.58019900	1.55852200	-0.45616300

C	0.87767400	2.04432500	0.81969600	F	-4.88503300	-4.44397600	-3.01646900
C	0.47644100	2.46161300	-1.52025800	F	-6.28465200	-2.21144600	-2.35876800
C	1.05988500	3.40794200	1.02891900	F	-5.10594300	-0.24265400	-0.97491500
H	0.95302100	1.35996200	1.65917900	F	-2.08253200	2.21142400	1.62425900
C	0.65948800	3.82413900	-1.31329800	F	-2.14520700	4.71839600	0.74891400
H	0.24662800	2.10279400	-2.51953400	F	-2.63338200	5.24980600	-1.86677000
C	0.94935900	4.29699000	-0.03657500	F	-3.09272300	3.20310100	-3.59526600
H	1.27331400	3.77866600	2.02422000	F	-3.02428600	0.68994900	-2.75901100
H	0.56290500	4.51678200	-2.14154500	F	-4.63183700	1.09871300	1.55749500
H	1.07729300	5.35968100	0.13055900	F	-5.36796000	0.47858300	4.04347500
H	0.79889400	-1.23883900	0.19593300	F	-4.01669900	-1.40865800	5.44894400
B	-2.42565400	-0.19747800	0.02989500	F	-1.90119300	-2.68326000	4.31204800
C	-2.60577000	1.31686700	-0.50682700	F	-1.16257300	-2.09571000	1.81031700
C	-2.84543200	1.64556300	-1.83395500	H	-1.16143700	-0.38527700	0.07217200
C	-2.38105200	2.40536500	0.33250800				
C	-2.87912500	2.95109600	-2.30353800	I4			
C	-2.40306700	3.71992000	-0.09428700				
C	-2.65348600	3.99473000	-1.42743400	Si	-2.17104800	0.37138400	0.27561100
C	-3.04843800	-1.38534700	-0.88313100	H	-2.23089500	-0.23754400	-3.40978300
C	-4.37900600	-1.32405000	-1.27987200	H	-1.52889200	-0.91676800	0.57681100
C	-2.38487100	-2.55090900	-1.23008300	C	-3.91586900	0.25613500	0.90885100
C	-5.00975200	-2.32635800	-1.99398700	C	-4.86406100	1.27927400	0.77791900
C	-2.97603600	-3.58108300	-1.94738800	C	-4.27775100	-0.91123100	1.59235000
C	-4.29876500	-3.46756700	-2.33086900	C	-6.14498200	1.12958400	1.29302600
C	-2.85939900	-0.46913300	1.57084400	H	-4.59750300	2.19884000	0.26765100
C	-2.20759600	-1.43029400	2.32963600	C	-5.55856600	-1.05993900	2.11745100
C	-3.93435300	0.15152200	2.19349600	H	-3.55630600	-1.71490400	1.70922000
C	-2.57059700	-1.75731400	3.62580700	C	-6.49296300	-0.04278900	1.96137300
C	-4.33405900	-0.14903200	3.48599500	H	-6.87171900	1.92538200	1.18082900
C	-3.64675700	-1.11054400	4.20703400	H	-5.82516600	-1.96821300	2.64431900
F	-1.09725000	-2.73991400	-0.88332100	H	-7.49180900	-0.15827500	2.36524900
F	-2.28288600	-4.67450600	-2.26392700	H	-1.40620400	1.55070200	0.72751600

C	-5.03678800	-1.41035300	-2.84986000	C	-2.44417700	5.52674900	0.53340700
C	-4.83793800	-2.35349800	-1.66409700	H	-4.41348800	4.82203000	0.03467000
C	-3.37247100	-2.69181800	-1.50358700	H	-0.37508100	6.06062700	0.79837900
C	-2.38788600	-1.82452100	-1.98887600	H	-2.79833300	6.18745500	1.31564600
C	-2.72771300	-0.41814100	-2.45290500	H	-1.85569200	2.35141700	-3.82157200
C	-4.23439300	-0.13660800	-2.60695600	B	1.58718800	-0.31330600	0.23572600
H	-3.73703400	-4.57741600	-0.54854000	C	1.17877800	-1.63857800	1.08266200
H	-4.70792100	-1.90224100	-3.77107600	C	1.52650900	-2.93528200	0.73663200
H	-5.22444500	-1.87487600	-0.75622800	C	0.27963400	-1.55042600	2.14004600
C	-2.97680500	-3.90816200	-0.93835200	C	0.99790000	-4.06135300	1.35029700
C	-1.04834600	-2.22812000	-1.99541600	C	-0.27560700	-2.64349800	2.77953400
H	-4.37157900	0.59207000	-3.40885300	C	0.08430000	-3.91790300	2.37527200
C	-0.67325700	-3.45201200	-1.46335300	C	2.81107800	-0.50083400	-0.81646000
C	-1.64109300	-4.28199500	-0.89929400	C	4.07074500	-0.87297300	-0.36632400
H	-0.29117300	-1.57922900	-2.42738900	C	2.72697400	-0.23307100	-2.16926400
H	0.36433500	-3.76113600	-1.49259100	C	5.17139900	-0.99352300	-1.19424500
H	-1.35269200	-5.23062000	-0.46000300	C	3.80031100	-0.33577900	-3.04185600
H	-4.60627400	0.32722400	-1.69071900	C	5.03258000	-0.71946100	-2.54707300
H	-6.09321100	-1.16196000	-2.96858300	C	1.93265000	1.00601200	1.12711500
H	-5.40119700	-3.27942800	-1.80049300	C	1.84679900	2.25577300	0.53347100
N	-2.19258900	0.62166800	-1.52821000	C	2.40205300	1.00728200	2.43308800
O	-0.85473900	0.99989400	-1.97888800	C	2.18818100	3.43791700	1.16663900
H	-0.08642000	0.60235000	-1.46431300	C	2.74122900	2.16801000	3.11347000
Si	-0.91205200	2.61583900	-2.72656500	C	2.63266900	3.39117200	2.47672100
H	0.47789600	2.81814600	-3.14660900	F	1.55067200	0.14921800	-2.72227000
C	-1.53375200	3.80715800	-1.46960000	F	3.65666500	-0.06611400	-4.33957000
C	-2.90269900	3.89689600	-1.18046700	F	6.07883700	-0.82529600	-3.36150500
C	-0.63388900	4.60793200	-0.75786900	F	6.35760200	-1.36388400	-0.71613600
C	-3.35432900	4.75393600	-0.18493400	F	4.24108800	-1.14821100	0.93309000
H	-3.61305100	3.28922200	-1.73307000	F	-0.14057300	-0.34374000	2.56138600
C	-1.08551000	5.45829700	0.24532000	F	-1.17600700	-2.48347300	3.75068600
H	0.42416600	4.56608400	-0.98183800	F	-0.46354400	-4.98762900	2.94646700

F	1.31157600	-5.28086700	0.90793700	H	-3.67814300	-4.62868400	-0.58147800
F	2.35550800	-3.17919500	-0.29264100	H	-4.75569600	-1.88731500	-3.69288600
F	2.54975600	-0.13638300	3.10819700	H	-5.19945100	-1.92486400	-0.66767200
F	3.17681000	2.11825800	4.37050500	C	-2.93566200	-3.93787200	-0.96815700
F	2.96161800	4.51332700	3.11031700	C	-1.05706200	-2.20307300	-2.02694100
F	2.11295900	4.61766000	0.54183200	H	-4.44433300	0.60245600	-3.28931100
F	1.42710600	2.34627200	-0.75347900	C	-0.65556400	-3.44182800	-1.54927400
H	0.56483200	-0.06538600	-0.40181300	C	-1.59659900	-4.30120400	-0.98330300
TS2				H	-0.32813800	-1.52858000	-2.46583200
				H	0.38173900	-3.74530800	-1.63097100
				H	-1.28808500	-5.26454000	-0.59157300
Si	-2.24877300	0.38571600	0.31998300	H	-4.64421700	0.30457700	-1.57343600
H	-2.29339500	-0.19232800	-3.34743400	H	-6.13405200	-1.18489400	-2.84525800
H	-1.61258900	-0.90763000	0.65101700	H	-5.38886800	-3.31243700	-1.73248100
C	-3.98123700	0.29585300	0.99879300	N	-2.22072400	0.62616000	-1.45553400
C	-4.89524100	1.35400600	0.90463300	O	-0.84126200	0.91873800	-1.81241100
C	-4.37284300	-0.86930500	1.66869900	H	0.22523500	0.30002100	-0.94901500
C	-6.17071500	1.24075300	1.44272400	Si	-0.91885400	2.41910800	-2.64755700
H	-4.60542000	2.27392400	0.40680500	H	0.45434500	2.67465700	-3.11075400
C	-5.64873500	-0.98328900	2.21444000	C	-1.52303300	3.74335800	-1.49529500
H	-3.67731200	-1.69897800	1.75938000	C	-2.88427600	3.87334300	-1.18743700
C	-6.54888900	0.06917600	2.09548500	C	-0.61137700	4.60339300	-0.87480700
H	-6.86985700	2.06443300	1.35962100	C	-3.31569600	4.82388200	-0.26960600
H	-5.93833200	-1.89165200	2.72915200	H	-3.60710100	3.22049200	-1.66778800
H	-7.54364900	-0.01823500	2.51627500	C	-1.03878800	5.54936000	0.05238900
H	-1.46317800	1.53344900	0.82001200	H	0.44280400	4.53517200	-1.11425500
C	-5.07125600	-1.41830400	-2.75503600	C	-2.39097300	5.65643600	0.35721600
C	-4.83197900	-2.38281400	-1.59370100	H	-4.37108000	4.91887900	-0.04050200
C	-3.35883300	-2.70684900	-1.47996900	H	-0.31550600	6.19713800	0.53334600
C	-2.39929300	-1.81109300	-1.96488800	H	-2.72748700	6.39168800	1.07859500
C	-2.76714500	-0.39562300	-2.38307600	H	-1.85645200	2.19409200	-3.76540600
C	-4.28088200	-0.13848400	-2.50360100	B	1.73415500	-0.34350600	0.27778000

C	1.25000500	-1.67572100	1.03005100	F	1.50203600	2.30366800	-0.77033100
C	1.59209300	-2.95646100	0.61263800	H	0.50984100	-0.26950100	-0.40236800
C	0.32329900	-1.62305100	2.07001900				
C	1.03890200	-4.10346500	1.15769300	I5			
C	-0.25848800	-2.74444600	2.63113800				
C	0.09966000	-3.99822400	2.16505300	C	2.22203000	-0.38909400	2.72713500
C	2.88051900	-0.47213700	-0.83772300	C	3.61376400	-0.54910100	2.11969300
C	4.15679800	-0.78400500	-0.38813100	C	3.59242000	-1.34119700	0.82793500
C	2.75821900	-0.24451700	-2.19640500	C	2.41473300	-1.53254000	0.09408600
C	5.25208500	-0.88251000	-1.22454200	C	1.08602400	-0.96377100	0.57691600
C	3.83080000	-0.33080000	-3.07199200	C	1.26483700	0.11090000	1.65090700
C	5.08328900	-0.65223700	-2.58181900	H	5.69231800	-1.75624200	0.92573600
C	1.92741100	0.99521300	1.13901400	H	1.87326500	-1.35318000	3.11448200
C	1.84649300	2.23890900	0.52918100	H	4.03025400	0.44479500	1.91674500
C	2.34082200	0.99918900	2.46507300	C	4.78102100	-1.90521000	0.35494600
C	2.12671200	3.42631200	1.18112200	C	2.45137200	-2.30266000	-1.07312100
C	2.62001000	2.16726800	3.15726000	H	0.28523500	0.37284000	2.05542100
C	2.50685600	3.38630100	2.51245500	C	3.63787700	-2.85529200	-1.53069500
F	1.56862800	0.07266000	-2.73193100	C	4.81412000	-2.64990000	-0.81404800
F	3.66432000	-0.10460100	-4.37207600	H	1.53089000	-2.45499800	-1.62448900
F	6.12051400	-0.73923800	-3.40541100	H	3.64638400	-3.44492600	-2.43965600
F	6.45428300	-1.19207300	-0.74964900	H	5.74806900	-3.07667500	-1.16027000
F	4.34101300	-1.01583300	0.91830100	H	1.68144900	1.01686300	1.19644000
F	-0.08975300	-0.44151400	2.54456700	H	2.25623600	0.30418500	3.56985000
F	-1.18143100	-2.62791500	3.58203100	H	4.29525700	-1.03434800	2.82311700
F	-0.47714400	-5.08594900	2.65707100	N	0.29346200	-0.52932600	-0.57659100
F	1.34396400	-5.29952100	0.65883500	O	-1.06352600	-0.27467000	-0.13318500
F	2.43648600	-3.14863000	-0.40744400	H	0.51788800	-1.79195200	1.02440300
F	2.50715500	-0.14407500	3.13186700	Si	0.71935800	0.82140500	-1.63541500
F	3.00578400	2.12712100	4.42823800	H	-0.26738800	0.74311100	-2.73354700
F	2.77877000	4.51226100	3.15839900	H	2.09618500	0.59812300	-2.12508600
F	2.06350500	4.59995500	0.55360700	C	0.64149400	2.49816700	-0.80317600

C	-0.50334800	2.91564100	-0.10851000	C	0.23142200	11.94915000	-5.84330900
C	1.74572100	3.35772100	-0.84179600	H	-4.28416100	11.94674800	-7.59277900
C	-0.53783300	4.15162100	0.52670600	H	-1.09861900	10.84953400	-4.55203400
H	-1.36402400	2.25780900	-0.04991800	H	-2.32962500	13.23750200	-5.98724600
C	1.71138100	4.59853600	-0.21130400	C	-3.37798800	11.50520900	-7.99542100
H	2.64769600	3.05511500	-1.36513300	C	-1.08003200	10.35301100	-9.00625700
C	0.56901000	4.99522400	0.47460000	H	1.14189300	11.89313800	-5.24802700
H	-1.42759900	4.45832300	1.06421400	C	-2.22797500	10.37298200	-9.78148200
H	2.57521700	5.25172200	-0.25259900	C	-3.38619100	10.95250700	-9.26657400
H	0.54038400	5.95899100	0.96953000	H	-0.17196700	9.89470600	-9.38634300
Si	-1.99645200	-1.52818600	-0.76784700	H	-2.22531800	9.94153100	-10.77527100
H	-1.51670700	-2.82320600	-0.23603600	H	-4.29581700	10.96644000	-9.85572500
H	-1.89975800	-1.49509500	-2.24221900	H	0.25614600	12.92167700	-6.34765600
C	-3.74134300	-1.20600800	-0.19799200	H	-0.96936300	12.54855200	-4.14523000
C	-4.45397000	-0.10235200	-0.68652100	H	-3.17078600	11.84721200	-5.32679300
C	-4.36774900	-2.04320500	0.73204800	N	0.39202500	9.49032200	-6.45365900
C	-5.74940400	0.15847700	-0.25619500	H	1.04922400	11.06529700	-7.61766200
H	-3.99393000	0.56058500	-1.41364000	O	1.74012500	9.22354400	-5.99532300
C	-5.66635800	-1.78830500	1.16257300	Si	2.81911200	8.70645700	-7.27244900
H	-3.83781400	-2.90451700	1.12639200	H	3.83214800	7.94650900	-6.52474500
C	-6.35635300	-0.68652500	0.66914000	H	1.97851500	7.90724400	-8.17614800
H	-6.28721900	1.01633400	-0.64221900	Si	-0.66239100	8.26186100	-5.72880900
H	-6.13825000	-2.44691000	1.88211200	H	-0.56771800	8.32966000	-4.25251100
H	-7.36742300	-0.48594300	1.00370100	H	-0.09287700	6.98013200	-6.19945700
I6'				Si	2.40700500	9.73766600	-4.19219600
				H	3.29616900	10.69791300	-4.86073800
				H	1.04968800	10.09075400	-3.76174600
C	-1.02414100	11.85419800	-4.98497900	C	3.00936300	8.05559100	-3.66189100
C	-2.25541500	12.15359800	-5.84099000	C	4.34545700	7.64379800	-3.76735300
C	-2.22246700	11.50268000	-7.20841200	C	2.09699600	7.19734500	-3.03328100
C	-1.06611600	10.91453700	-7.72769300	C	4.75424700	6.41805500	-3.25474200
C	0.22238800	10.87365600	-6.92665800	H	5.07837300	8.28130600	-4.24460300

C	2.50480200	5.96907000	-2.52357700	C	5.22550500	14.39811500	-3.29954200
H	1.06288200	7.49873200	-2.90726400	C	6.12380700	12.51179300	-4.44799500
C	3.83558300	5.58060900	-2.62840900	C	6.03658000	13.88463900	-4.29381700
H	5.79351200	6.12146100	-3.33522500	C	2.37445300	11.78302300	-0.99850200
H	1.78816300	5.32773700	-2.02552200	C	2.17004800	11.72622300	0.37113200
H	4.15920600	4.63369100	-2.21251500	C	1.40450600	12.47314100	-1.71184800
C	3.57090600	10.18739200	-8.10019200	C	1.07158500	12.30164600	0.99481400
C	4.61587000	10.88743600	-7.47820000	C	0.29558300	13.06114900	-1.13440700
C	3.10801300	10.63947800	-9.34322200	C	0.12670000	12.96980200	0.23757100
C	5.15976500	12.02289100	-8.06819100	C	4.34307200	9.87394600	-1.05283200
H	5.01955300	10.54466400	-6.52915900	C	3.55670000	8.82497300	-0.58489100
C	3.65525800	11.77068100	-9.93778700	C	5.71063300	9.67831600	-0.93962600
H	2.31392000	10.10460600	-9.85520400	C	4.06831300	7.65184500	-0.06681800
C	4.67521300	12.46567100	-9.29542000	C	6.26796700	8.50854100	-0.43953100
H	5.96251700	12.55529300	-7.57298200	C	5.44256500	7.48787900	-0.00838800
H	3.28712100	12.10918000	-10.89862300	F	1.54090900	12.61059900	-3.04524600
H	5.09944800	13.35014200	-9.75539700	F	-0.60459100	13.71212800	-1.87359100
C	-2.45927000	8.44335600	-6.17660500	F	-0.93166000	13.52494000	0.81997100
C	-2.96563900	8.00088800	-7.40446700	F	0.91744900	12.21608500	2.31483100
C	-3.35498800	8.95363000	-5.22792400	F	3.04487100	11.10201800	1.16826800
C	-4.32427700	8.08380100	-7.68317100	F	5.50903400	10.37146200	-3.82180200
H	-2.29419600	7.59362700	-8.15356000	F	6.90464800	11.99264200	-5.39928600
C	-4.71400100	9.04636900	-5.50841100	F	6.72678400	14.69298200	-5.09144900
H	-2.99099400	9.28005200	-4.25815300	F	5.14233100	15.71603700	-3.13186700
C	-5.19834800	8.61105000	-6.73748700	F	3.74656400	14.12488000	-1.54964300
H	-4.70115200	7.74216500	-8.64007100	F	6.57822900	10.62521000	-1.32266600
H	-5.39400000	9.44707900	-4.76584600	F	7.59145800	8.36089000	-0.37457000
H	-6.25774600	8.67654800	-6.95631000	F	5.95959800	6.35223800	0.45297400
B	3.60977000	11.10702800	-1.79256200	F	3.26712300	6.67486500	0.35658600
C	4.53326500	12.15377800	-2.61857800	F	2.21947100	8.92698200	-0.64890900
C	4.49907600	13.53645300	-2.48642400	H	2.98329800	10.46142100	-2.71483100
C	5.38269000	11.69477000	-3.61768100				

I6				H	0.69309500	10.54043500	-3.37103100
C	-1.91553400	12.29249800	-4.43979000	C	3.31966900	9.68290800	-3.96446300
C	-3.27260800	12.34955700	-5.13595500	C	4.53985100	10.28738500	-3.63399700
C	-3.32471900	11.50058700	-6.38638600	C	3.25743000	8.28638500	-4.06850300
C	-2.16497900	11.10018300	-7.05494800	C	5.67291100	9.51146800	-3.41650300
C	-0.78157100	11.39402200	-6.49959900	H	4.61329300	11.36747400	-3.57166900
C	-0.81053500	12.51813400	-5.46528600	C	4.39443200	7.51280500	-3.87048600
H	-5.46696900	11.43771200	-6.40172400	H	2.32172000	7.79579600	-4.32026900
H	-1.78411500	11.31815200	-3.95308800	C	5.60136200	8.12730600	-3.54405500
H	-3.48417000	13.38783000	-5.42304000	H	6.61266000	9.98644300	-3.16296500
C	-4.56332500	11.12911900	-6.91695600	H	4.34065000	6.43535300	-3.96836100
C	-2.26056400	10.37162000	-8.24321700	H	6.48810200	7.52437100	-3.38910200
H	0.16713900	12.63970000	-4.99875000	C	3.61284900	10.22482300	-7.68939700
C	-3.49390600	10.01448000	-8.76223800	C	4.82256200	10.00038200	-7.01427300
C	-4.65347100	10.38851100	-8.08467500	C	3.62920400	10.97693100	-8.87432500
H	-1.34837100	10.10734800	-8.76937900	C	6.00016200	10.57189900	-7.47658600
H	-3.55595600	9.45999400	-9.69058100	H	4.85063200	9.37651700	-6.12835400
H	-5.62509300	10.11313800	-8.47703900	C	4.81700800	11.51486600	-9.35799700
H	-0.99313000	13.45326300	-5.99958700	H	2.71221000	11.16148300	-9.42278800
H	-1.86630900	13.04656900	-3.65217100	C	5.99708200	11.32973900	-8.64720500
H	-4.07421800	12.04772500	-4.45779000	H	6.92386500	10.41656800	-6.93214900
N	-0.27616100	10.11705800	-5.96353100	H	4.80491500	12.08999700	-10.27598000
H	-0.12546700	11.67231500	-7.33330800	H	6.91976900	11.77189100	-9.00568500
O	1.17626900	10.14035600	-5.80568100	C	-0.41663200	7.17689300	-6.10605000
Si	2.01727100	9.41216800	-7.25372500	C	0.31100800	6.20694200	-5.40787400
H	2.17355500	8.01186300	-6.83790000	C	-0.57631100	7.02830500	-7.49065900
H	1.00051800	9.65490000	-8.28266300	C	0.89513400	5.13470500	-6.07665800
Si	-1.05166700	8.69555500	-5.23344700	H	0.42727400	6.28877000	-4.33093600
H	-2.49558700	8.93328400	-5.36851700	C	0.00183200	5.95782700	-8.16122300
H	-0.63319200	8.58278400	-3.81564900	H	-1.15149300	7.76081900	-8.04941600
Si	1.84308200	10.74940800	-4.25834700	C	0.74899800	5.01743900	-7.45476400
H	2.22510800	12.15362800	-4.39781500	H	1.46096100	4.39316600	-5.52527300

H	-0.12545300	5.85545300	-9.23226000	F	0.14601600	16.84386600	-13.18704400
H	1.20808400	4.18777800	-7.97902700	F	1.34653800	15.14732700	-14.93609000
B	1.19113600	13.79422900	-9.30532800	F	2.49039800	12.85520600	-14.02036500
C	-0.10517200	14.40869600	-8.53164200	F	2.43213100	12.26494500	-11.41988500
C	-0.10006600	15.45588200	-7.62221100	H	1.05144700	12.58878900	-9.26643800
C	-1.35582800	13.86362300	-8.79587900				
C	-1.24540000	15.92018700	-6.99028600	TS3			
C	-2.52567100	14.29213800	-8.18855200				
C	-2.46533900	15.33021700	-7.27365700	C	-1.99815700	12.21424600	-4.54881500
C	2.61234200	14.09551900	-8.55586400	C	-3.33200500	12.29130100	-5.28441600
C	3.67594000	14.83522900	-9.05361700	C	-3.35594600	11.50303100	-6.57014500
C	2.87364100	13.46862800	-7.34715500	C	-2.18038900	11.16507800	-7.26330100
C	4.91585900	14.90544600	-8.42969500	C	-0.79681900	11.50365000	-6.66676100
C	4.08484700	13.51328200	-6.68494600	C	-0.84735400	12.48807300	-5.50996000
C	5.12560500	14.23567800	-7.23891900	H	-5.49145400	11.43879200	-6.65691500
C	1.21095200	14.22083600	-10.87824300	H	-1.88123800	11.23379600	-4.07682200
C	1.82490400	13.40228100	-11.81418800	H	-3.54230300	13.33750500	-5.54431900
C	0.66207300	15.38536400	-11.39540100	C	-4.57041600	11.16576700	-7.15988900
C	1.88395200	13.68518500	-13.16825100	C	-2.22973100	10.50656100	-8.50068400
C	0.69200100	15.71017100	-12.74332000	H	0.11693600	12.48676300	-5.00198800
C	1.30561400	14.85145100	-13.63766600	C	-3.44838500	10.17971800	-9.06489300
F	1.91630700	12.69656300	-6.78261000	C	-4.61985200	10.50110600	-8.38016100
F	4.27716000	12.83834800	-5.54266400	H	-1.29692000	10.26785700	-8.99914500
F	6.31809700	14.26110000	-6.64567800	H	-3.49116500	9.68073800	-10.02420700
F	5.91326300	15.60454300	-8.97367500	H	-5.58122600	10.24097600	-8.80691200
F	3.56659400	15.51929000	-10.20134300	H	-0.95607200	13.48449000	-5.94472300
F	-1.47195000	12.86553800	-9.68383100	H	-1.98114300	12.94541900	-3.73919700
F	-3.69860500	13.72320700	-8.46577700	H	-4.15348400	11.96350900	-4.64367000
F	-3.57349500	15.74449600	-6.65629300	N	-0.63076000	10.12634900	-6.41458300
F	-1.18651300	16.92302500	-6.11166300	H	-0.12520700	11.82857300	-7.46667200
F	1.04244700	16.08828400	-7.31566400	O	1.19332500	9.89587600	-5.88325000
F	0.08467600	16.28702600	-10.58610300	Si	1.99528800	9.22357000	-7.27116200

H	2.28396300	7.82397200	-6.90730900	C	-0.55463300	6.86515100	-7.31582300
H	1.00673600	9.34719200	-8.35383600	C	0.95308700	5.38356900	-5.50425400
Si	-1.37884800	8.80528200	-5.42335000	H	0.29847600	6.79603000	-4.02757300
H	-2.79909200	8.81300000	-5.81268200	C	0.14219500	5.74349500	-7.74782400
H	-1.21423000	8.99612500	-3.97065700	H	-1.13787000	7.43904400	-8.03067300
Si	1.81537600	10.40900600	-4.36624200	C	0.90180200	5.00673500	-6.84206300
H	2.10216000	11.84831300	-4.37846500	H	1.53690100	4.80469300	-4.79801600
H	0.72499600	10.09691400	-3.42403500	H	0.09731200	5.44426400	-8.78798500
C	3.39236500	9.48604900	-4.03324200	H	1.44934600	4.13496000	-7.17974100
C	4.52623200	10.21363300	-3.64819000	B	1.19149300	13.81340200	-9.23053000
C	3.50369800	8.09740700	-4.18560100	C	-0.08864600	14.49244000	-8.47550200
C	5.74008900	9.57123800	-3.42878900	C	-0.05122500	15.52346600	-7.54752900
H	4.46986600	11.29127300	-3.54347100	C	-1.35740400	13.99793400	-8.75318400
C	4.71943500	7.45595300	-3.97936300	C	-1.18194100	16.00675700	-6.90108100
H	2.64262300	7.51049100	-4.48707100	C	-2.51127600	14.44195000	-8.12779500
C	5.83865700	8.19423500	-3.60326800	C	-2.41875800	15.45526400	-7.18799900
H	6.61040800	10.14608200	-3.13626700	C	2.61450800	14.07448200	-8.47598900
H	4.79554700	6.38362400	-4.11442200	C	3.69165600	14.80465300	-8.95647400
H	6.78776700	7.69544000	-3.44676800	C	2.86246900	13.40933100	-7.28423400
C	3.53235700	10.13282000	-7.78607900	C	4.93293600	14.83410700	-8.33315100
C	4.77007400	10.02896400	-7.13189700	C	4.07538600	13.41225100	-6.62447000
C	3.46879100	10.86625800	-8.98014400	C	5.12952700	14.12846100	-7.16163000
C	5.89125800	10.68068500	-7.63020400	C	1.20201000	14.22760200	-10.80345200
H	4.86615800	9.43603400	-6.22912000	C	1.43834500	13.30096100	-11.80537600
C	4.59735200	11.49763100	-9.49387600	C	0.96139300	15.52229400	-11.24191200
H	2.53084600	10.96365400	-9.51624700	C	1.42101500	13.61594700	-13.15663800
C	5.80546700	11.41619300	-8.81138600	C	0.93214300	15.88363300	-12.57755400
H	6.83423100	10.61104800	-7.10078400	C	1.16072000	14.91743200	-13.54387800
H	4.52125700	12.06200200	-10.41631700	F	1.88848700	12.65379500	-6.73013800
H	6.68185800	11.92588300	-9.19639200	F	4.25334500	12.71020200	-5.49860500
C	-0.49955000	7.26721800	-5.97470500	F	6.32450900	14.10906400	-6.57246000
C	0.25300100	6.50748100	-5.07402300	F	5.94702900	15.52007500	-8.86483200

F	3.59628700	15.51393600	-10.09085300	C	-4.96821000	-5.20762100	-11.67936200
F	-1.50534500	13.01885100	-9.65921700	C	-5.97711600	-4.75770100	-10.81746400
F	-3.70111100	13.90224000	-8.40321600	C	-3.65949600	-4.76387700	-11.45887200
F	-3.51266500	15.88075100	-6.55366500	C	-5.68752600	-3.89370100	-9.76683200
F	-1.09187200	16.98865500	-6.00292200	H	-7.00276400	-5.08464800	-10.96539700
F	1.10804600	16.11010900	-7.22432100	C	-3.36587300	-3.89548900	-10.41305900
F	0.77327400	16.50346700	-10.34683700	H	-2.85624100	-5.11131400	-12.10130100
F	0.69747600	17.14387300	-12.94813200	C	-4.37983700	-3.46157500	-9.56538700
F	1.13833900	15.24250800	-14.83592500	H	-6.47926400	-3.55414200	-9.10915000
F	1.65174000	12.68248600	-14.08348600	H	-2.34548400	-3.56751400	-10.25194300
F	1.71475400	12.01888500	-11.50196400	H	-4.15201700	-2.78764100	-8.74757700
H	1.00529300	12.61741600	-9.17530300	H	-6.52186600	-6.04537400	-13.80958800

O(SiH₂Ph)₂

I7

O	-5.71514100	-7.91655700	-12.31941100	C	-2.81842100	0.40785200	3.89308900
Si	-5.42160300	-8.71458800	-10.89866300	C	-3.74988400	1.04513700	2.81824200
H	-5.22715600	-10.14137200	-11.22886800	C	-4.16868600	0.26944500	1.55796600
H	-6.56890800	-8.54216200	-9.97918200	C	-3.43595600	-0.76687100	0.94907400
C	-3.89730700	-8.00185300	-10.08515900	C	-1.60418200	-0.14239000	2.11044400
C	-3.99825700	-7.20345000	-8.94026800	C	-1.30022700	0.11674200	3.51373600
C	-2.63298000	-8.18098000	-10.66174100	H	-5.95521000	1.44026200	1.36213000
C	-2.87264200	-6.60421500	-8.38534100	H	-3.24725400	-0.54804000	4.19947000
H	-4.96873200	-7.03447400	-8.48390400	H	-3.32216000	2.00409600	2.50152100
C	-1.50520700	-7.57906800	-10.11388400	C	-5.36209800	0.63988200	0.93137600
H	-2.52428000	-8.79704000	-11.55020300	C	-3.84387100	-1.39310400	-0.22529700
C	-1.62578000	-6.79056600	-8.97328000	H	-0.92480300	-0.71920300	4.09773700
H	-2.96974900	-5.98281600	-7.50264500	C	-5.03187200	-0.99263000	-0.81734000
H	-0.53400700	-7.72767300	-10.57146000	C	-5.79363700	0.01623600	-0.23152400
H	-0.74813900	-6.32116900	-8.54393400	H	-3.22018400	-2.15535700	-0.67539200
Si	-5.34769500	-6.45936500	-13.01432800	H	-5.35395800	-1.45391500	-1.74190700
H	-4.15395000	-6.60010400	-13.87863700	H	-6.71780500	0.33539300	-0.69757300

H	-0.67168900	0.99704800	3.63020500	C	0.24006800	0.48390300	-2.33823700
H	-2.81299600	1.08031700	4.75064400	C	1.09948300	-0.59496900	-2.49669200
H	-4.67163300	1.29850800	3.34503200	C	0.07881400	1.27029400	-3.46900500
N	-2.26457100	-1.18109700	1.68502900	C	1.72474300	-0.91809100	-3.68785800
H	-1.64913800	0.73639700	1.47457300	C	0.69253000	0.99127500	-4.68246100
Si	-2.02475200	-2.91520500	2.20347800	C	1.51789900	-0.11306400	-4.79501800
H	-3.28363200	-3.34057200	2.84314000	F	0.79712200	-0.78295500	1.42948500
H	-0.89839200	-2.82762300	3.14716000	F	2.81683400	0.08977900	2.91930300
C	-1.66573900	-3.83762600	0.64170300	F	3.92278500	2.53486300	2.46104100
C	-0.61949000	-3.40049000	-0.18360800	F	2.94269400	4.10728100	0.47788700
C	-2.45410000	-4.91974500	0.23320400	F	0.88321000	3.25252400	-1.02607800
C	-0.37375300	-4.03036400	-1.39762800	F	-2.64441200	0.38111400	-2.66112600
H	-0.00425600	-2.55420500	0.10352500	F	-4.95171400	1.70734400	-2.68313900
C	-2.19971400	-5.55463700	-0.97791000	F	-5.42572000	3.67602800	-0.87804700
H	-3.27474200	-5.26417500	0.85422300	F	-3.51219100	4.29417200	0.96382800
C	-1.16369600	-5.10695200	-1.79232900	F	-1.21875000	2.99334900	1.01763700
H	0.43153100	-3.67575600	-2.02963400	F	-0.70684400	2.35585600	-3.44282000
H	-2.81255600	-6.39191100	-1.28911400	F	0.49453400	1.77522500	-5.74334700
H	-0.97256700	-5.59699800	-2.73961800	F	2.10920900	-0.39778000	-5.95408600
B	-0.44536100	0.69993700	-0.87243900	F	2.51416700	-1.99162700	-3.78011300
C	-1.76829700	1.66258100	-0.88137200	F	1.35895500	-1.40115500	-1.44871100
C	-2.06871500	2.67799600	0.01356200	H	-0.82824100	-0.38984600	-0.51222200
C	-2.79114900	1.38371700	-1.78429500				
C	-3.26882700	3.37737200	0.02230400	2a-Si			
C	-3.99444500	2.06070600	-1.82397000				
C	-4.24032000	3.06890700	-0.90699000	C	-9.54187500	1.06885000	-1.65566000
C	0.74742100	1.20619000	0.12400400	C	-9.29362100	0.83143100	-0.15886200
C	1.35033100	2.44344000	-0.06701200	C	-9.80790100	-0.48091500	0.38414200
C	1.29686100	0.44287200	1.13771200	C	-9.33834500	-1.71795100	-0.09437300
C	2.40653900	2.90742900	0.69531100	C	-8.75211600	-1.23618600	-2.44638700
C	2.35056600	0.86410500	1.93734600	C	-8.60627500	0.28034100	-2.56920600
C	2.91133600	2.10644000	1.70968200	H	11.11340900	0.46275900	1.79318100

H	10.58336400	0.82617800	-1.89499700				
H	-8.21551700	0.89686300	0.03264300	I8'			
C	10.74231300	-0.48670800	1.42137900				
C	-9.78536900	-2.90415700	0.49264600	Si	7.37171500	2.39229300	-3.59584000
H	-8.79378200	0.55996700	-3.61113800	B	8.34460200	4.32580400	-5.56075300
C	10.69836800	-2.88636500	1.53997900	C	9.92278100	4.24921200	-5.24908200
C	11.18654800	-1.66984300	2.00136600	C	10.89563900	3.85153200	-6.15616400
H	-9.40550200	-3.84211900	0.10361000	C	10.37041200	4.42452400	-3.94426300
H	11.03442800	-3.81689700	1.98169600	C	12.21572500	3.61911600	-5.79259500
H	11.90614800	-1.63954700	2.81081800	C	11.66991100	4.19637600	-3.53826300
H	-7.56719300	0.55425000	-2.34644600	C	12.60168000	3.78188600	-4.47597000
H	-9.41107700	2.13533700	-1.85873000	C	7.89982200	4.00544600	-7.07731300
H	-9.76229600	1.63634400	0.41185700	C	7.83217100	5.02503400	-8.01598700
N	-8.37963900	-1.80017900	-1.14645900	C	7.59082300	2.73938600	-7.54511100
H	-9.78933700	-1.52375300	-2.65276800	C	7.46319800	4.81584900	-9.33415500
Si	-6.72888800	-2.09541800	-0.69081500	C	7.21303600	2.48426900	-8.85294000
H	-5.94065700	-2.13507300	-1.94504900	C	7.14617500	3.53417900	-9.75248100
H	-6.64749100	-3.37618500	0.05077300	C	7.51298300	5.56537600	-4.94548700
C	-6.07269000	-0.73425500	0.41896700	C	6.15277200	5.43372300	-4.70881600
C	-5.27739900	0.30163600	-0.08596900	C	8.04796800	6.81103500	-4.65236100
C	-6.49596500	-0.65474700	1.75289600	C	5.36072800	6.44089400	-4.18739000
C	-4.91954900	1.38541700	0.71026000	C	7.29060500	7.85311900	-4.13992400
H	-4.93516200	0.26539000	-1.11623500	C	5.93882200	7.66613900	-3.90340900
C	-6.14725400	0.42977100	2.55088900	F	7.66899300	1.67609600	-6.72345000
H	-7.11741200	-1.44177800	2.17185200	F	6.92111400	1.24832400	-9.25270000
C	-5.36000500	1.45211700	2.02843200	F	6.78761500	3.31210500	-11.01246400
H	-4.30084300	2.17719700	0.30408100	F	7.41474900	5.82469500	-10.20051300
H	-6.48893800	0.47890900	3.57819100	F	8.16319300	6.27459300	-7.66545000
H	-5.08756500	2.29778300	2.64907000	F	9.49175600	4.77614400	-2.99065300
H	-8.13171800	-1.71869600	-3.20659700	F	12.02740700	4.33679000	-2.26349500
				F	13.85038500	3.52224200	-4.10368900
Path B				F	13.10625600	3.21499500	-6.69703800

F	10.60021600	3.64063300	-7.44480300	C	2.49869700	-2.44065300	-3.07609700
F	9.34398900	7.05610900	-4.86301600	C	1.31000700	-1.96767000	-3.63205200
F	7.84722000	9.03173800	-3.87230700	H	4.42798000	-1.90178800	-2.31018000
F	5.20290400	8.65403700	-3.40633500	H	2.63806100	-3.50073000	-2.90459600
F	4.06240400	6.24268300	-3.95566200	H	0.52148000	-2.66073700	-3.89985000
F	5.54650700	4.25718400	-4.96567900	H	3.45260400	2.40362300	-1.65596300
H	7.89520700	3.28423800	-4.91677300	H	2.99590500	3.65307100	-3.80968300
H	6.40756200	1.70349400	-4.45966900	H	1.33951300	1.91107800	-4.67813500
C	9.05834600	1.69248300	-3.24123100	N	5.54913200	0.26580100	-2.33366900
C	9.63728100	1.89068400	-1.98022700	O	6.53230100	1.25206000	-2.00624200
C	9.81504700	1.07197000	-4.24305800	H	7.24161200	0.72735100	-1.60819600
C	10.93999700	1.47448300	-1.72407100				
H	9.08677800	2.40972500	-1.20007900	I8			
C	11.11971400	0.66504800	-3.98905400				
H	9.39215500	0.92837300	-5.23197400	Si	7.95070500	2.51722000	-2.73726600
C	11.68301000	0.86808300	-2.73138600	B	8.10841700	-1.05854400	-0.29225200
H	11.38116600	1.64737500	-0.75026000	C	9.30309300	-1.95540200	-0.93684500
H	11.70172300	0.19894700	-4.77539300	C	10.56389600	-2.18397800	-0.40469800
H	12.70516600	0.56317300	-2.54087500	C	9.11885900	-2.47434200	-2.21253900
H	6.99526700	3.58311800	-2.82793700	C	11.55859100	-2.88995800	-1.06891800
C	3.19896700	2.58183500	-3.79051800	C	10.07553400	-3.18450200	-2.91083000
C	1.90201600	1.78309400	-3.75097700	C	11.31413500	-3.39496500	-2.33074700
C	2.13796100	0.30853600	-3.51298400	C	8.43738100	-0.40664000	1.16232600
C	3.33162300	-0.17338800	-2.95639100	C	8.66102700	-1.19006100	2.28579900
C	4.41014800	0.78300600	-2.59251200	C	8.43785500	0.95438500	1.39359400
C	4.04769700	2.24157500	-2.56316800	C	8.89830100	-0.66732400	3.54441100
H	0.21712600	-0.24266000	-4.28444100	C	8.66624900	1.53364400	2.63190800
H	3.76192000	2.34422400	-4.69807000	C	8.90216000	0.70929700	3.71671500
H	1.26718900	2.16736900	-2.94334400	C	6.65420900	-1.80878700	-0.19221300
C	1.13888800	-0.60970300	-3.84587500	C	5.55469400	-1.02585100	0.12470400
C	3.50128000	-1.54856300	-2.74355800	C	6.34830100	-3.13872400	-0.44644800
H	4.92408700	2.87892400	-2.48698400	C	4.25050800	-1.47938400	0.17417000

C	5.05163700	-3.63770700	-0.43521900	C	1.79889200	0.37788100	-2.25350200
C	3.99272300	-2.80600500	-0.12180900	C	2.66489000	-0.75596800	-2.74748800
F	8.17890500	1.82806000	0.37613300	C	4.05456700	-0.62004700	-2.88882100
F	8.65265300	2.85818100	2.78827200	C	4.71439400	0.61721900	-2.40969200
F	9.12547200	1.23251700	4.91974200	C	3.87808000	1.67527200	-1.74734000
F	9.12060400	-1.45987700	4.59150900	H	1.01667600	-2.11209000	-2.91775200
F	8.66572600	-2.52244100	2.16069500	H	2.59060300	1.98923600	-3.44876500
F	7.94734000	-2.27788400	-2.84424300	H	1.56067600	0.19490400	-1.19990800
F	9.84280700	-3.61324200	-4.15421100	C	2.08764900	-1.99308200	-3.03925600
F	12.27294800	-4.03318700	-3.00200600	C	4.83363900	-1.70306500	-3.32547400
F	12.76139300	-3.05358400	-0.51313400	H	4.38690200	2.63565100	-1.80527100
F	10.91575800	-1.69422500	0.79497900	C	4.23895500	-2.91638800	-3.61619400
F	7.30895200	-4.02071800	-0.74823600	C	2.85972300	-3.06383400	-3.46269000
F	4.81149000	-4.90975500	-0.75116000	H	5.90767200	-1.59235400	-3.39090600
F	2.74384900	-3.26605400	-0.12198100	H	4.84909400	-3.75393000	-3.93138500
F	3.23890000	-0.64650000	0.44959500	H	2.39069900	-4.01892300	-3.66624800
F	5.73020600	0.30654900	0.35255600	H	3.78674300	1.41255800	-0.68769700
H	7.94429000	-0.15708000	-1.07459600	H	1.90415300	2.50998400	-1.91230200
H	7.23941300	2.90778800	-3.96013000	H	0.85318700	0.37082400	-2.79929700
C	9.32011500	1.32399300	-3.00306900	N	5.98878300	0.63738700	-2.55778100
C	10.38061100	1.25479700	-2.08911300	O	6.56497500	1.79603000	-1.83244400
C	9.36002100	0.53097700	-4.15861500	H	6.80343100	1.45185100	-0.93754500
C	11.46537800	0.42180000	-2.33393300				
H	10.35747100	1.84905800	-1.18134000				
C	10.44765100	-0.29709500	-4.40385800	TS4			
H	8.54199500	0.56134000	-4.87055700				
C	11.50281200	-0.34281100	-3.49630700	Si	8.38528000	1.89899000	-2.76228600
H	12.27822600	0.36654300	-1.61937000	B	7.62846600	-0.64452900	0.56170700
H	10.47147300	-0.91097000	-5.29616100	C	8.81666200	-1.06847000	-0.45139200
H	12.35313300	-0.98683800	-3.69141000	C	10.04339600	-0.42027800	-0.33966000
H	8.27662000	3.61750000	-1.82144500	C	8.77971300	-2.09089900	-1.38896900
C	2.49247200	1.72641700	-2.39132000	C	11.17621800	-0.79110000	-1.03787000

C	9.89650900	-2.49976800	-2.10430000	C	10.82341000	0.89547000	-3.69567900
C	11.10584100	-1.86071300	-1.91366200	C	8.91248800	-0.39335900	-4.40725800
C	8.09712000	-0.57058500	2.11705500	C	11.65922700	0.07696900	-4.44694800
C	9.10166300	-1.34856700	2.67762000	H	11.25906000	1.70534200	-3.11784900
C	7.40737000	0.24364700	3.00567100	C	9.75066100	-1.22077500	-5.14636900
C	9.41712000	-1.30631800	4.02803500	H	7.84573200	-0.58962900	-4.39694700
C	7.69452000	0.31986700	4.35680100	C	11.12183100	-0.98401800	-5.16848700
C	8.71173400	-0.46645800	4.87113200	H	12.72786900	0.25347400	-4.45137000
C	6.22183600	-1.44024100	0.49238800	H	9.33493900	-2.05341500	-5.70042900
C	4.97713100	-0.84279800	0.39256900	H	11.77357300	-1.63439700	-5.73924300
C	6.20296700	-2.81950000	0.65788500	H	9.17910700	2.71396000	-1.82778000
C	3.78639600	-1.55351100	0.39504600	C	3.30031500	1.88094700	-3.04898700
C	5.04293700	-3.57248700	0.63076500	C	2.40044500	0.81777700	-2.42943500
C	3.82134400	-2.93139100	0.49086600	C	2.96557000	-0.56107800	-2.66092300
F	6.40203100	1.00730900	2.55025400	C	4.34778300	-0.75600300	-2.78588000
F	7.00676200	1.12768300	5.16081700	C	5.25192600	0.38678500	-2.51772800
F	9.00533800	-0.41672600	6.16571900	C	4.70247900	1.78828200	-2.45450200
F	10.39061000	-2.06860900	4.52074400	H	1.05857100	-1.53517000	-2.58692800
F	9.82100300	-2.19173900	1.92923500	H	3.34557500	1.73246300	-4.13183000
F	7.65049700	-2.75495700	-1.65815400	H	2.31844100	0.98828600	-1.34937800
F	9.80533400	-3.49073500	-2.98896600	C	2.12711300	-1.67746400	-2.70427300
F	12.18467100	-2.24586900	-2.58586000	C	4.86680300	-2.04568600	-2.97899700
F	12.31758900	-0.11721700	-0.90683300	H	5.39411800	2.45971000	-2.96523900
F	10.16001200	0.62603600	0.49539500	C	4.01947100	-3.13671500	-3.02559300
F	7.35697600	-3.47092300	0.84864400	C	2.64315300	-2.95217600	-2.87403500
F	5.08288400	-4.89793100	0.74950000	H	5.93733800	-2.17960700	-3.05628400
F	2.69439600	-3.63536200	0.46282000	H	4.42507800	-4.13142500	-3.16370600
F	2.61558300	-0.92165100	0.29841500	H	1.97669800	-3.80620100	-2.89064400
F	4.87222300	0.49135000	0.25554000	H	4.69283600	2.09055400	-1.40344200
H	7.33527800	0.63429800	0.43174400	H	2.89812000	2.87918400	-2.87058500
H	7.58208800	2.71637700	-3.69063200	H	1.39017800	0.86971500	-2.83972000
C	9.43940700	0.67192900	-3.66392900	N	6.46267800	0.05817300	-2.25017100

O	7.20599200	1.17708700	-1.72119600	Si	-6.90096500	1.45645700	1.36076100
H	7.38128600	0.77278700	-0.48958500	H	-6.71375300	2.51412900	0.34648100
				H	-8.32464500	1.10484800	1.52755000
H ₂				C	-6.19221200	1.96358100	3.01016200
				C	-4.83655100	2.28971100	3.16128100
H	4.19116400	-0.97917700	0.35025900	C	-7.02207500	2.03473500	4.13550800
H	3.45054900	-0.97917700	0.35025900	C	-4.33089900	2.67303100	4.39770800
				H	-4.17130000	2.23178600	2.30613800
I9				C	-6.51954600	2.42393900	5.37374100
				H	-8.07425800	1.78219600	4.04810200
C	-3.97689500	-3.20171900	-0.49495600	C	-5.17279000	2.74251500	5.50470500
C	-2.56601600	-3.15935700	0.08787000	H	-3.28018200	2.91797000	4.49963800
C	-1.95224500	-1.79660600	-0.12376700	H	-7.17665700	2.47446900	6.23394400
C	-2.75878700	-0.65004600	-0.08536100	H	-4.77782200	3.04336000	6.46807500
C	-4.20659200	-0.78936700	0.20843200				
C	-4.85687300	-2.14888900	0.17314200	I10'			
H	0.03758500	-2.54029900	-0.40434900				
H	-3.92410200	-3.01083000	-1.57104800	Si	6.52935100	2.12762300	-4.63187000
H	-2.61149100	-3.37899100	1.16161300	B	8.44017200	4.19624700	-5.83283100
C	-0.58618200	-1.65336000	-0.36960300	C	9.83945400	3.70420400	-5.16956200
C	-2.18781700	0.60951100	-0.30398100	C	10.98965000	3.37516500	-5.87208200
H	-5.82529100	-2.05499800	-0.32034100	C	9.87643700	3.37214300	-3.81989000
C	-0.82962600	0.73493300	-0.54429800	C	12.08015200	2.73848000	-5.29170000
C	-0.02331400	-0.40180800	-0.57468900	C	10.92932600	2.72911200	-3.20193200
H	-2.82790200	1.48273500	-0.28760800	C	12.04710400	2.40397000	-3.95235700
H	-0.39852400	1.71388300	-0.71545000	C	8.48817300	4.48572700	-7.42322900
H	1.03887500	-0.31105100	-0.76865300	C	9.04631600	5.65673600	-7.91367100
H	-5.07225900	-2.43557500	1.20939200	C	7.98496400	3.61905000	-8.37739200
H	-4.42064100	-4.18970600	-0.35940300	C	9.10612900	5.96308200	-9.26174800
H	-1.92937300	-3.92114400	-0.36658300	C	8.02574300	3.88154100	-9.73810400
N	-4.83777100	0.27605500	0.51932800	C	8.58821300	5.06462900	-10.18170700
O	-6.18829100	0.03687900	0.78660600	C	7.65324500	5.38483000	-5.05122400

C	6.28647200	5.52352900	-5.25858300	H	11.10500800	-1.21353600	-3.68969000
C	8.19153500	6.24524400	-4.10556800	H	6.35912200	3.42947700	-4.01489600
C	5.48024300	6.39559400	-4.54787200	C	2.23520600	2.18711800	-1.39181900
C	7.42475700	7.14572300	-3.38021500	C	2.36631500	3.61785600	-1.92694200
C	6.06194900	7.22044700	-3.60225300	C	3.78722600	4.06659800	-1.70808600
F	7.43405400	2.44411300	-8.01569400	C	4.82159900	3.15070900	-1.96282900
F	7.53349200	3.00654600	-10.61769000	C	4.44238000	1.86915800	-2.57076600
F	8.63661900	5.33737500	-11.48332100	C	3.13442400	1.23421900	-2.18297300
F	9.65656300	7.09930100	-9.68774400	H	3.33293000	6.05246700	-1.04278600
F	9.58455700	6.53566200	-7.05725100	H	2.51411000	2.18014700	-0.33554500
F	8.80072700	3.62657400	-3.04679200	H	2.11457600	3.64250500	-2.99350000
F	10.87067400	2.39464700	-1.91247000	C	4.11834200	5.32558300	-1.21498100
F	13.06513200	1.75557000	-3.39207200	C	6.14542200	3.46324200	-1.63124700
F	13.14718400	2.41900700	-6.02553500	H	3.34677000	0.31188300	-1.63501700
F	11.09733600	3.62069100	-7.18617400	C	6.45537900	4.71228900	-1.12126000
F	9.49760700	6.21339500	-3.81767100	C	5.44140900	5.65032900	-0.93478800
F	7.97656000	7.90944000	-2.43528000	H	6.93397000	2.73475300	-1.77702500
F	5.30827700	8.04860500	-2.87998500	H	7.48345300	4.95812300	-0.88533200
F	4.16008600	6.42815300	-4.73856700	H	5.68363000	6.63779800	-0.55895400
F	5.66840800	4.71675600	-6.13990800	H	2.64446700	0.92338100	-3.11122600
H	7.70130700	3.18707500	-5.73384800	H	1.20458500	1.83807800	-1.46273100
H	5.79203600	1.88430600	-5.88083900	H	1.67986500	4.29334600	-1.41582400
C	7.95930800	0.97548300	-4.32068000	N	5.19562100	1.30970200	-3.46749300
C	8.19171600	0.40659700	-3.06436500	O	4.82297500	0.02049700	-3.77586500
C	8.86476200	0.71136800	-5.35583700	Si	4.45524100	-0.58071900	-5.34082300
C	9.31922400	-0.37689700	-2.83658900	H	3.68269300	-1.77212300	-4.95203300
H	7.49245300	0.56745000	-2.24966900	H	3.64388000	0.43424100	-6.04323300
C	9.98426300	-0.07971300	-5.13348100	C	5.96951000	-1.03546800	-6.31051800
H	8.69657600	1.13501700	-6.34127000	C	6.80283900	-2.06777400	-5.85730200
C	10.22022800	-0.61388400	-3.86932600	C	6.29168000	-0.38596000	-7.50726200
H	9.49725800	-0.79408900	-1.85288200	C	7.92818900	-2.43728200	-6.58154700
H	10.67643200	-0.27278300	-5.94537800	H	6.57736600	-2.58295600	-4.92834700

C	7.41786500	-0.75564600	-8.23551800	F	-2.23007800	1.25763700	4.20879400
H	5.67293800	0.42801100	-7.87181100	F	-0.77583000	2.35584000	2.24324400
C	8.23386000	-1.78193100	-7.77221400	F	1.23525700	1.82467100	-2.73161000
H	8.57093900	-3.22965200	-6.21696900	F	0.02152500	3.05623400	-4.75444800
H	7.65990800	-0.23226700	-9.15290500	F	-2.58657000	3.81641300	-4.54131700
H	9.11384300	-2.06895200	-8.33618400	F	-3.97059900	3.21894500	-2.28491500
I10				F	-2.79842500	1.99043100	-0.25100200
				F	0.50575400	3.95115500	0.11921300
				F	2.75776700	5.09733400	0.97245800
Si	-0.14101700	-3.60023100	-2.42308000	F	4.89498300	3.58138600	1.68046700
B	0.09096100	0.98074300	-0.24848700	F	4.73434900	0.86594400	1.52633200
C	-0.71010000	1.84512600	-1.37709500	F	2.48821000	-0.30493100	0.70246900
C	-2.03733600	2.24503500	-1.32832600	H	0.53182200	0.02440500	-0.81952100
C	-0.05839100	2.17038900	-2.56047900	H	-0.66849300	-3.96613900	-1.10811600
C	-2.67592700	2.90486800	-2.36999200	C	0.96714800	-4.87298600	-3.19755600
C	-0.65293500	2.82544900	-3.62361700	C	0.92953000	-5.05035500	-4.58796900
C	-1.98169400	3.19929200	-3.52698400	C	1.83940000	-5.67093800	-2.44250700
C	-0.85103200	0.39186900	0.93893300	C	1.75062500	-5.98479900	-5.20880400
C	-1.18083800	1.08789800	2.09277100	H	0.24744700	-4.46271900	-5.19358200
C	-1.36309100	-0.89140600	0.86660400	C	2.66335200	-6.60111200	-3.06440600
C	-1.94114100	0.54832000	3.11742200	H	1.87737600	-5.57317600	-1.36279200
C	-2.12154500	-1.47982100	1.86559200	C	2.62217700	-6.75563300	-4.44695200
C	-2.41145800	-0.75048100	3.00428000	H	1.70703600	-6.11314000	-6.28344400
C	1.39019400	1.76868400	0.34647700	H	3.33361600	-7.20869000	-2.46832700
C	2.50487800	1.04413300	0.74630200	H	3.26399800	-7.48297000	-4.92965200
C	1.52230400	3.14621100	0.45149400	H	-1.18406400	-3.14392800	-3.35591500
C	3.68502000	1.62135600	1.18582600	C	4.37246600	-0.92309100	-1.83122000
C	2.68030500	3.76827800	0.89464100	C	4.75415100	-2.40644900	-1.94858000
C	3.77296000	3.00016000	1.25926900	C	3.91369100	-3.17507000	-0.96379500
F	-1.13258200	-1.66218900	-0.22457000	C	2.55823200	-2.82958200	-0.84873900
F	-2.56302400	-2.73559500	1.74311600	C	2.04241100	-1.84318400	-1.79458500
F	-3.13863200	-1.28982700	3.98138700	C	2.90956200	-0.70358500	-2.22858200

H	5.46046400	-4.43720400	-0.18718600				
H	4.52888500	-0.59918300	-0.79956900	Si	-2.37759400	-1.72729600	-2.94662200
H	4.57219100	-2.76083500	-2.97032400	B	0.21965800	0.74742200	0.32788300
C	4.42002500	-4.14454400	-0.10550200	C	-1.20529600	1.51077200	0.38424900
C	1.76215600	-3.34155900	0.18097700	C	-2.17627500	1.35947600	1.36946100
H	2.49269300	0.22088300	-1.81953400	C	-1.55342900	2.39838100	-0.62864900
C	2.29477500	-4.28478200	1.04654600	C	-3.42315300	1.96572600	1.30754700
C	3.61269500	-4.70672000	0.87971800	C	-2.79155800	2.99693800	-0.74309800
H	0.75816500	-2.96109100	0.32369000	C	-3.74648400	2.77162900	0.23362700
H	1.69390900	-4.67604300	1.85741900	C	0.42614600	-0.46923600	1.37452100
H	4.02759600	-5.44898600	1.55110100	C	1.52744700	-0.65768500	2.20572600
H	2.80897500	-0.61715900	-3.31623400	C	-0.55089600	-1.45017900	1.50208700
H	5.00528200	-0.30983600	-2.47304500	C	1.67069000	-1.75528800	3.04392000
H	5.81202200	-2.55854200	-1.73307200	C	-0.44620400	-2.56651300	2.30739300
N	0.86533800	-2.02775600	-2.31298500	C	0.68491700	-2.72266500	3.08975800
O	0.32518000	-0.95426000	-2.96490700	C	1.51401000	1.68169500	0.11580300
Si	0.12034700	-0.75181200	-4.64900200	C	2.71256900	1.09011100	-0.26501700
H	1.13800000	0.19155500	-5.14822900	C	1.56609700	3.06056700	0.27172600
H	0.33529300	-2.08497300	-5.25315600	C	3.87289400	1.79071900	-0.52453500
C	-1.60027600	-0.07415600	-4.77165600	C	2.71237300	3.80536400	0.02626000
C	-2.50598500	-0.25296100	-3.71904300	C	3.86998800	3.16940200	-0.38151300
C	-2.00235500	0.65957500	-5.89571800	F	-1.67452900	-1.34628200	0.78005500
C	-3.78861200	0.28130900	-3.79498600	F	-1.40645600	-3.49121200	2.32359100
H	-2.19590900	-0.77288100	-2.81834700	F	0.81769800	-3.78380200	3.87697400
C	-3.28402900	1.19015400	-5.97058600	F	2.75247100	-1.88078400	3.81020900
H	-1.30738500	0.83900200	-6.71035600	F	2.52608900	0.23059600	2.26338400
C	-4.17760100	1.00098500	-4.91938700	F	-0.65317800	2.72621500	-1.56483800
H	-4.47352900	0.15880200	-2.96392500	F	-3.07423600	3.78561200	-1.78487500
H	-3.57962500	1.76997900	-6.83630700	F	-4.95178500	3.32256700	0.14287300
H	-5.16938000	1.43413200	-4.96777700	F	-4.32781600	1.74920300	2.26325100
				F	-1.95978300	0.61655300	2.45927500
TS5				F	0.49946600	3.75323100	0.68497300

F	2.70694500	5.12744600	0.18427200	H	-0.66645000	-2.36885600	-0.71210200
F	4.97089900	3.86999700	-0.62754400	H	0.27639300	-4.62640300	-0.42107500
F	4.97837800	1.16210600	-0.92289100	H	2.23462600	-5.32138600	-1.79255800
F	2.76235400	-0.24367400	-0.40477900	H	0.54524600	0.93118300	-3.96136200
H	0.15731900	0.09341200	-0.93426300	H	2.84976100	0.91231000	-4.14504400
H	-3.16325500	-1.20147300	-4.07871600	H	3.41082400	-1.53497000	-4.30453800
C	-3.40524200	-1.86456100	-1.41029500	N	-1.12159300	-0.43938500	-2.79023000
C	-3.52795300	-3.08607200	-0.73977800	O	-1.73739000	0.80871800	-2.95712000
C	-4.04629700	-0.73476100	-0.88553800	Si	-2.02253200	1.49806600	-4.49713400
C	-4.27039900	-3.17845000	0.43241800	H	-3.39770800	2.01045800	-4.36903700
H	-3.02616800	-3.96965800	-1.12396200	H	-1.87932700	0.41383600	-5.49215900
C	-4.79513500	-0.82843900	0.28119100	C	-0.82154500	2.84963400	-4.94550000
H	-3.94679500	0.22574800	-1.38512300	C	0.08647500	2.63919700	-5.99267700
C	-4.90302000	-2.04981700	0.94125800	C	-0.79891400	4.08197200	-4.27950200
H	-4.34720700	-4.12555800	0.95244300	C	0.99903200	3.62324400	-6.35743900
H	-5.29344900	0.04660600	0.68191600	H	0.08393500	1.69502700	-6.53006900
H	-5.47870700	-2.11835900	1.85653200	C	0.11493300	5.06558700	-4.64048500
H	-1.71745600	-2.99757200	-3.28662900	H	-1.49123100	4.27439300	-3.46828100
C	2.45759300	0.20123700	-3.41431200	C	1.01475600	4.83648700	-5.67728800
C	2.41571000	-1.20515300	-4.00264900	H	1.69341400	3.44521200	-7.16990700
C	1.84542700	-2.16073300	-2.98886300	H	0.12493300	6.01199800	-4.11327400
C	0.76119400	-1.76806200	-2.19204500	H	1.72575100	5.60498400	-5.95676200
C	0.17387200	-0.40303000	-2.37462300				
C	1.05044400	0.66797600	-3.03247600	Path C			
H	3.20278000	-3.75309000	-3.43649100	I11'			
H	3.13817600	0.20166400	-2.56574300				
H	1.78624400	-1.20914900	-4.90156900	C	2.80208100	-2.27999900	-2.08659000
C	2.35861800	-3.44677200	-2.82858600	C	3.79091500	-2.15426000	-0.93282600
C	0.19829200	-2.66792200	-1.28700500	C	3.45709700	-0.95794700	-0.07775400
H	1.07532600	1.57856800	-2.43729000	C	2.12718800	-0.54374600	0.08836900
C	0.71921100	-3.94385500	-1.13670400	C	1.03946300	-1.32399800	-0.54947300
C	1.81100700	-4.33095600	-1.90738100	C	1.37975100	-2.40129000	-1.54816300

H	5.49642100	-0.55375000	0.43694100	C	-2.09244900	-5.80698800	2.90496800
H	2.88262500	-1.40069900	-2.73217700	C	-3.23700000	-6.45599300	3.34692500
H	3.75891500	-3.06523700	-0.32340600	C	-1.75723700	-4.66201200	3.61966700
C	4.46673400	-0.23808500	0.56295100	C	-4.00854700	-5.99440100	4.40565600
C	1.83303400	0.57537500	0.88015100	C	-2.49812200	-4.16384300	4.67286200
H	0.63896900	-2.38518800	-2.34952300	C	-3.64323700	-4.83715100	5.06491400
C	2.84758700	1.27839300	1.50330200	C	-1.78322000	-7.48998400	0.76979900
C	4.17106600	0.86700500	1.34584000	C	-1.30643300	-8.73589800	1.14965700
H	0.80136500	0.88006900	1.00130200	C	-2.68793100	-7.48872100	-0.27769300
H	2.61369000	2.14329600	2.11128200	C	-1.68396700	-9.91368200	0.52775300
H	4.97050300	1.41396400	1.83117000	C	-3.09223400	-8.64188100	-0.93129500
H	1.26720200	-3.37037100	-1.04794900	C	-2.58260900	-9.86266200	-0.52528900
H	3.02767400	-3.15894500	-2.69175000	C	0.32491000	-6.08255200	1.58980300
H	4.81287800	-2.06105500	-1.30420600	C	1.02371000	-5.86016400	0.41217400
N	-0.14962900	-1.02629800	-0.16835100	C	1.11047900	-6.18944500	2.72766100
O	-1.13395700	-1.87586300	-0.80440800	C	2.39496300	-5.69048900	0.34957100
Si	-2.34403400	-0.91691600	-1.62649800	C	2.48995700	-6.03918500	2.71093900
H	-1.54804000	-0.13354000	-2.58556900	C	3.13601400	-5.77708400	1.51481200
H	-3.17527100	-1.96177400	-2.24678200	F	-3.23791700	-6.33552800	-0.70017100
C	-3.30985800	0.10446500	-0.42803700	F	-3.96397000	-8.58900400	-1.93811100
C	-2.74199400	1.21208700	0.21535100	F	-2.95832800	-10.98136300	-1.13857000
C	-4.62977300	-0.25250800	-0.12547600	F	-1.20152300	-11.08851500	0.92847700
C	-3.47406500	1.93599600	1.14836200	F	-0.46030700	-8.83293400	2.18434800
H	-1.72131000	1.50556900	-0.00768400	F	-0.68167800	-3.94637600	3.24955700
C	-5.36524400	0.47841900	0.79985900	F	-2.14655800	-3.03719200	5.29052400
H	-5.08294000	-1.11721500	-0.59982900	F	-4.39339900	-4.35882500	6.05374400
C	-4.78548400	1.56901100	1.43909800	F	-5.11296400	-6.64465500	4.77366400
H	-3.02622400	2.78781500	1.64597600	F	-3.68524800	-7.56630900	2.74436800
H	-6.38312200	0.18878400	1.03139300	F	0.55042100	-6.42812800	3.91629700
H	-5.35556100	2.13519900	2.16634300	F	3.19901700	-6.13269200	3.83364400
Si	-1.49735400	-3.57176100	0.11398900	F	4.45362600	-5.59880600	1.48296300
B	-1.29365100	-6.16030500	1.54482100	F	2.99901000	-5.41415400	-0.81127800

F	0.35004800	-5.73557200	-0.74805100	H	0.85058500	1.77353500	-1.46438200
H	-1.64793600	-5.21568200	0.76506300	H	1.85201600	4.03911200	-1.54688900
H	-1.86888300	-4.18684500	-1.16610800	H	4.02680900	4.46090500	-0.43262300
C	-2.84596000	-2.95902300	1.23454000	H	2.44113600	-2.05329800	0.99992500
C	-2.60432900	-1.86391100	2.07521200	H	4.75674100	-2.08432800	0.52774300
C	-4.06597200	-3.63640700	1.33454100	H	5.46838000	0.25396500	1.07481900
C	-3.55989200	-1.45937000	2.99866900	N	0.55539600	-0.38533400	-0.20981800
H	-1.66166800	-1.32817600	2.01179100	O	-0.03847200	-1.75117800	-0.19544300
C	-5.02429700	-3.22958000	2.25817700	Si	-1.42791700	-1.62300900	-1.33814400
H	-4.25729200	-4.50289300	0.70789600	H	-0.83454400	-1.08410200	-2.55959000
C	-4.76781400	-2.14584000	3.09337200	H	-1.87435900	-3.02160500	-1.39382900
H	-3.36046800	-0.61628200	3.64891200	C	-2.73941100	-0.59493600	-0.53257900
H	-5.96148600	-3.76819700	2.33789700	C	-2.53323600	0.71855000	-0.08704100
H	-5.50761400	-1.84039200	3.82454000	C	-4.00953600	-1.16754700	-0.38735800
H	-0.12971600	-3.54589700	0.63356400	C	-3.57047200	1.43008000	0.50330900
I11				H	-1.55766600	1.17903000	-0.19217200
				C	-5.05067900	-0.44772300	0.18772500
				H	-4.18597100	-2.19069100	-0.70637800
C	4.20892600	-1.23479900	0.11761900	C	-4.82886000	0.84863700	0.63848400
C	4.40890000	0.01495100	0.97460600	H	-3.40070300	2.44176700	0.85180200
C	3.68696000	1.16859600	0.32688100	H	-6.02768700	-0.90359300	0.29569000
C	2.44027900	0.94973200	-0.27742100	H	-5.63676400	1.40911900	1.09400900
C	1.83616100	-0.39659800	-0.16884100	Si	-0.11275200	-2.69282600	1.32852300
C	2.72445800	-1.59575200	0.04600400	B	1.45644600	-2.59918700	-3.37578600
H	5.20453300	2.62596800	0.72620700	C	0.39758900	-3.80844500	-3.08351800
H	4.59900100	-1.03705700	-0.88123100	C	-0.77545000	-4.08030700	-3.77266900
H	4.01836900	-0.15882000	1.98467300	C	0.57738100	-4.57493900	-1.93627200
C	4.23880000	2.44596000	0.26746600	C	-1.71301600	-5.01961400	-3.35471500
C	1.78329000	1.98144300	-0.95634000	C	-0.32982600	-5.51039500	-1.47510100
H	2.50979100	-2.32609700	-0.73769900	C	-1.49618700	-5.73147200	-2.19073200
C	2.35171600	3.24318600	-1.00942700	C	1.17413200	-1.71749400	-4.71027500
C	3.57639000	3.47656700	-0.38704000	C	1.22582800	-2.28749000	-5.97437800

C	0.96846800	-0.34813100	-4.68382800	C	-3.87063700	-4.38264800	1.56276900
C	1.06627800	-1.56862200	-7.14447400	H	-1.99653200	-4.88122800	0.65438200
C	0.80390500	0.41561000	-5.83182100	C	-4.56334500	-3.47264600	2.35653200
C	0.85397000	-0.20021500	-7.06840800	H	-4.46724400	-1.63186700	3.46563100
C	3.01351100	-3.08107100	-3.41669400	H	-4.36623800	-5.27065300	1.18982800
C	3.99070100	-2.11592700	-3.21271800	H	-5.60441100	-3.65262400	2.59775700
C	3.49181100	-4.36384500	-3.63439200	H	0.53154900	-1.77545900	2.27794300
C	5.34792700	-2.38715000	-3.19009200				
C	4.84321600	-4.68046900	-3.62996600	TS6			
C	5.77818200	-3.68604900	-3.40251800				
F	0.91159900	0.32067400	-3.51707300	C	-1.16188500	3.59590700	-2.23496100
F	0.60038900	1.73318800	-5.75574600	C	-0.62335600	4.91035900	-1.63484800
F	0.69800900	0.51518000	-8.18124300	C	-0.87606800	4.87783500	-0.15220200
F	1.11348800	-2.16356900	-8.33726600	C	-0.56801900	3.70388300	0.55928900
F	1.42636300	-3.60871500	-6.08422000	C	0.08004000	2.63551600	-0.32252200
F	1.68505500	-4.40589200	-1.18953800	C	-0.35517000	2.39471700	-1.73579200
F	-0.11424300	-6.18191800	-0.33871500	H	-1.87347500	6.75940300	0.01622600
F	-2.39683800	-6.60576800	-1.74568000	H	-2.21196800	3.48160200	-1.95704400
F	-2.83456200	-5.21426500	-4.04668500	H	0.44803800	4.99960800	-1.84766700
F	-1.10685200	-3.39371200	-4.87484500	C	-1.57288600	5.85832200	0.53809000
F	2.64527200	-5.38128400	-3.84593900	C	-0.91637800	3.49327300	1.89084200
F	5.25226200	-5.93319000	-3.83573800	H	-0.90772000	1.45574900	-1.75960200
F	7.07828600	-3.97484800	-3.38542000	C	-1.59097400	4.50818500	2.55552900
F	6.23746600	-1.42067800	-2.94761300	C	-1.90384500	5.68469500	1.88311700
F	3.62644600	-0.83908300	-2.99417000	H	-0.68241500	2.55267200	2.36917100
H	1.35878000	-1.85873900	-2.43068400	H	-1.87941500	4.37422900	3.58964600
H	0.63686800	-3.91214600	1.00495100	H	-2.43555700	6.47265700	2.40263200
C	-1.88387000	-3.00646600	1.72965300	H	0.55897500	2.25354400	-2.31567600
C	-2.59271500	-2.10364600	2.53503000	H	-1.10108300	3.62244800	-3.32318500
C	-2.53430100	-4.15530800	1.25693200	H	-1.12183100	5.77233000	-2.07681200
C	-3.92493700	-2.33726700	2.84807900	N	1.04626800	2.46690700	0.40582500
H	-2.10596500	-1.20924000	2.91095200	O	2.05124200	0.85751700	-0.41019200

Si	2.30644100	-0.17484400	0.92423100	C	-3.98368800	-0.74566300	-3.02577400
H	1.09664300	-0.06032300	1.75109700	C	-4.55178800	0.51177600	-2.91809900
H	2.53248300	-1.54036400	0.41203800	F	-1.13971600	0.46496900	2.75732200
C	3.86648600	0.38186200	1.78099700	F	-2.52532100	-0.22792500	4.91800100
C	4.07680200	1.72548600	2.11906900	F	-4.33988000	-2.24993500	4.80802400
C	4.88556800	-0.54032400	2.04053800	F	-4.74449200	-3.57469000	2.47121900
C	5.27302100	2.13381800	2.69759400	F	-3.35482000	-2.88846800	0.27785300
H	3.30233900	2.46125900	1.92388900	F	0.01846400	-0.47048300	-2.41504300
C	6.07967800	-0.13630200	2.62919100	F	1.95822400	-2.04777700	-3.34660600
H	4.75670200	-1.58210100	1.76271200	F	2.69532700	-4.27137800	-1.97795400
C	6.27513500	1.20135500	2.95419200	F	1.40684400	-4.91548000	0.33467900
H	5.42434800	3.17634600	2.95235500	F	-0.50469500	-3.36403000	1.29519500
H	6.86161000	-0.86212200	2.81988500	F	-2.49989100	-2.36399300	-2.29895500
H	7.20738300	1.51906900	3.40659900	F	-4.36788100	-1.55628100	-4.01137800
Si	3.05884700	1.12889100	-1.74827300	F	-5.47325300	0.91305800	-3.79074600
B	-1.43539300	-0.73190300	0.03860900	F	-4.66235400	2.57904000	-1.79231900
C	-0.35382900	-1.82736000	-0.51171400	F	-2.80954100	1.78683500	-0.05010300
C	0.04768900	-2.98949400	0.13268800	H	-0.80472500	0.27357300	0.26764700
C	0.32870900	-1.56533200	-1.69448700	H	2.36517200	0.57222200	-2.92382000
C	1.05285400	-3.82399500	-0.34315200	C	4.69845900	0.30505600	-1.46373100
C	1.33289600	-2.36494500	-2.20755000	C	5.78106100	1.02189300	-0.93672400
C	1.70762400	-3.50573100	-1.51708000	C	4.84910500	-1.06897200	-1.69507100
C	-2.20703300	-1.16897700	1.40409400	C	6.97849100	0.38272000	-0.64267200
C	-3.14155000	-2.19607600	1.40589700	H	5.68405300	2.08484600	-0.73916100
C	-2.03205700	-0.53620700	2.62159600	C	6.04431600	-1.71234800	-1.39137500
C	-3.86199400	-2.57645600	2.52329000	H	4.03316300	-1.64457900	-2.12208500
C	-2.73276800	-0.87804500	3.77016400	C	7.10736500	-0.98568700	-0.86483000
C	-3.65604300	-1.90495600	3.71855700	H	7.80580000	0.94681100	-0.22882300
C	-2.57379400	-0.33899600	-1.07217500	H	6.14568200	-2.77600200	-1.57115800
C	-3.18467700	0.90653400	-1.00191300	H	8.03928000	-1.48607200	-0.62858300
C	-3.01553100	-1.14360000	-2.11409200	H	3.20381800	2.59793500	-1.84734200
C	-4.14574000	1.35031500	-1.89478400				

I12				H	4.76382800	1.06199800	2.06631800
C	-1.36936300	0.15830800	-3.89628200	C	5.84128300	3.53110200	0.01131900
C	-0.95357300	1.52261900	-4.50402200	H	4.75265400	4.30660000	-1.67363700
C	-1.27447700	2.79200200	-3.72717400	H	6.68826800	2.56471300	1.73394300
C	-0.84380100	3.00247800	-2.40855500	H	6.69484200	4.18119400	-0.14199900
C	-0.11775000	0.75457600	-2.03355700	Si	3.02188300	-0.95000300	-1.84854300
C	-0.38010900	-0.42050800	-2.83544100	B	-1.29528200	-0.76142400	0.73744000
H	-2.31344200	3.74114300	-5.33797400	C	-0.15100800	-1.71300700	1.39491400
H	-2.36460400	0.23148300	-3.45954200	C	0.29791600	-1.70239300	2.70705600
H	0.12523500	1.50427600	-4.70481400	C	0.57104400	-2.54250600	0.54405800
C	-1.95869800	3.84909600	-4.31933900	C	1.38689200	-2.44535700	3.14886400
C	-1.05228400	4.16840900	-1.69364600	C	1.66113200	-3.29529200	0.93542000
H	-0.80526300	-1.22053600	-2.22860500	C	2.07998800	-3.23826700	2.25565000
C	-1.73910100	5.19955300	-2.32196300	C	-2.07061600	0.23921000	1.75525700
C	-2.18914300	5.03606700	-3.62744600	C	-2.85531000	-0.25782000	2.78684300
H	-0.71133900	4.23963100	-0.66956400	C	-2.08632900	1.61510900	1.61229500
H	-1.92843700	6.12174800	-1.78852500	C	-3.59017300	0.54221800	3.64234200
H	-2.72797800	5.83899600	-4.11488400	C	-2.80910800	2.45956000	2.44339400
H	0.54861800	-0.76624200	-3.29229600	C	-3.56474000	1.91773300	3.46603100
H	-1.40879400	-0.57946300	-4.69862300	C	-2.43292300	-1.56342600	-0.11707300
H	-1.44026900	1.61128300	-5.47517200	C	-3.16942400	-0.84257600	-1.04736600
N	-0.20355900	1.88683000	-1.82066600	C	-2.76341600	-2.90735400	-0.02635800
O	1.95528500	-0.08146800	-0.89217900	C	-4.14346500	-1.39252800	-1.86175900
Si	2.21000200	0.65332100	0.59878800	C	-3.74076600	-3.50176400	-0.81411800
H	0.95264400	1.33858500	0.94475600	C	-4.43338500	-2.74149000	-1.74037800
H	2.59662900	-0.35701100	1.60658300	F	-1.38523900	2.21525300	0.63034600
C	3.63743600	1.84380100	0.40384900	F	-2.78539900	3.78289100	2.26188200
C	3.65748800	2.76436400	-0.65212200	F	-4.26607700	2.70937600	4.27519600
C	4.74310200	1.78614700	1.25753300	F	-4.32110500	0.01708000	4.62600300
C	4.74996800	3.60064600	-0.85118200	F	-2.90669900	-1.58218300	2.98518400
H	2.81310200	2.82497300	-1.33446800	F	0.21497600	-2.63135400	-0.75244900
C	5.83576600	2.62654200	1.06750500	F	2.32825400	-4.05970500	0.06498100

F	3.14825000	-3.93186700	2.64551000	H	-2.38625700	0.30915900	-3.50016900
F	1.78701200	-2.37547100	4.41820900	H	0.23526500	1.42880700	-4.62073100
F	-0.27897100	-0.92216100	3.63130500	C	-1.70982500	3.89987400	-4.38446700
F	-2.12808800	-3.70923200	0.83530100	C	-0.98046300	4.17975100	-1.70019800
F	-4.01658400	-4.79959100	-0.69451700	H	-0.95586400	-1.25156600	-2.23063200
F	-5.36526600	-3.29981800	-2.50893600	C	-1.54784000	5.24953600	-2.38089300
F	-4.78547800	-0.64682200	-2.76548200	C	-1.91014700	5.10551000	-3.71568600
F	-2.91301000	0.47297100	-1.21891200	H	-0.71163900	4.23543700	-0.65370500
H	-0.69389500	-0.07977900	-0.06125300	H	-1.71329900	6.18693300	-1.86631400
H	2.48636100	-2.31710900	-1.99291500	H	-2.35634100	5.93849600	-4.24456100
C	4.71595300	-0.95874700	-1.07648500	H	0.47499500	-0.80418700	-3.18408700
C	5.70693600	-0.06692400	-1.50572100	H	-1.42372400	-0.56237900	-4.69280500
C	4.99305300	-1.79459000	0.01371600	H	-1.27226900	1.61546000	-5.48569300
C	6.93589700	-0.00517100	-0.86046400	N	-0.27905600	1.84858800	-1.75585900
H	5.51159900	0.59925100	-2.34034200	O	1.93798500	-0.10960700	-0.85676300
C	6.21857200	-1.72749600	0.66815800	Si	2.19294200	0.63638800	0.62487600
H	4.25218200	-2.51206100	0.35428800	H	0.92539100	1.29946400	0.98039600
C	7.18882100	-0.83108300	0.23107500	H	2.60658000	-0.35944400	1.63676300
H	7.69036900	0.69535800	-1.19844900	C	3.59444900	1.85385400	0.41135400
H	6.41627100	-2.37735100	1.51240700	C	3.57073800	2.78821600	-0.63238200
H	8.14429500	-0.77816000	0.73995600	C	4.72429800	1.80240200	1.23313200
H	3.07209800	-0.27025000	-3.16639400	C	4.64438900	3.64395400	-0.85057400
TS7				H	2.70591500	2.84537900	-1.28913100
				C	5.79832300	2.66206200	1.02397500
				H	4.77859900	1.06803600	2.03109500
				C	5.76041700	3.58016500	-0.01976300
C	-1.37742700	0.17759600	-3.89269700	H	4.61312900	4.36060600	-1.66312400
C	-0.85106100	1.50995400	-4.48594700	H	6.67012000	2.60480900	1.66539700
C	-1.14253500	2.80465800	-3.74008900	H	6.59933600	4.24543600	-0.18807300
C	-0.79678400	2.99649500	-2.39385300	Si	3.00297300	-0.92636300	-1.85408700
C	-0.23717000	0.70836200	-1.94076900	B	-1.32363800	-0.78474000	0.74218000
H	-1.99609000	3.80762600	-5.42592200	C	-0.16412700	-1.72426100	1.38838700

C	0.28564800	-1.72055500	2.70058400	H	-0.73101300	-0.09864100	-0.07059200
C	0.56169800	-2.54311800	0.53043100	H	2.48950000	-2.29860900	-2.02991000
C	1.37731200	-2.46287300	3.13630400	C	4.70799800	-0.92507000	-1.10569300
C	1.65627200	-3.29259400	0.91557400	C	5.68751300	-0.02519300	-1.54349600
C	2.07391300	-3.24521100	2.23649300	C	5.00260000	-1.76065100	-0.01974900
C	-2.09345100	0.21291900	1.76678200	C	6.92345800	0.04334500	-0.91197800
C	-2.86957300	-0.29632700	2.79931900	H	5.47786100	0.64183300	-2.37397800
C	-2.11475400	1.58967200	1.63675900	C	6.23493300	-1.68681000	0.62089500
C	-3.60067800	0.49329000	3.66738200	H	4.26975500	-2.48295200	0.32862500
C	-2.83368600	2.42416400	2.48119600	C	7.19447000	-0.78331300	0.17447900
C	-3.58034600	1.87052800	3.50398500	H	7.66928200	0.74986800	-1.25670100
C	-2.46580700	-1.59727400	-0.09501900	H	6.44658600	-2.33671900	1.46171200
C	-3.22335000	-0.88958400	-1.01895900	H	8.15537000	-0.72532300	0.67246800
C	-2.78560900	-2.94270100	0.01340400	H	3.02273100	-0.21221500	-3.15482000
C	-4.20689700	-1.45281800	-1.81234400				
C	-3.77302000	-3.54991200	-0.75166300	I13			
C	-4.48632300	-2.80232500	-1.67258200				
F	-1.42284700	2.19964500	0.65477800	C	-1.45896700	0.29719400	-3.89388300
F	-2.81483500	3.74886900	2.31196800	C	-0.86423600	1.53697900	-4.57711300
F	-4.27789300	2.65222700	4.32556700	C	-1.16680300	2.77815400	-3.78343700
F	-4.32274100	-0.04338700	4.65106400	C	-0.76804900	2.90313200	-2.43997500
F	-2.91440600	-1.62258900	2.98602100	C	0.13073100	0.73928600	-1.88294100
F	0.20494200	-2.62280100	-0.76573700	C	-0.52207900	-0.24269000	-2.82099500
F	2.32843600	-4.04462700	0.03856400	H	-2.21198300	3.71622400	-5.39469500
F	3.14532700	-3.93645800	2.62082400	H	-2.42794600	0.55909600	-3.46212000
F	1.77760900	-2.40084600	4.40587500	H	0.21967400	1.40622900	-4.68036700
F	-0.29380900	-0.94975800	3.63072700	C	-1.90336000	3.81301700	-4.35900100
F	-2.13188900	-3.73239200	0.87200400	C	-1.10520900	4.06253100	-1.73272400
F	-4.03925800	-4.84778500	-0.61465100	H	-1.02779800	-0.98885400	-2.19705000
F	-5.42784600	-3.37342400	-2.41908200	C	-1.85643400	5.07232400	-2.31474600
F	-4.86920700	-0.71982000	-2.71077200	C	-2.25533700	4.94992900	-3.64098900
F	-2.97662500	0.42530400	-1.20791300	H	-0.75330600	4.14192900	-0.71134300

H	-2.11552900	5.95433300	-1.74165600	Si	0.85333300	2.69857900	-0.06036500
H	-2.83105800	5.73478000	-4.11663400	H	-0.28603900	3.19869700	0.71645900
H	0.30563700	-0.78461700	-3.29558300	H	1.36726100	1.34814000	0.21504900
H	-1.63990000	-0.49378300	-4.62545900	C	1.91685400	3.94497800	-0.94312300
H	-1.26992100	1.65369700	-5.58335700	C	2.05401800	5.24658100	-0.44989400
N	0.03545100	1.99422700	-1.71431900	C	2.64832900	3.57246400	-2.07538100
H	0.83036500	0.24926100	-1.19841600	C	2.90242700	6.15298200	-1.07648800
I14'				H	1.51484800	5.54393700	0.44483000
				C	3.49627000	4.47680500	-2.70505500
				H	2.58962600	2.55537600	-2.45163500
C	-0.59542800	0.40862000	-4.27897000	C	3.62450400	5.76818000	-2.20297800
C	0.18210200	1.72389300	-4.44339700	H	3.01111000	7.15495300	-0.67807500
C	-0.55480300	2.91833500	-3.89377400	H	4.07145600	4.16932900	-3.56983300
C	-0.73600300	3.07750000	-2.51300300	H	4.29771800	6.47045200	-2.68058900
C	-0.41493400	0.84794100	-1.80345100	B	2.63814600	3.10973900	2.42537700
C	-1.28185800	0.32333300	-2.89688700	C	2.01408500	3.90288000	3.69264600
H	-0.92859900	3.80872200	-5.80097900	C	2.61016000	3.80260300	4.94199700
H	-1.37562300	0.32411200	-5.03760300	C	0.88509400	4.70001800	3.63529600
H	1.14006900	1.63137900	-3.92250500	C	2.12284600	4.43648700	6.07086500
C	-1.06342500	3.90998600	-4.72996500	C	0.35889000	5.35359000	4.73972900
C	-1.38384600	4.18979400	-1.98465300	C	0.98191300	5.21649200	5.96660200
H	-2.18544400	0.94017600	-2.91869400	C	2.76172000	1.53029800	2.77823800
C	-1.88738600	5.15817000	-2.84203300	C	3.94363000	0.84033900	3.00380000
C	-1.72559600	5.01820600	-4.21568900	C	1.60427000	0.77611400	2.90859100
H	-1.50402400	4.29023600	-0.91327900	C	3.98181900	-0.51010100	3.31812100
H	-2.39892200	6.02065000	-2.43456700	C	1.59443500	-0.57410200	3.21408400
H	-2.11014700	5.77558600	-4.88736600	C	2.79945600	-1.22197500	3.42316800
H	-1.56731800	-0.70318800	-2.67282900	C	3.94433800	3.79609900	1.75801700
H	0.08674500	-0.43224300	-4.41593200	C	4.50378800	3.21306000	0.62727500
H	0.41264500	1.88997500	-5.49601500	C	4.48158800	5.02697800	2.10356500
N	-0.19332700	2.09754800	-1.60490200	C	5.49132700	3.79946700	-0.13819200
H	0.06152400	0.16000100	-1.10783800	C	5.48288300	5.65058800	1.36935500

C	5.98248300	5.03930400	0.23643100	C	-2.60611300	-1.66644800	-0.02299100
F	0.40626300	1.35989900	2.71320100	C	-2.65128400	-2.22514700	1.24591800
F	0.44837500	-1.25156200	3.30629800	H	-1.97062100	-0.01994700	-1.20374600
F	2.82042100	-2.51925900	3.71988400	H	-3.08941500	-2.15038400	-0.86207500
F	5.14306700	-1.13114200	3.52225800	H	-3.16546700	-3.16291700	1.41368400
F	5.12289200	1.46602400	2.92498600	H	0.08746900	3.09380300	3.17773700
F	0.24147900	4.89232900	2.46796100	H	-1.33944300	1.94398600	4.65241700
F	-0.73444700	6.10993200	4.63146600	H	-0.85558200	-0.35279600	4.19358800
F	0.49360300	5.83473100	7.03907000	N	-0.69012900	1.45901500	0.54486300
F	2.73283400	4.31332400	7.24901100	Si	-0.05970400	1.71530300	-1.20953800
F	3.73387900	3.08495700	5.07907800	H	0.82576500	2.86722100	-1.00986600
F	4.03231400	5.71001100	3.16685300	H	-1.24345700	1.96781500	-2.04478500
F	5.94582600	6.84777400	1.73272600	C	0.82845700	0.16029900	-1.68144700
F	6.90937300	5.64273800	-0.50445700	C	1.90951200	-0.30055400	-0.91965300
F	5.94901300	3.20971900	-1.24338000	C	0.43927300	-0.56659800	-2.81239500
F	4.03427500	2.02618200	0.19985900	C	2.58008300	-1.46400100	-1.27510400
H	1.76620300	3.18436300	1.53172200	H	2.23261200	0.25011700	-0.04078400
114				C	1.11415600	-1.72738400	-3.17316000
				H	-0.39634100	-0.22826800	-3.41765400
				C	2.18159000	-2.17631400	-2.40285600
C	-1.45964000	1.65020200	3.60868000	H	3.41280700	-1.81430600	-0.67753100
C	-0.75935800	0.31369000	3.33687800	H	0.80655400	-2.28118500	-4.05168000
C	-1.36685500	-0.35801300	2.13785000	H	2.70572200	-3.08253700	-2.68188600
C	-1.35627000	0.21054900	0.85552600	H	0.01237300	3.30438600	0.86687900
C	-0.51017300	2.47206200	1.33085600	B	-2.94182300	4.10541300	-0.65344300
C	-0.85960600	2.74480400	2.74416600	C	-3.53641100	5.43715000	0.08694600
H	-2.06766500	-2.00604100	3.29563100	C	-2.71105900	6.54970900	0.19393000
H	-2.53051800	1.55088200	3.42691500	C	-4.82272000	5.61378000	0.57625600
H	0.31317300	0.48252200	3.18362000	C	-3.10693100	7.75082100	0.75840100
C	-2.03552600	-1.57060300	2.30388100	C	-5.26184800	6.79826900	1.15021600
C	-1.95926300	-0.45528400	-0.21289800	C	-4.39803700	7.87461200	1.24199500
H	-1.48994900	3.64225800	2.70485800	C	-2.90287400	4.45907400	-2.24426400

C	-4.07931100	4.65067300	-2.95683200	C	-1.25137600	-0.02717400	1.65515900
C	-1.74019500	4.69010100	-2.95851100	C	-1.36226300	0.46736400	0.35221100
C	-4.11838100	5.02128000	-4.28810600	C	-0.79833000	2.86325300	0.53738100
C	-1.72745500	5.06262500	-4.29623500	C	-1.04022000	3.16513000	1.99602400
C	-2.92565800	5.23138400	-4.96360100	H	-1.79628600	-1.62753600	2.96067000
C	-3.74599000	2.73024200	-0.28090600	H	-2.45589000	1.81984200	2.95462600
C	-4.01832600	2.42576900	1.04860300	H	0.44298000	1.02482000	2.46015600
C	-4.16014500	1.75306700	-1.17538800	C	-1.85899200	-1.24808200	1.94697700
C	-4.63862300	1.26588200	1.47827200	C	-2.02935600	-0.26666300	-0.62740100
C	-4.80899900	0.58601400	-0.79537200	H	-1.75626100	3.98708400	2.06090700
C	-5.04300000	0.33160900	0.54096800	C	-2.60988500	-1.48965500	-0.32076000
F	-0.53312000	4.54115400	-2.37974200	C	-2.52859000	-1.98142900	0.97535500
F	-0.57510300	5.25943300	-4.94084400	H	-2.11808000	0.12883000	-1.63429300
F	-2.93631900	5.58891900	-6.24632900	H	-3.13922600	-2.03903400	-1.08951500
F	-5.27635900	5.17971100	-4.92975000	H	-2.98873300	-2.92771100	1.23048200
F	-5.25346000	4.44943300	-2.34132600	H	-0.07677100	3.59698900	2.29906300
F	-5.71984100	4.61878200	0.52517200	H	-1.18631600	2.44848400	3.98161200
F	-6.50746100	6.91167200	1.61430400	H	-0.54068300	0.17473800	3.64629300
F	-4.80387900	9.01898700	1.78974000	N	-0.70617800	1.68611100	-0.07062900
F	-2.26642000	8.78460700	0.83957500	Si	0.23897200	1.59529500	-1.64017200
F	-1.45260300	6.49209500	-0.27375600	H	1.20895100	2.69368500	-1.51111700
F	-3.90065600	1.85789300	-2.49039700	H	-0.68687000	1.76237700	-2.77588100
F	-5.11648400	-0.34335500	-1.70326500	C	1.02008100	-0.08797900	-1.67144900
F	-5.59764900	-0.81622000	0.92217600	C	1.84956400	-0.50853000	-0.62409000
F	-4.83503900	1.03328400	2.77893400	C	0.77802300	-0.96631200	-2.73278200
F	-3.67149000	3.29840800	2.01563000	C	2.41905700	-1.77528000	-0.63599000
H	-1.80026900	3.97042700	-0.26743100	H	2.05251800	0.15544400	0.21173600
TS8				C	1.35205800	-2.23333300	-2.74969000
				H	0.13058700	-0.66534300	-3.55055900
				C	2.16992300	-2.63756800	-1.70059700
C	-1.39233900	2.05560100	2.98374200	H	3.05572900	-2.09162300	0.18138500
C	-0.58784800	0.77477700	2.73716100	H	1.15744400	-2.90481700	-3.57716000

H	2.61364300	-3.62597200	-1.71034400	F	-5.27965200	-0.34815600	-1.93678200
H	-0.23262600	3.65016900	0.04514800	F	-5.76038300	-1.06493600	0.63053400
B	-3.24145000	3.99208900	-0.47716700	F	-5.17993500	0.67545600	2.64650500
C	-3.57051900	5.27852700	0.44864000	F	-4.16465400	3.06917300	2.09953300
C	-2.56035400	6.18429000	0.74048400	H	-2.09637500	3.60892900	-0.11262900
C	-4.82630000	5.60737600	0.94010800				
C	-2.75515200	7.34064000	1.47663100	TS9			
C	-5.06811900	6.75734700	1.67545700	C	-2.51868600	12.83733800	-4.57172500
C	-4.02598500	7.62916900	1.94396000	C	-3.44381900	12.29603600	-5.66857800
C	-3.08696200	4.48865400	-2.01068500	C	-2.79848600	11.42079800	-6.72685100
C	-4.21167800	4.85893700	-2.73609600	C	-1.41628400	11.23875200	-6.85274300
C	-1.88275000	4.64746200	-2.66878000	C	-0.45078100	11.81193800	-5.85196400
C	-4.15805500	5.33104700	-4.03466100	C	-1.11743100	13.10931800	-5.06414200
C	-1.77610900	5.11281500	-3.97106700	H	-4.69953300	10.98376700	-7.61342300
C	-2.92509700	5.45862800	-4.65745800	H	-2.50146500	12.17823100	-3.70412300
C	-4.13250300	2.66719700	-0.23398500	H	-3.90212200	13.13805500	-6.19700700
C	-4.44038700	2.26118900	1.06026800	C	-3.62714000	10.83823800	-7.69144800
C	-4.47244000	1.75231600	-1.22090000	C	-0.89490500	10.53753300	-7.94014300
C	-4.98080900	1.02834900	1.37720700	H	-0.42550500	13.43904200	-4.29390100
C	-5.05325700	0.52269400	-0.95212200	C	-1.72722400	9.96797800	-8.88769800
C	-5.29016100	0.14705900	0.35545300	C	-3.10532400	10.11321300	-8.75336500
F	-0.72091000	4.32992600	-2.05707900	H	0.17793600	10.47290200	-8.05219100
F	-0.58595200	5.22631800	-4.56007400	H	-1.30449600	9.44045100	-9.73348000
F	-2.85048700	5.90882500	-5.90630300	H	-3.77317900	9.68422900	-9.49077500
F	-5.26614800	5.66186600	-4.69403000	H	-1.10234700	13.82263500	-5.89112100
F	-5.41894200	4.74000200	-2.17002500	H	-2.91261400	13.79396200	-4.21501000
F	-5.86995300	4.80032600	0.72567000	H	-4.27087900	11.74833700	-5.20931400
F	-6.28895200	7.03363200	2.12953300	N	-0.05950700	11.10064600	-4.75146100
F	-4.24355100	8.73423400	2.65051900	H	0.41308000	12.32710800	-6.29883900
F	-1.74527700	8.16971100	1.73801100	O	1.70929200	10.07075400	-5.08461400
F	-1.30666000	5.93962200	0.31085500	Si	2.33999600	9.09947800	-6.35520100
F	-4.17086200	1.97881700	-2.50935300	H	3.05814100	7.99534400	-5.68809700

H	1.17096400	8.62691100	-7.11417700	C	0.35607400	5.97435200	-5.53106200
Si	-0.90642900	9.60730300	-4.07687800	H	0.83410600	7.28121400	-3.90121500
H	-2.29680500	10.08785900	-3.94481400	C	-1.43215100	6.69804800	-6.98194300
H	-0.24270500	9.42516800	-2.77756900	H	-2.36831600	8.55966600	-6.48277600
Si	2.46098200	11.12496200	-3.96755600	C	-0.45019100	5.76971900	-6.64674900
H	2.32097300	12.51066400	-4.44042600	H	1.11142900	5.24547900	-5.26318900
H	1.79806000	10.88545200	-2.67408000	H	-2.06565000	6.53351400	-7.84540900
C	4.27248400	10.69663900	-3.89053100	H	-0.31877700	4.88057000	-7.25184200
C	5.22617900	11.68368700	-4.16816300	B	1.09978000	13.77768200	-8.73183800
C	4.71852200	9.40091700	-3.59611100	C	-0.23648700	14.61625400	-8.28485900
C	6.58419900	11.38303800	-4.17876500	C	-0.29432500	15.80704100	-7.57313600
H	4.91011700	12.69816100	-4.38218300	C	-1.47570500	14.06340200	-8.59973600
C	6.07447600	9.09371500	-3.61287500	C	-1.48136800	16.36160200	-7.10932100
H	4.00319200	8.61851600	-3.35940900	C	-2.68233200	14.58430100	-8.16212400
C	7.00712600	10.08463400	-3.91219000	C	-2.68324600	15.73485400	-7.39104900
H	7.30589400	12.15920700	-4.40394700	C	2.49210400	14.20775700	-7.98897300
H	6.40568400	8.08579100	-3.39338100	C	3.73963900	14.27577000	-8.59575200
H	8.06350200	9.84398300	-3.93021300	C	2.53609000	14.34824800	-6.60720700
C	3.47175200	10.05728300	-7.47949700	C	4.93223000	14.41484500	-7.89679100
C	4.82417700	10.27778100	-7.17557700	C	3.69071100	14.53223200	-5.87128900
C	2.98636700	10.51991600	-8.71154800	C	4.91194600	14.53821700	-6.52255000
C	5.64645700	10.97482700	-8.05357300	C	1.15916200	13.78991400	-10.35585000
H	5.24664300	9.89599900	-6.25237600	C	0.91157400	12.67870200	-11.14282000
C	3.81010800	11.20446600	-9.59720200	C	1.39121600	14.96862000	-11.04949200
H	1.95914500	10.34276500	-9.00568700	C	0.90952700	12.71637800	-12.53066100
C	5.13884700	11.44237900	-9.26290200	C	1.40035500	15.05574900	-12.42970000
H	6.68438200	11.15115900	-7.79478800	C	1.15506100	13.91388300	-13.17665900
H	3.41015900	11.56724900	-10.53665400	F	1.39130700	14.28315900	-5.88925300
H	5.77612500	11.99878600	-9.94032000	F	3.64847400	14.66417700	-4.54018900
C	-0.77343000	8.07583700	-5.10697900	F	6.04445600	14.64246000	-5.82534000
C	0.19461600	7.12251600	-4.76473800	F	6.10018300	14.39493700	-8.54143800
C	-1.60017000	7.84235300	-6.21151300	F	3.87475300	14.16123000	-9.92611800

F	-1.54367200	12.95905000	-9.35144300	H	-6.01106000	0.39037800	2.03417500
F	-3.84061400	13.98624100	-8.45704200	N	-2.34327900	-0.63593600	2.60884800
F	-3.83194700	16.23600600	-6.93817000	H	-2.25699500	0.80756200	1.17481100
F	-1.47813900	17.48926100	-6.39741700	Si	-2.25164200	-2.41451200	3.06947000
F	0.82263100	16.48020200	-7.27166000	H	-3.60620700	-2.99709100	3.05023300
F	1.64270000	16.09151000	-10.36025800	H	-1.72479000	-2.30907500	4.44173100
F	1.64048500	16.21174400	-13.05079400	C	-1.13896000	-3.13864200	1.78051000
F	1.15669500	13.97110800	-14.50780100	C	-0.01117200	-2.42383100	1.35295800
F	0.67343400	11.61365900	-13.24621500	C	-1.47637700	-4.32916000	1.12724500
F	0.66704100	11.47714100	-10.58704900	C	0.74330100	-2.87303400	0.27675600
H	0.90000000	12.63647600	-8.37401600	H	0.26359600	-1.49143500	1.83628000
				C	-0.70996100	-4.78745400	0.06129400
I15				H	-2.35588900	-4.88873400	1.42909300
C	-4.38352100	0.23508600	3.40885800	C	0.39065600	-4.05338100	-0.37110500
C	-4.92354000	0.35291200	1.95516500	H	1.58963800	-2.28945400	-0.06685000
C	-4.60258900	-0.69813100	0.87118500	H	-0.98340100	-5.70497800	-0.44549100
C	-3.28249700	-1.01502000	0.46307500	H	0.96762700	-4.39385300	-1.22229300
C	-2.42432200	-0.24937100	1.37726000	B	-0.21232900	0.80175700	-1.04236400
C	-2.85195800	0.37471100	3.56084000	C	-1.34720600	1.94527000	-0.74368700
H	-6.66079600	-1.03191700	0.38641800	C	-1.22370600	3.03988400	0.10087900
H	-4.69728900	-0.72144100	3.83631400	C	-2.64068900	1.70902900	-1.20701700
H	-4.62955600	1.33517100	1.56140600	C	-2.30668000	3.79844400	0.53150700
C	-5.63393600	-1.26843700	0.13010500	C	-3.74825300	2.43166300	-0.79613600
C	-2.99448700	-1.84709300	-0.60401000	C	-3.57863300	3.48457500	0.08912700
H	-2.50895400	0.16090700	4.57171000	C	1.20810900	1.00797100	-0.26337100
C	-4.05457900	-2.41816500	-1.29904500	C	2.46484300	1.11771500	-0.84275900
C	-5.36339700	-2.12770100	-0.93228200	C	1.22718400	0.96321400	1.12472000
H	-1.96411500	-2.04315500	-0.87637600	C	3.64468100	1.15737500	-0.10766700
H	-3.85386800	-3.08075700	-2.13134800	C	2.36962700	0.99041300	1.89961700
H	-6.18687900	-2.56659100	-1.48233200	C	3.60047900	1.08833200	1.27138000
H	-2.49933600	1.36359900	3.25578600	C	-0.05923000	0.56810800	-2.64070700
H	-4.85875700	1.01751700	4.00526900	C	-0.14933400	-0.67640900	-3.23874900

C	0.13988100	1.63067400	-3.51023600	C	-3.02387700	-2.34157100	-0.58975500
C	-0.06496100	-0.86998700	-4.60997700	H	-2.61367900	-0.50195300	4.45094500
C	0.23131700	1.48714200	-4.88324100	C	-4.11786400	-2.37490000	-1.45132400
C	0.12407500	0.22143800	-5.43731300	C	-5.06675200	-1.36417500	-1.38900700
F	0.05718000	0.88400600	1.80236900	H	-2.28269600	-3.13463600	-0.62318900
F	2.30052700	0.91656200	3.23062500	H	-4.22614300	-3.18627800	-2.16122200
F	4.72165900	1.11835800	1.98765000	H	-5.92403300	-1.37714500	-2.05169700
F	4.82245800	1.25907100	-0.72314500	H	-1.65982700	0.42556600	3.30061800
F	2.61592500	1.19003200	-2.17214900	H	-3.95223900	1.28443900	3.49276600
F	-2.87681100	0.68694500	-2.04075600	H	-4.49221700	1.56505700	1.20599800
F	-4.97591500	2.10258600	-1.20093500	N	-2.12416500	-1.51405800	2.70028300
F	-4.63453500	4.17157600	0.52271100	H	-1.02863400	-2.14210200	1.02958000
F	-2.13462400	4.81779200	1.37300400	Si	-2.92079800	-2.99833200	3.12607400
F	-0.03074900	3.40511800	0.58817100	H	-4.31435600	-3.15550200	2.62332800
F	0.28076300	2.86926100	-3.01534000	H	-2.95708300	-3.02822600	4.60811500
F	0.42609900	2.54071100	-5.67768900	C	-1.92815700	-4.40735600	2.39239000
F	0.20811200	0.05766300	-6.75663300	C	-0.54403300	-4.48569700	2.59687300
F	-0.16441800	-2.09290700	-5.13759900	C	-2.53996800	-5.39341300	1.61154600
F	-0.32683900	-1.78491500	-2.49514300	C	0.20349400	-5.51864600	2.04342600
H	-0.68627600	-0.21205900	-0.55322000	H	-0.04564400	-3.72256400	3.18773400
2a'-Si				C	-1.79614100	-6.43113000	1.05562200
C	-3.77046800	0.40131800	2.87199100	H	-3.60868900	-5.34556200	1.42624100
C	-3.69758400	0.84142700	1.40009200	C	-0.42404400	-6.49413900	1.27240700
C	-3.82764400	-0.28586500	0.39984200	H	1.27329300	-5.56477500	2.21068700
C	-2.86731200	-1.30889300	0.33112500	H	-2.28568500	-7.18662000	0.45217800
C	-1.70874800	-1.33241500	1.30645400	H	0.15738600	-7.29996300	0.83977000
C	-2.49667200	-0.28010600	3.38596000	H	-1.13778500	-0.39868300	1.24334200
H	-5.65951600	0.45968900	-0.42344100				
H	-4.62741400	-0.26754600	3.00673800				
H	-2.75003600	1.37023900	1.23739400				
C	-4.91627200	-0.32980000	-0.46813800				

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