Supplementary Materials for

Mechanistic Insight Into the Stereoselective Cationic Polymerization of N-Vinylcarbazole

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1. Materials and Methods

1.1. General Considerations

Prior to use, *N*-vinylcarbazole was recrystallized twice from hexanes, dried under vacuum overnight, and stored in a N_2-filled glovebox freezer. Scandium(III) trifluoromethanesulfonate 99.995% trace metal purity was purchased and used from MilliporeSigma (St. Louis, MO). Me-NVC-OMe was prepared according to literature.[1] Unless otherwise noted, solvents were dried and degassed using a Pure Process Technology solvent purification system and then subsequently stored over molecular sieves (3Å) in a N_2-filled glovebox. Other reagents whose syntheses are not described in Section 2 were purchased from commercial sources (Alfa Aesar (Ward Hill, MA), MilliporeSigma (St. Louis, MO), Oakwood Products (West Columbia, SC), Acros Organics (Geel, Belgium), and TCI America (Portland, OR)) and used without further purification. All syntheses were performed under inert atmosphere (N_2 or Ar) using flame-dried or oven-dried glassware unless specified otherwise. Qualitative TLC analysis was performed on 250 mm thick, 60 Å, glass backed, F254 silica (SiliCycle, Quebec City, Canada). Visualization was accomplished with UV light, exposure to *p*-anisaldehyde solution followed by heating, or exposure to $KMnO_4$ solution followed by heating. Flash chromatography was performed using SiliCycle silica gel (230-400 mesh). NMR spectra were recorded using a Bruker DRX 400 MHz, Bruker AVANCE III 500 MHz, or Bruker AVANCE III 600 MHz CryoProbe spectrometer. Chemical shifts δ (ppm) are referenced to tetramethylsilane (TMS) using the residual solvent as an internal standard (^{1}H and ^{13}C). For ^{1}H NMR: $CDCl_3$, 7.26 ppm and $C_2D_2Cl_4$, 6.04 ppm. For ^{13}C NMR: $CDCl_3$, 77.16 ppm and $C_2D_2Cl_4$, 73.78 ppm. Coupling constants (J) are expressed in hertz (Hz). The use of ^{1}H NMR to quantify tacticity of poly(*N*-vinylcarbazole) has been established and reported previously. Circular dichroism (CD) measurements were collected on a Chirascan Plus instrument with a wavelength range of 250-350 nm in 1.0 nm steps with 4.000 sec scans per point. Samples were observed in a 1 mm quartz cuvette at 0.1 mg/mL in HPLC grade, filtered THF. The sample temperature was controlled using a Quantum Northwester TC125 unit with Julabo AWC100 water bath. A Savitzky-Golay smoothing filter with window size < 8 was applied to the chromatogram. Optical rotations were collected using a Jasco P-1010 polarimeter at 25 ºC, using a 2 mL cell with 1 dm path length. All samples were prepared in HPLC grade methanol. HPLC data was collected using a Perkin Elmer Flexar HPLC system equipped with a Perkin Elmer PDA detector and Daicel CHIRALPAK IA column.

1.2. Macromolecular Characterization

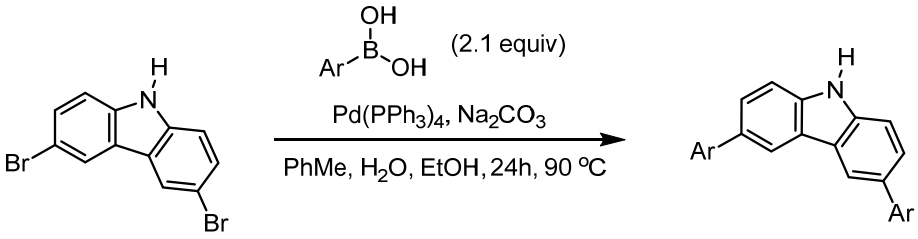
Gel permeation chromatography (GPC) was performed on a Tosoh EcoSEC Elite GPC system equipped with a TSKgel Super HM-M (17392) column maintained at 40 °C with an RI detector and a Tosoh LENSTM 3 multi-angle light scattering detector (MALS) Tetrahydrofuran was used as the mobile phase at a flow rate of 0.5 mL/min. Molecular weight and dispersity data are reported relative to polystyrene standards. For highly isotactic samples, high temperature gel permeation chromatography (HT GPC) spectra were obtained using a Tosoh EcoSEC-HT GPC using TSKgel GMHHR-M columns. 1,2,4-trichlorobenzene (TCB) was prepared with 200 ppm dibutylhydroxytoluene (BHT) by stirring overnight and was the mobile phase. The flow rate was set to 1 mL/min and samples were prepared at concentrations of 2 mg/mL in TCB with 200 ppm

BHT. The instrument was calibrated using 17 polystyrene standards in the range of 580 to 5,480,000 Da. A calibration curve was created using refractive index detection against 2 mg/mL polystyrene standards in TCB with 200 ppm BHT at 140 °C. A tandem multi-angle light scattering (MALS) detector could also be employed on the HT GPC via a Wyatt DAWN 8 heated flow cell instrument.

2. Experimental Section

2.1. Initiator and Monomer Synthesis

General Carbazole 3,6-difunctionalization (1a-d):



Accessing aryl disubstituted carbazoles **(1a-e)**, an semi-optimized procedure was developed utilizing a Suzuki-Miyaura coupling with 3,6-dibromocarbazole.

$Pd(PPh_3)_4$ (43.8 mg, 37.9 mmol) was added to a mixture of boronic acid (2.1 Eq, 5.17 mmol), 3,6-dibromo-9H-carbazole (.800 g, 1.00 Eq, 2.46 mmol), sodium carbonate (1.04 g, 4 Eq, 9.85 mmol), EtOH (5 mL), and Toluene (24 mL) under a nitrogen atmosphere. The reaction was heated to reflux at 90 C for 24 h. After being cooled to room temperature, the mixture was diluted with distilled water. The organic layer was separated, dried over anhydrous MgSO4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography with pentane/dichloromethane (3:1) to afford a white solid.

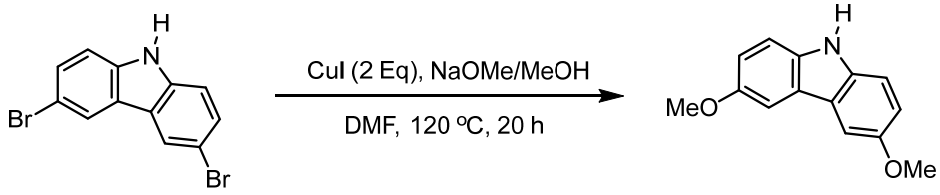
(1a) 3,6-diphenyl-9H-carbazole:
Matches literature reported values.[2]
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 2H), 7.80 – 7.71 (m, 8H), 7.51 (t, *J* = 1.6 Hz, 4H), 7.38 (t, *J* = 1.3 Hz, 2H), 5.95 (q, 1H), 3.32 (s, 3H), 1.87 (d, *J* = 1.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 141.88, 139.09, 133.16, 129.07, 128.82, 128.26, 127.32, 126.62, 125.51, 124.30, 118.89, 110.84, 84.24, 55.93, 20.22.

(1b) 3,6-di(naphthalen-2-yl)-9H-carbazole:
Matches literature reported values.[3]
^{1}H NMR(CDCl3, 300 MHz) 8.53 (s, 2H), 8.19 (s, 3H), 8.01-7.83 (m, 10H), 7.61-7.47 (m, 6H).
^{13}C NMR (75 MHz, CDCl3) 139.7, 139.5, 134.1, 133.2, 132.5, 128.6, 128.3, 127.9, 126.4, 126.3, 126.1, 125.9, 125.8, 124.3, 119.5, 111.3

(1c) 3,6-di(phenanthren-9-yl)-9H-carbazole:
^{1}H NMR (600 MHz, CDCl3) δ 8.40 (d, J = 1.8 Hz, 3H), 8.32 (d, J = 9.2 Hz, 2H), 8.27 (d, J = 7.8 Hz, 2H), 8.21 (d, J = 7.6 Hz, 2H), 8.17 (d, J = 7.6 Hz, 2H), 8.16 – 8.10 (m, 6H), 8.07 – 7.98 (m, 4H), 7.78 (dd, J = 8.3, 1.6 Hz, 2H), 7.72 (d, J = 8.3 Hz, 2H).
^{13}C NMR (151 MHz, CDCl3) δ 139.31, 138.54, 132.83, 131.55, 131.06, 130.33, 129.03, 128.86, 128.22, 127.51, 127.37, 127.23, 125.97, 125.66, 125.06, 124.98, 124.71, 124.66, 123.65, 122.45, 110.61.

(1d) 3,6-di(pyren-1-yl)-9H-carbazole:
Matches literature reported values.[4]
50% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.40 (d, J = 1.8 Hz, 3H), 8.32 (d, J = 9.2 Hz, 2H), 8.27 (d, J = 7.8 Hz, 2H), 8.21 (d, J = 7.6 Hz, 2H), 8.17 (d, J = 7.6 Hz, 2H), 8.16 – 8.10 (m, 6H), 8.07 – 7.98 (m, 4H), 7.78 (dd, J = 8.3, 1.6 Hz, 2H), 7.72 (d, J = 8.3 Hz, 2H).
^{13}C NMR (151 MHz, CDCl3) δ 139.31, 138.54, 132.83, 131.55, 131.06, 130.33, 129.03, 128.86, 128.22, 127.51, 127.37, 127.23, 125.97, 125.66, 125.06, 124.98, 124.71, 124.66, 123.65, 122.45, 110.61.

3,6-dimethoxy-9H-carbazole (1e):

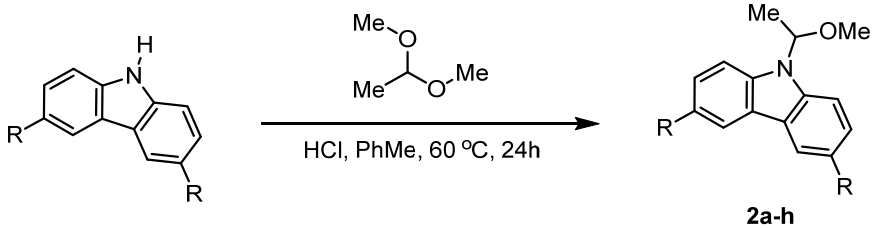


Using a procedure outlined by Louillat *et al*.[5]

3,6-dibromo-9H-carbazole (4.00 g, 1.0 Eq, 12.3 mmol) and copper(I) iodide (4.69 g, 2 Eq, 24.6 mmol) are placed in a Schlenk reactor under N2 atmosphere. DMF (1.0 mL) and a solution of MeONa/MeOH (5.4 M, 3.5 mL) are added. The reactor is sealed under N2 and heated at 120 °C for 20 h. The crude is then directly filtered over a SiO2 plug in ethyl acetate. The crude is then reduced, and purified over SiO2 gel column chromatography in pentane/CH2Cl2 = 6/4, then pentane/CH2Cl2 = 1/1, then pure CH2Cl2 (1L). 55% isolated yield (white solid). Note: the NMR signals of this molecule are very broad, consistent with the literature.

^{1}H NMR (600 MHz, CDCl3) δ (ppm): 8.1-7.7 (br, 1H, NH), 7.53 (br s, 2H), 7.4-7.2 (br, 2H), 7.09 (dd, 3 J = 8.8 Hz, J = 2.3 Hz). 3.97 (s, 6H, CH3O).
^{13}C NMR (151 MHz, CDCl3) δ (ppm): 153.72 (br), 135.32 (br), 123.87, 115.38 (br), 111.69 (br), 103.00, 56.22

General Hemiaminal Synthesis, With 3,6-Substitution (2a-h):



2a-h

To a 2-dram vial was added 3,6-substitued carbazole (1 Eq, 313 µmol), 1,1-dimethoxyethane (56.4 mg, 70.4 µL, 2 Eq, 626 µmol), hydrogen chloride (1 M, 1 drop), and toluene (2.5 mL). The reaction mixture was capped, put under N2 atmosphere, and heated to 60 °C and allowed to react

overnight. The reaction was cooled and poured into deionized water. The organic layer was collected, dried over MgSO4, and concentrated under reduced pressure. The crude reaction mixture was purified by column chromatography 1:4 dichloromethane:pentanes solvent mixture to yield pure product.

(2a) 3,6-di-tert-butyl-9-(1-methoxyethyl)-9H-carbazole:
White crystalline solid, 51% yield.
1H NMR (600 MHz, CDCl3) δ 8.11 (d, J = 1.9 Hz, 2H), 7.59 – 7.47 (m, 4H), 5.86 (q, J = 6.1 Hz, 1H), 3.25 (s, 3H), 1.78 (d, J = 6.1 Hz, 3H), 1.48 (s, 18H).
13C NMR (151 MHz, CDCl3) δ 142.20, 137.65, 123.55, 123.53, 123.36, 116.22, 109.86, 83.92, 77.24, 77.03, 76.81, 55.73, 34.66, 32.01, 20.06.
HR-MS (ESI+)($C_{22}H_{28}N)^+$([M-OMe]) Expected: 306.22217, Found: 306.2232
FT-IR (powder) ν_{max}/cm^{-1}: 2953, 2865, 1606, 1491, 1393, 1238, 1099, 1034, 817, 736, 618, 564

(2b) 3,6-dichloro-9-(1-methoxyethyl)-9H-carbazole:
White crystalline solid, 89% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.02 (d, J = 2.1 Hz, 2H), 7.57 (d, J = 8.7 Hz, 2H), 7.44 (dd, J = 8.7, 2.1 Hz, 2H), 5.82 (q, J = 6.1 Hz, 1H), 3.23 (s, 3H), 1.77 (d, J = 6.1 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 137.91, 126.58, 125.45, 123.85, 120.22, 111.69, 84.39, 77.24, 77.03, 76.81, 55.90, 20.14.
HR-MS (ESI+)($C_{14}H_{10}Cl_2N)^+$([M-OMe]) Expected: 262.01903, Found: 262.0202
FT-IR (powder) ν_{max}/cm^{-1}: 2989, 2952, 2822, 1471, 1435, 1280, 1097, 859, 730, 623, 522

(2c) 3,6-dibromo-9-(1-methoxyethyl)-9H-carbazole:
White crystalline solid, 91% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.17 (d, J = 1.9 Hz, 2H), 7.62 – 7.47 (m, 4H), 5.82 (q, J = 6.1 Hz, 1H), 3.22 (s, 3H), 1.77 (d, J = 6.1 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 138.05, 129.23, 124.30, 123.28, 112.78, 112.13, 84.36, 55.93, 20.14.
HR-MS (ESI+)($C_{14}H_{10}Br_2N)^+$([M-OMe]) Expected: 349.91799, Found: 349.9181
FT-IR (powder) ν_{max}/cm^{-1}: 2985, 2928, 2821, 1588, 1469, 1310, 1045, 799, 635, 492

(2d) 9-(1-methoxyethyl)-3,6-diphenyl-9H-carbazole
White crystalline solid, 67%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 2H), 7.80 – 7.71 (m, 8H), 7.51 (t, J = 1.6 Hz, 4H), 7.38 (t, J = 1.3 Hz, 2H), 5.95 (q, 1H), 3.32 (s, 3H), 1.87 (d, J = 1.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 141.88, 139.09, 133.16, 129.07, 128.82, 128.26, 127.32, 126.62, 125.51, 124.30, 118.89, 110.84, 84.24, 55.93, 20.22.
HR-MS (ESI+)($C_{26}H_{20}N)^+$([M-OMe]) Expected: 346.15957, Found: 346.1595
FT-IR (powder) ν_{max}/cm^{-1}: 2986, 1595, 1474, 1318, 1100, 879, 868

(2e) 9-(1-methoxyethyl)-3,6-di(naphthalen-2-yl)-9H-carbazole
White crystalline solid, 89% yield.

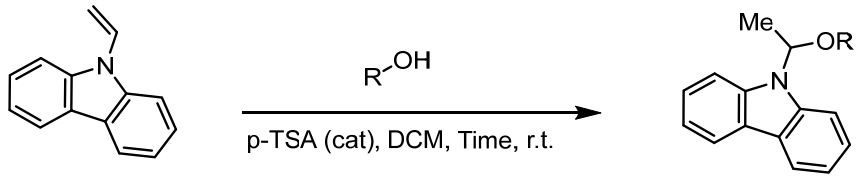
^{1}H NMR (600 MHz, CDCl3) δ 8.55 (dd, J = 10.4, 1.8 Hz, 4H), 8.25 – 8.14 (m, 5H), 8.01 – 7.84 (m, 20H), 7.79 (d, J = 8.5 Hz, 2H), 7.60 (d, J = 8.3 Hz, 2H), 7.58 – 7.49 (m, 8H), 6.00 (q, J = 6.1 Hz, 1H), 3.35 (s, 3H), 1.90 (d, J = 6.0 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 139.53, 139.36, 139.21, 133.90, 133.11, 132.35, 132.32, 128.43, 128.40, 128.112, 128.111, 127.69, 127.68, 126.27, 126.25, 126.10, 126.05, 125.96, 125.80, 125.65, 125.61, 125.58, 124.46, 124.20 119.27, 119.21, 111.10, 110.99, 84.31, 77.24, 77.03, 76.82, 55.95, 20.26. *Note: Hindered rotation of 2-naphthyl group + stereocenter of the methine must break symmetry of the compound, thus showing each individual carbon.*
HR-MS (ESI+)($C_{34}H_{24}N$)$^+$([M-OMe]) Expected: 446.19087, Found: 446.1909
FT-IR (powder) ν_{max}/cm^{-1}: 3051, 2984, 1598, 1492, 1462, 1275, 806, 736, 475

(2f) 9-(1-methoxyethyl)-3,6-di(phenanthren-9-yl)-9H-carbazole
White crystalline solid, 74% yield. Very acid/water sensitive.
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.86 – 8.71 (m, 6H), 8.32 (dd, *J* = 1.7, 0.7 Hz, 2H), 8.08 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.93 (dt, *J* = 7.9, 1.6 Hz, 3H), 7.86 – 7.81 (m, 5H), 7.71 – 7.68 (m, 6H), 6.08 (q, *J* = 6.1 Hz, 1H), 3.45 (s, 3H), 1.98 (d, *J* = 6.0 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 139.28, 139.01, 132.34, 131.73, 130.70, 129.88, 128.62, 128.28, 127.90, 127.23, 126.81, 126.48, 126.38, 123.77, 123.52, 122.90, 122.54, 121.82, 110.44, 110.34, 84.40, 56.08, 20.31.
HR-MS (ESI+)($C_{42}H_{28}N$)$^+$([M-OMe]) Expected: 546.22217, Found: 546.2220
FT-IR (powder) ν_{max}/cm^{-1}: 2988, 1605, 1526, 1308, 766, 616

(2g) 9-(1-methoxyethyl)-3,6-di(pyren-1-yl)-9H-carbazole
Pale yellow crystalline solid, 55% yield. very acid/water sensitive.
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 2.0 Hz, 2H), 8.35 (d, *J* = 9.3 Hz, 2H), 8.28 (d, *J* = 2.4 Hz, 2H), 8.21 (dd, *J* = 7.7, 1.1 Hz, 3H), 8.17 (dt, *J* = 7.8, 1.4 Hz, 3H), 8.14 – 8.10 (m, 6H), 8.05 – 8.02 (m, 4H), 7.91 (d, *J* = 8.4 Hz, 2H), 6.12 (q, *J* = 6.1 Hz, 1H), 3.49 (s, 3H), 2.02 (d, *J* = 6.1 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 139.32, 139.01, 138.41, 132.82, 131.56, 131.07, 130.36, 129.02, 128.88, 128.18, 127.49, 127.37, 127.22, 125.96, 125.65, 125.00, 124.70, 124.64, 123.93, 122.38, 110.59, 110.49, 84.47, 56.13, 20.37.
HR-MS (ESI+)($C_{42}H_{28}N$)$^+$([M-OMe]) Expected: 594.22217, Found: 594.2225
FT-IR (powder) ν_{max}/cm^{-1}: 3035, 2955, 1600, 1481, 1306, 1124, 841, 472

(2h) 3,6-dimethoxy-9-(1-methoxyethyl)-9H-carbazole
Ran at room temperature instead of 60 ºC. Off-white crystalline solid, 43%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 4H), 7.09 (dd, *J* = 8.9, 2.5 Hz, 2H), 5.80 (q, *J* = 6.1 Hz, 1H), 3.96 (s, 6H), 3.24 (s, 3H), 1.76 (d, *J* = 6.0 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 153.60, 134.76, 123.85, 114.96, 111.32, 103.01, 84.08, 56.08, 55.64, 20.10.
HR-MS (ESI+)($C_{16}H_{16}NO_2$)$^+$([M-OMe]) Expected: 254.11810, Found: 254.1181
FT-IR (powder) ν_{max}/cm^{-1}: 2993, 2932, 2829, 1606, 1471, 1293, 1197, 802, 733, 687

General Hemiaminal Synthesis, Anion Substitution (3a-c):



3a-c

For 3a-c: 9-vinyl-9H-carbazole (250 mg, 1 Eq, 1.29 mmol) was suspended in alcohol (20 Eq, 25.9 mmol) and DCM (1 mL), and p-TSA (0.1 Eq, 129 µmol) was added at 23 °C. The reaction is allowed to stir for 5 minutes to 3 hours (MeOH = 5 mins, EtOH 30 mins, (*S*)-sec-butanol = 1 hr, and iPrOH = 3 hours). The reaction is quenched with the addition of 5 mL of saturated aqueous sodium carbonate. 20 mL of deionized water is added and an additional 30 mL of DCM. The aqueous phase is washed 2 x 30 mL DCM and the organic phase is dried over Na2SO4, concentrated under vacuum, and yields a white solid. The crude solid purified by column chromatography with a gradient of 0 to 15% DCM in pentanes to yield pure product. *Note: If alcohols are significantly wet a co-eluting side-product is formed that can be removed by running a second column with 10% EtOAc in hexanes. Hemiaminals should be stored in a freezer dry as they are susceptible to hydrolysis to carbazole and aldehyde.

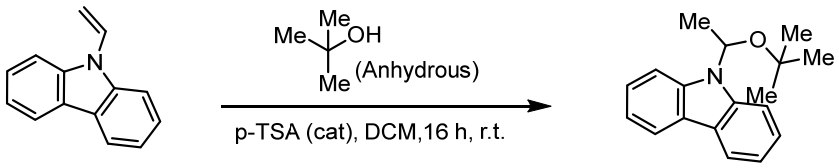
(3a) 9-(1-ethoxyethyl)-9H-carbazole:
White crystalline solid, 98% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.20 – 8.03 (m, 2H), 7.68 (d, J = 8.3 Hz, 2H), 7.53 – 7.41 (m, 2H), 7.28 (ddd, J = 7.8, 7.1, 0.9 Hz, 2H), 6.04 (q, J = 6.1 Hz, 1H), 3.55 – 3.29 (m, 2H), 1.82 (d, J = 6.1 Hz, 3H), 1.19 (t, J = 7.0 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 139.17, 125.70, 123.56, 120.30, 119.36, 110.59, 110.51, 82.24, 63.49, 20.24, 14.92.
HR-MS (ESI+)($C_{14}H_{12}N$)$^{+}$([M-OMe]) 194.09697, Found: 194.0972
FT-IR (powder) ν_{max}/cm^{-1}: 3059, 2973, 2928, 1593, 1481, 1377, 1255, 1149, 753, 599

(3b) 9-(1-isopropoxyethyl)-9H-carbazole:
Clear viscous oil, 45% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.12 (dt, J = 7.7, 0.9 Hz, 2H), 7.68 (d, J = 8.3 Hz, 2H), 7.47 (ddd, J = 8.3, 7.1, 1.2 Hz, 2H), 7.30 – 7.24 (m, 2H), 6.15 (q, J = 6.1 Hz, 1H), 3.53 (hept, J = 6.1 Hz, 1H), 1.78 (d, J = 6.1 Hz, 3H), 1.25 (d, J = 6.0 Hz, 3H), 1.04 (d, J = 6.2 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 139.20, 125.65, 123.55, 120.28, 119.30, 110.57, 79.18, 68.15, 22.98, 20.89, 20.48.
HR-MS (ESI+)($C_{14}H_{12}N$)$^{+}$([M-OMe]) 194.09697, Found: 194.0967
FT-IR (powder) ν_{max}/cm^{-1}: 3059, 2968, 2933, 1596, 1483, 1314, 1129, 1002, 748

(3c) 9-(1-((S)-2-methylbutoxy)ethyl)-9H-carbazole
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 7.7 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.47 (ddd, *J* = 8.3, 7.1, 1.3 Hz, 2H), 7.27 (d, *J* = 7.4 Hz, 2H), 5.99 (qd, *J* = 6.1, 1.3 Hz, 1H), 3.32 – 3.01 (m, 2H), 1.81 (dd, *J* = 6.1, 1.2 Hz, 3H), 1.65 (dq, *J* = 13.1, 6.1 Hz, 1H), 1.52 – 1.34 (m, 1H), 1.15 – 1.00 (m, 1H), 0.86 (t, *J* = 6.7 Hz, 3H), 0.81 (dt, *J* = 11.3, 7.4 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.17, 125.63, 123.54, 120.26, 119.30, 110.60, 82.85, 82.75, 77.26, 77.05, 76.84, 73.48, 34.90, 34.79, 26.26, 26.00, 20.15, 16.77, 16.46, 11.41, 11.13.
HR-MS (ESI+)$(C_{14}H_{12}N)^+$([M-OMe]) 194.09697, Found: 194.0966
FT-IR (powder) ν_{max}/cm^{-1}: 3058, 2975, 2970, 1594, 1480, 1320, 1002, 766

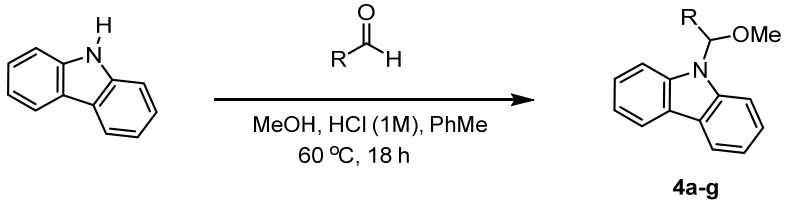
9-(1-(tert-butoxy)ethyl)-9H-carbazole (3d):



9-vinyl-9H-carbazole (250 mg, 1 Eq, 1.29 mmol) was suspended in tert-butanol (20 Eq, 25.9 mmol) freshly dried from CaH_2 and anhydrous DCM (1 mL), and dried p-TSA (0.1 Eq, 129 µmol) was added at 23 °C. The reaction is allowed to stir overnight. The reaction is quenched with the addition of 5 mL of saturated aqueous sodium carbonate. 20 mL of deionized water is added and an additional 30 mL of DCM. The aqueous phase is washed 2 x 30 mL DCM and the organic phase is dried over Na2SO4, concentrated under vacuum, and yields a white solid. The crude solid purified by column chromatography with a gradient of 0 to 15% DCM in pentanes to yield pure product.

(3d) 9-(1-(tert-butoxy)ethyl)-9H-carbazole:
White crystalline solid, 63% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.10 (d, J = 7.7 Hz, 2H), 7.71 (s, 2H), 7.52 – 7.39 (m, 2H), 7.25 (t, J = 7.4 Hz, 2H), 6.22 (q, J = 6.2 Hz, 1H), 1.72 (d, J = 6.2 Hz, 3H), 1.14 (s, 9H).
^{13}C NMR (151 MHz, CDCl3) δ 138.62, 125.47, 123.50, 120.22, 118.96, 75.08, 27.93, 22.13.
HR-MS (ESI+)$(C_{14}H_{12}N)^+$([M-OMe]) 194.09697, Found: 194.0970
FT-IR (powder) ν_{max}/cm^{-1}: 3051, 2979, 1593, 1451, 1306, 1101, 951, 746

General Hemiaminal Synthesis, Alpha Substitution (4a-g):



To 9H-carbazole (200 mg, 1 Eq, 1.20 mmol) were added Toluene (4 mL), methanol (76.6 mg, 96.8 µL, 2 Eq, 2.39 mmol), and aldehyde (235 mg, 255 µL, 2 Eq, 2.39 mmol), followed by the addition of hydrogen chloride (1 molar, 1 drop) at room temperature. The reaction mixture was

heated at 60 °C with stirring for 18 h. The reaction was allowed to cool to room temperature before washing the organic layer with with deionized water. The organic layer was isolated, dried over Na2SO4, and the volatile organics were removed under reduced pressure. The crude mixture was purified by column chromatography with 15% DCM in pentanes yield pure product.

(4a) 9-(1-methoxypropyl)-9H-carbazole:
White crystalline solid, 74% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.14 (d, 2H), 7.67 (d, J = 8.3 Hz, 2H), 7.48 (t, J = 1.3 Hz, 2H), 7.30 (t, 2H), 5.67 (t, 1H), 3.25 (s, 3H), 2.31 (td, 2H), 0.86 (t, J = 7.5 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 125.72, 123.53, 120.30, 119.44, 110.69, 89.10, 55.89, 27.28, 9.80.
HR-MS (ESI+)($C_{15}H_{14}N)^{+}$([M-OMe]) 208.11262, Found: 208.1121
FT-IR (powder) ν_{max}/cm^{-1}: 3063, 2965, 2929, 2987, 1595, 1448, 1300, 1060, 816, 749

(4b) 9-(1-methoxy-2-methylpropyl)-9H-carbazole:
White crystalline solid, 81% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.14 (dt, J = 7.7, 1.0 Hz, 2H), 7.65 (s, 2H), 7.49 – 7.43 (m, 2H), 7.31 – 7.24 (m, 2H), 5.26 (d, J = 9.3 Hz, 1H), 3.22 (s, 3H), 2.79 (dh, J = 9.0, 6.7 Hz, 1H), 1.28 (d, J = 6.6 Hz, 3H), 0.60 (d, J = 6.8 Hz, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 125.65, 123.39, 120.23, 119.35, 93.17, 56.17, 32.57, 19.58, 18.45.
HR-MS (ESI+)($C_{16}H_{16}N)^{+}$([M-OMe]) 222.12827, Found: 222.1290
FT-IR (powder) ν_{max}/cm^{-1}: 3057, 2928, 1593, 1448, 1308, 1224, 1052, 723

(4c) 9-(1-methoxy-2-phenylethyl)-9H-carbazole:
White crystalline solid, 87% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.11 (d, J = 7.7 Hz, 2H), 7.56 (s, 1H), 7.42 (t, J = 7.7 Hz, 2H), 7.29 – 7.22 (m, 3H), 7.22 – 7.12 (m, 3H), 7.12 – 6.99 (m, 2H), 5.84 (t, J = 6.5 Hz, 1H), 3.59 (dd, J = 13.9, 6.6 Hz, 1H), 3.38 (dd, J = 13.9, 6.4 Hz, 1H), 3.24 (s, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 136.60, 129.30, 128.35, 126.71, 125.72, 123.54, 120.23, 119.47, 88.83, 55.97, 40.54.
HR-MS (ESI+)($C_{18}H_{18}N)^{+}$([M-OMe]) 270.12827, Found: 270.1280
FT-IR (powder) ν_{max}/cm^{-1}: 3097, 2926, 1596, 1482, 1403, 1351, 1122, 749, 615

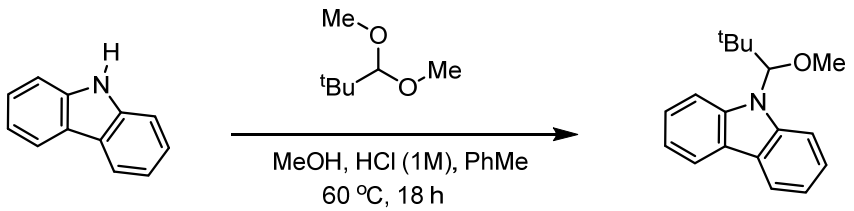
(4d) 9-(cyclopropyl(methoxy)methyl)-9H-carbazole:
White crystalline solid, 41% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.13 (dt, J = 7.8, 1.0 Hz, 2H), 7.67 (d, J = 8.2 Hz, 2H), 7.47 (dddd, J = 9.5, 7.8, 4.5, 1.2 Hz, 3H), 7.28 – 7.23 (m, 1H), 5.17 (d, J = 7.2 Hz, 1H), 3.21 (s, 3H), 1.85 (tdt, J = 8.2, 7.2, 5.0 Hz, 1H), 0.85 – 0.65 (m, 2H), 0.51 – 0.34 (m, 2H).
^{13}C NMR (151 MHz, CDCl3) δ 139.63, 125.77, 123.51, 120.28, 119.47, 110.59, 90.86, 55.96, 14.97, 3.58, 2.29.
HR-MS (ESI+)($C_{16}H_{14}N)^{+}$([M-OMe]) 220.11262, Found: 220.1120
FT-IR (powder) ν_{max}/cm^{-1}: 3050, 2900, 2815, 1594, 1483, 1448, 1318, 1222, 1086, 755

(4e) 9-(cyclobutyl(methoxy)methyl)-9H-carbazole:
White crystalline solid, 88% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.11 (dt, J = 7.7, 0.9 Hz, 2H), 7.68 (d, J = 8.7 Hz, 2H), 7.46 (ddd, J = 8.2, 7.1, 1.2 Hz, 2H), 7.28 – 7.25 (m, 2H), 5.69 (d, J = 9.1 Hz, 1H), 3.42 (h, J = 8.2 Hz, 1H), 3.22 (s, 3H), 2.38 – 2.24 (m, 1H), 2.15 (dq, J = 11.5, 8.6 Hz, 1H), 1.95 – 1.83 (m, 2H), 1.76 – 1.64 (m, 2H).
^{13}C NMR (151 MHz, CDCl3) δ 125.67, 123.43, 120.21, 119.37, 91.72, 56.06, 38.49, 25.89, 23.98, 18.13.
HR-MS (ESI+)$(C_{17}H_{16}N)^{+}$([M-OMe]) 234.12827, Found: 234.1284
FT-IR (powder) ν_{max}/cm^{-1}: 3057, 2981, 2900, 1593, 1447, 1318, 1222, 1188, 1091, 723

(4f) 9-(cyclopentyl(methoxy)methyl)-9H-carbazole:
White crystalline solid, 85% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.13 (dt, J = 7.8, 1.0 Hz, 2H), 7.65 (br, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.27 (d, J = 7.4 Hz, 2H), 5.40 (d, J = 9.7 Hz, 1H), 3.21 (s, 3H), 3.09 (dq, J = 9.1, 7.7 Hz, 1H), 2.17 – 2.03 (m, 1H), 1.81 – 1.60 (m, 3H), 1.60 – 1.50 (m, 1H), 1.43 (dddd, J = 15.7, 14.2, 7.2, 4.3 Hz, 1H), 1.19 – 1.04 (m, 2H).
^{13}C NMR (151 MHz, CDCl3) δ 125.64, 123.47 (br), 120.24, 119.35, 112.85 (br), 108.58 (br), 91.94, 55.97, 43.87, 30.13, 28.41, 25.49, 25.09.
HR-MS (ESI+)$(C_{18}H_{18}N)^{+}$([M-OMe]) 248.14392, Found: 248.1434
FT-IR (powder) ν_{max}/cm^{-1}: 3055, 2941, 2868, 2824, 1594, 1482, 1448, 1316, 1105, 1166, 750, 737

(4g) 9-(cyclohexyl(methoxy)methyl)-9H-carbazole:
White crystalline solid, 67% yield.
^{1}H NMR (600 MHz, CDCl3) δ 8.12 (t, J = 6.6 Hz, 2H), 7.75 (s, 1H), 7.45 (q, J = 6.8 Hz, 2H), 7.27 (d, J = 7.3 Hz, 3H), 5.32 (dd, J = 9.3, 5.2 Hz, 1H), 3.20 (d, J = 5.2 Hz, 3H), 2.56 – 2.21 (m, 2H), 1.85 (dq, J = 11.8, 3.9 Hz, 1H), 1.72 – 1.60 (m, 1H), 1.54 – 1.46 (m, 1H), 1.39 – 1.10 (m, 3H), 1.09 – 0.79 (m, 3H).
^{13}C NMR (151 MHz, CDCl3) δ 125.64, 123.38 (br), 120.21, 119.31, 112.04 (br), 108.89 (br), 92.08, 56.10, 41.54, 30.16, 28.43, 26.23, 25.62, 25.54.
HR-MS (ESI+)$(C_{19}H_{20}N)^{+}$([M-OMe]) 262.15957, Found: 262.1602
FT-IR (powder) ν_{max}/cm^{-1}: 3055, 2924, 2852, 1593, 1448, 1318, 1144, 749, 722

9-(1-methoxy-2,2-dimethylpropyl)-9H-carbazole (4h):

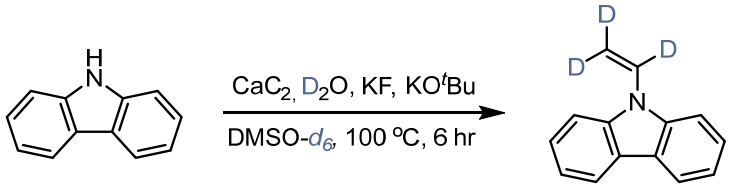


Accessing **#a** using the parent aldehyde as outlined above did not provide product. Using 1,1-dimethoxy-2,2-dimethylpropane instead, which should be generated in-situ, provided product in moderate yields.

To 9H-carbazole (200 mg, 1 Eq, 1.20 mmol) were added Toluene (4 mL), methanol (76.6 mg, 96.8 µL, 2 Eq, 2.39 mmol), and 1,1-dimethoxy-2,2-dimethylpropane (2 Eq, 2.39 mmol), followed by the addition of hydrogen chloride (1 molar, 1 drop) at room temperature. The reaction mixture was heated at 60 °C with stirring for 18 h. The reaction was allowed to cool to room temperature before washing the organic layer with with deionized water. The organic layer was isolated, dried over Na2SO4, and the volatile organics were removed under reduced pressure. The crude mixture was purified by column chromatography with 15% DCM in pentanes to yield 9-(1-methoxy-2,2-dimethylpropyl)-9H-carbazole (123 mg, 460 µmol, 38.5 %).

^{1}H NMR (600 MHz, CDCl3) δ 8.11 (td, J = 7.8, 1.0 Hz, 2H), 7.91 (d, J = 8.4 Hz, 1H), 7.53 – 7.35 (m, 3H), 7.28 – 7.20 (m, 2H), 5.38 (s, 1H), 3.18 (s, 3H), 1.13 (s, 9H).
^{13}C NMR (151 MHz, CDCl3) δ 141.66, 139.37, 125.47, 125.39, 123.56, 123.25, 120.06, 119.65, 119.20, 119.08, 114.59, 109.91, 95.93, 56.96, 39.79, 27.07.
HR-MS (ESI+)($C_{17}H_{18}N)^+$([M-OMe]) 236.14392, Found: 236.1439
FT-IR (powder) ν_{max}/cm^{-1}: 3058, 2919, 1594, 1446, 1298, 1106, 746, 722

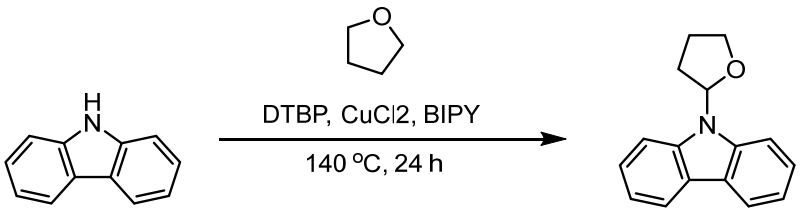
d^{3}-*N*-vinylcarbazole Synthesis (5a):



The procedure by Ledovskaya *et al*[6] was modified for an abundance of caution which allowed for lower pressures of acetylene—which required an extended reaction period.

A 100-ml glass pressure flask was loaded with 9H-carbazole (400 mg, 1 Eq, 2.39 mmol), CaC2 (613 mg, 4 Eq, 9.56 mmol), potassium tert-butoxide (537 mg, 2 Eq, 4.78 mmol) and potassium fluoride (139 mg, 1 Eq, 2.39 mmol). Then dimethyl sulfoxide-d6 (201 mg, 6 mL, 1 Eq, 2.39 mmol) and D_2O (345 uL, 8 eq, 19.1 mmol) were added, the flask was immediately sealed, and the mixture was stirred at 100 °C for overnight. After that, the reaction mixture was cooled to r.t. and extracted with hexane (5 x 100 mL). The solvent from the hexane extract was evaporated, and the residue was purified by column chromatography with hexane as an eluent to yield 9-(vinyl-d3)-9H-carbazole (.360 g, 1.83 mmol, 76.7 %) as a slightly off-white crystalline solid. The NMR spectra matched that of literature values.
^{1}H NMR (400 MHz, CDCl3): 8.10 (d, J = 7.7 Hz, 2 H), 7.68 (d, J = 8.3 Hz, 2 H), 7.52–7.47 (m, 2 H), 7.34–7.30 (m, 2 H).
^{13}C NMR (101 MHz, CDCl3): 139.5 (2 C), 129.3 (t, J = 26.7 Hz, CD=),126.4 (2 × CH), 124.1 (2 C), 120.7 (2 × CH), 120.4 (2 × CH), 110.6 (2 ×CH), 101.4 (quint, J = 24.5 Hz, =CD2).

9-(tetrahydrofuran-2-yl)-9H-carbazole (6a)



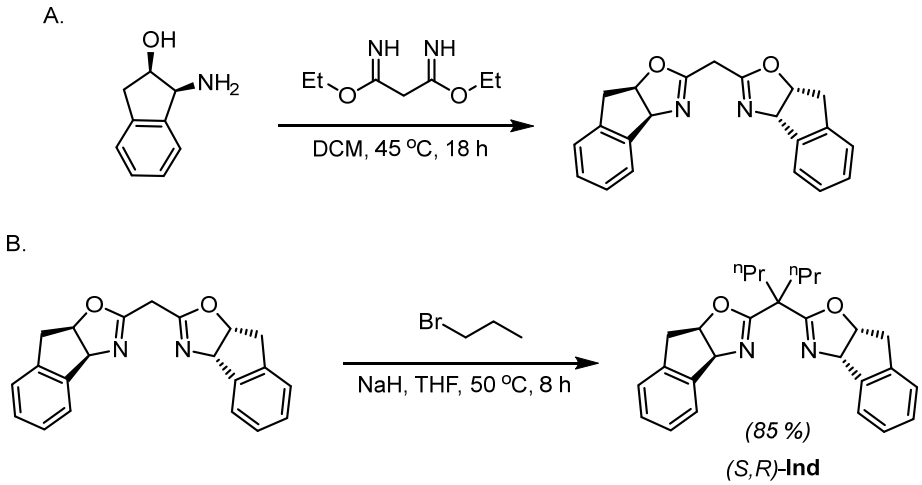
According to the following procedure.[7]

DTBP (1.5 mmol) was added to a mixture of indole/ carbazole (0.50 mmol), CuCl2 (0.05 mmol), 2,2′-bipyridine (0.05 mmol), and ether (2 mL) in a Schlenk tube at room temperature under an air atmosphere. The tube was then placed into a preheated oil bath (140 °C) and stirred for 15 h. After completion of reaction, the reaction tube was allowed to cool to room temperature, quenched with water, and diluted with ethyl acetate. The organic layer was separated, and the aqueous layer was washed with ethyl acetate (~10 mL × 3). The filtrate was concentrated under reduced pressure. The crude products were purified by column chromatography on silica gel with 10% dichloromethane in pentanes to afford the desired product with 66% yield. The NMR spectra matched that of literature values.

^{1}H NMR (400 MHz, CDCl3) δ 8.10 (d, J = 7.7 Hz, 2H), 7.54 (d, J = 8.2 Hz, 2H), 7.49 – 7.40 (m, 2H), 7.26 (d, J = 7.4 Hz, 2H), 6.51 (t, J = 6.7 Hz, 1H), 4.53 – 4.35 (m, 1H), 4.10 (td, J = 8.0, 5.4 Hz, 1H), 2.61 – 2.16 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.19, 125.67, 123.89, 120.29, 119.54, 110.36, 86.50, 77.24, 77.03, 76.82, 68.16, 29.40, 25.68.

(3aS,3a'S,8aR,8a'R)-2,2'-(heptane-4,4-diyl)bis(3a,8a-dihydro-8H-indeno[1,2-d]oxazole) (*S,R)*-**Ind** Ligand:

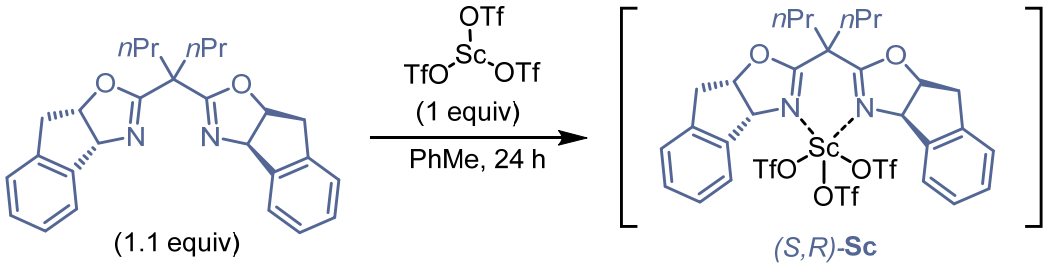


(*S,R)*-**Ind** was prepared using a modified literature preparation by Reisman and company to access larger quantities of material.[8]

A. Bis((3aS,8aR)-3a,8a-dihydro-8H-indeno[1,2-d]oxazol-2-yl)methane. An oven-dried 2-L three-necked, round-bottomed flask equipped with a 6.5 cm × 2.0 cm Teflon-coated elliptical stir bar is fitted with a thermometer, a reflux condenser and a rubber septum. The system is connected to a continuous nitrogen flow and then charged with (1R,2S)-(+)-cis-1-amino-2-indanol (1, 22.2 g, 149 mmol, 2.1 equiv), diethyl malonimidate dihydrochloride (2, 16.4 g, 71 mmol, 1 equiv), and 1 L of dichloromethane. The system is heated to 45 °C (internal temperature 43 °C) under an atmosphere of nitrogen in an oil bath for 18 h, stirring at 600 rpm. The reaction is removed from the stir plate, allowed to cool to 23 °C, and poured into to a separatory funnel (4 L). Water (1 L) is added as a single addition. The layers are separated and the aqueous layer is extracted with dichloromethane (800 mL). The combined organic layers are dried with anhydrous sodium sulfate (150 g, stirred for 5 min). The solution is filtered over a plug of cotton into an Erlenmeyer flask (3 L), then concentrated under reduced pressure (40 °C, 420 mmHg) into a 1 L flask. A 6.5 cm × 2.0 cm Teflon-coated elliptical stir bar stir bar is added to the 1 L flask containing the crude material, followed by EtOH (675 mL). The mixture is heated in a water bath to 80 °C with stirring. After 5 min at 80 °C, the flask is removed from the water bath. The solution is stirred, with precipitation of the product, until it reaches 23 °C. The resulting white solid is filtered through a medium porosity fritted filter funnel and transferred into a 250 mL round-bottomed flask. The solid is dried at 0.004 mmHg for 12 h to provide 16.4 g (70% yield) of bis((3aS,8aR)-3a,8a-dihydro-8H-indeno[1,2-d]oxazol-2-yl)methane.

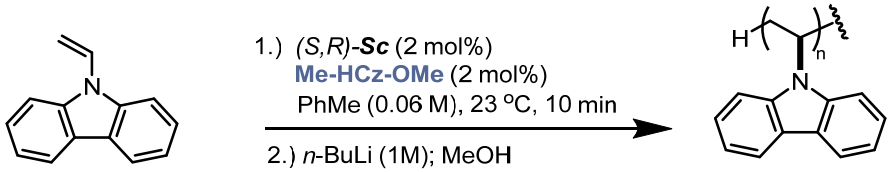
B. (3aS,3a'S,8aR,8a'R)-2,2'-(Cyclopropane-1,1-diyl)bis(3a,8a-dihydro-8H-indeno[1,2-d]-oxazole) (4) . A flame-dried 1-L three-necked round-bottomed flask equipped with a 3.5 x 1.5 cm Teflon-coated elliptical stir bar is fitted with a thermometer, a reflux condenser and a rubber septum. The system is connected to a continuous nitrogen flow and charged with 3 (14.9 g, 45 mmol, 1 equiv) and anhydrous THF (350 mL). The mixture is stirred at 0 °C in an ice bath for 15 min. Sodium hydride (5.4 g, 135 mmol, 3.0 equiv) is added to the resulting solution in five approximately equal portions over 5 min, and the reaction is stirred at 0 °C for 5 min at 700 rpm. n-propylbromide (135 mmol, 1.5 equiv) is added via syringe dropwise over 10 min. The reaction is removed from the ice bath and warmed to 23 °C, and then heated to 50 °C in an oil bath for 8 h. The reaction is removed from the oil bath and allowed to cool to 23 °C, then cooled to 0 °C with an ice bath. The septum is removed and the excess base is quenched by adding sat. NH4Cl (300 mL) over 30 sec. The reaction is diluted with water (200 mL) and the layers are separated. The aqueous layer is extracted with dichloromethane (2 x 300 mL), and the combined organic layers are dried with anhydrous sodium sulfate (150 g, stirred for 5 min). The solution is filtered over a plug of cotton into an Erlenmeyer flask (2 L) and then concentrated under reduced pressure (40 °C, 450-15 mmHg) into a 1 L flask. The crude material is loaded onto silica gel and separated with a 10 to 90% gradient EtOAc in hexanes to yield pure (3aS,3a'S,8aR,8a'R)-2,2'-(heptane-4,4-diyl)bis(3a,8a-dihydro-8H-indeno[1,2-d]oxazole) in 85% yield.

2.2.General Procedure for the In-situ Synthesis of Lewis Acid-BOX Complexes



To a 5-mL vial equipped with a magnetic stir bar in a glove box under inert atmosphere (N2) was added scandium triflate (25.9 µmol, 1 equiv.) and (3aS,3a'S,8aR,8a'R)-2,2'-(heptane-4,4-diyl)bis(3a,8a-dihydro-8H-indeno[1,2-d]oxazole) (31 µmol, 1.2 equiv.) and 0.5 mL of toluene to create a 0.0518 M solution. The suspension was stirred overnight at room temperature vigorously to yield a clear solution which was stored in a -40 °C glovebox freezer. No appreciable change in reactivity was noticed for up to a month, but with depreciating % mm values after 3 days. A significantly lower resulting isotacticity was observed when using lower purity metal triflates (e.g. 98% vs. 99.995%)

2.3. General Procedure for the Lewis Acid Catalyzed Polymerization of NVC



To a 5-mL vial equipped with a magnetic stir bar in a glove box under inert atmosphere (N_2) was added 9-(1-methoxyethyl)-9H-carbazole (1.17 mg, 5.18 µmol, 51.8 mM in PhMe, 100 µL), toluene (1.4 mL), and ligated Lewis acid-BOX complex (5.18 µmol, 51.8 mM in PhMe, 100 µL) and was allowed to stir vigorously for 5 minutes after which a solution of *N*-vinyl carbazole (50 mg, 258 µmol) in 0.5 mL of toluene was added. The reaction was quenched after 10 minutes with a stock solution of 1.0 M *n*-BuLi in hexanes, allowed to stir briefly, and a subsequent addition of dry MeOH. The solvent was removed under reduced pressure to yield crude polymer. The crude polymer was dissolved in 3 mL of dichloromethane and precipitated into MeOH two times to yield pure polymer and was analyzed by GPC and NMR for molecular weight, dispersity, and tacticity.

2.4. Tabulated Polymerization Data

Table S1: Tabulated Tacticity and GPC Data from Figure 3 and 8.

Initiator	T (°C)	[NVC]	mm %[a]	M_n (kDa)$_{RI}$	$Đ_{RI}$	[θ]
Me-HCz-OMe	23	0.12	90.6 ± 0.076	21.7	4.7	760
Me-HCz-OEt	23	0.12	87.5 ± 0.079	22.6	4.2	660
Me-HCz-OiPr	23	0.12	86.6 ± 0.072	21.5	4.9	500
Me-HCz-OtBu	23	0.12	85.7 ± 0.126	22.9	4.3	600
Me-HCz-OPh	23	0.12	85.5 ± 0.057	14.8	5.6	660
HCz-THF	23	0.12	89.5 ± 0.124	18.9	3.8	445
Me-HCz-O-(S)-Me^{S}Bu	23	0.12	88.9 ± 0.076[b]	26.2	4.3	740
Me-HCz-O-(S)-Me^{S}Bu	23	0.12	86.5 ± 0.076[c]	25.4	4.2	-240
Et-HCz-OMe	23	0.12	91	22.6	4.5	660
iPr-HCz-OMe	23	0.12	91	23.6	4.3	1040
tBu-HCz-OMe	23	0.12	91	25.8	3.3	480
Bn-HCz-OMe	23	0.12	91	23.0	4.5	950
cyPr-HCz-OMe	23	0.12	91	24.5	4.4	650
cyBu-HCz-OMe	23	0.12	91	28.2	4.2	1090
cyPn-HCz-OMe	23	0.12	91	25.3	4.2	850
Cy-HCz-OMe	23	0.12	91	28.5	4.1	680
Me-ClCz-OMe	23	0.12	91	20.1	4.8	1190
Me-BrCz-OMe	23	0.12	91	19.1	4.9	600
Me-tBuCz-OMe	23	0.12	91	20.6	4.4	640
Me-2naphCz-OMe	23	0.12	91	30.8	3.3	910
Me-OMeCz-OMe	23	0.12	91	28.9	3.5	510
Me-PhCz-OMe	23	0.12	91	21.2	4.5	750
Me-1-PhenCz-OMe	23	0.12	91	27.4	4.3	820
Me-4-PyrCz-OMe	23	0.12	91	24.0	4.6	820
α-chloroisobutylvinylether	23	0.12	73	2.1	3.7	--
Me-HCz-NEt2	23	0.12	--	--	--	--
thiophenol	23	0.12	--	--	--	--
H2O	23	0.12	87	12.5	4.8	--

[a]Tacticity was determined by ^{1}H-NMR in $C_2D_2Cl_4$ at 100 °C. [b](S,R)-indane ligand was utilized and [c](R,S)-indane was employed.

2.5. Pseudo-First Order Kinetics

The cationic polymerization of *N*-vinyl carbazole, facilitated by catalyst *(S,R)*-**Sc** and initiator **Me-HCz-OMe** may be represented as:

$$M + C \rightarrow P$$

Under the assumption that there are negligible side-reactions taking place in the formation of polymer (P), *N*-vinylcarbazole (M) will always be present in a large excess over the catalyst-initiator (C). As such, pseudo-first-order kinetics are valid for rate calculations. In this scenario, the following rate law applies:

$$d[P]/dt = k[M][C]_0 = k[M]$$

The integrated form of the rate equation is represented as:

$$\ln[M] = \ln[M]_0 - kt$$

This equation indicates that plotting -ln[M] versus t (s) should give a linear plot where k is equal to the slope of the line.

2.6. Kinetic Experiments and Data Analysis

The rate of *N*-vinylcarbazole conversion to polymer was analyzed by running individual reactions and quenching with ^{n}BuLi (method outlined in **2.3**) with subsequent ^{1}H-NMR analysis of the relative concentration of NVC and p(NVC). This method was required due to convoluted IR stretching frequencies of the vinyl group and resulting polymer absorbances and rapid rates preventing reliable measurements by taking aliquots. Basified MeOH solutions were ineffective at stopping polymerization due to rapid activation via (*S,R)*-**Sc** and subsequent Markovnikov addition to remaining monomer to yield **Me-HCz-OMe**.

The monomer concentration was determined using the following protocol. After quenching (*vide supra*), the reaction was allowed to warm to room temperature and all solvent was removed under reduced pressure to yield a crude reaction mixture of NVC and p(NVC), which was then completely dissolved in 1.0 mL of $CDCl_3$ to ensure a homogenous solution. 0.1 mL of the crude solution was added to 0.5 mL of $CDCl_3$ and analyzed via ^{1}H-NMR (ns = 16, delay = 4 seconds). The vinyl peak of *N*-vinyl carbazole (1H, 5.73-5.54 ppm) and three distinct aryl protons of the polymer (3H, 6.86-6.00 ppm) were integrated relative to one another to yield % conversion—assuming polymer was the sole product. Knowing the % conversion allowed for the calculation of the monomer concentration present immediately prior to quenching. Using an internal standard also gave results within 1% error of the method outlined above.

A total of five data points were typically used to calculate a pseudo first order rate constant (5, 10, 15, 20, and 30 seconds). Analysis of the stereoselective polymerization using *(S,R)*-**Sc** ([NVC] = 0.06 M, [*(S,R)*-**Sc**] = 0.0012 M, [**Me-HCz-OMe**] = 0.0012 M, in PhMe) were ran three times at each temperature disclosed. The data points plotted below and in **Figure 4** are the average of the three runs, with the standard error (S.E. = σ/Σ_n, where Σ_n = # of runs (3)) added above and below.

Table S2: Tabulated Kinetics Data

T (°C)	Time (s)	Conv % (run1)	Conv % (run2)	Conv % (run3)	Average Conv.	Average -ln(nvc)	STD Error
-20	5	8.8	1.8	2.3	4.30	2.906	0.000
-20	10	13.4	3.6	4.4	4.01	2.957	0.000
-20	15	19.4	5.3	6.2	10.30	3.029	0.000
-20	20	23.3	5.9	6.7	11.98	3.079	0.000
-20	30	37.7	9.6	8.1	18.46	3.287	0.000
					rate	0.007	0.003
0	5	12.2	11.8	14.4	12.83	2.951	0.008
0	10	18.7	22.0	21.5	20.73	3.046	0.011
0	15	30.4	25.7	29.0	28.36	3.147	0.016
0	20	35.6	36.1	36.5	36.06	3.261	0.003
0	30	44.2	44.8	44.6	44.58	3.404	0.003
					rate	0.018	0.000
23	5	29.2	33.9	38.0	33.69	3.226	0.032
23	10	42.9	52.6	56.5	50.68	3.527	0.065
23	15	59.2	66.7	69.0	64.93	3.868	0.067
23	20	67.1	74.1	78.1	73.11	4.141	0.096
23	30	72.5	87.0	85.5	81.63	4.565	0.190
					rate	0.064	0.003
-10	5	6.6	11.2	16.3	11.38	2.935	0.026
-10	10	15.6	18.9	18.9	17.80	3.010	0.011
-10	15	23.0	25.4	30.0	26.14	3.117	0.023
-10	20	29.6	31.3	34.0	31.63	3.194	0.015
-10	30	39.2	42.2	44.8	42.08	3.360	0.023
					rate	0.017	0.000
10	5	21.3	26.5	31.3	26.40	3.121	0.032
10	10	27.7	42.9	43.9	38.16	3.301	0.067
10	15	36.8	58.8	58.8	51.46	3.557	0.117
10	20	42.4	63.7	64.9	57.00	3.684	0.131
10	30	59.5	72.5	74.6	68.87	4.002	0.118
					rate	0.035	0.004
5	5	15.0	18.3	19.5	17.61	3.007	0.013
5	10	32.1	33.8	31.9	32.62	3.208	0.007
5	15	41.3	43.5	38.6	41.14	3.344	0.020
5	20	47.4	52.9	45.5	48.59	3.481	0.036
5	30	58.5	60.6	62.1	60.40	3.740	0.022
					rate	0.029	0.000

Kinetic data was collected for the alkyl based initiators shown in Figure 3 to probe the effect of initiator structure on rates of polymerization. Under our working hypothesis, a decrease in rate would increase selectivity if conformer equilibration is unaffected. However, since we observe a decrease in rate and selectivity going from -OMe to -OtBu, it suggests a large decrease in ΔG between chain-end stereoisomers or a decrease in ΔG‡ for conformer equilibration potentially arising from the separated ion-pair and increased bulk around the alkoxy portion of the anion. The large difference in k_{obs} between -OMe and the other substitutions could also arise from a change in the rate determining step, as described in Figure 4B.

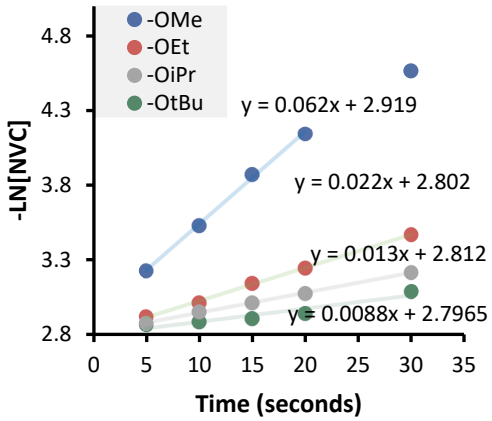


Figure S1: Pseudo 1st-order kinetic plot with increasing sized alkoxy anions during polymerization of NVC, [NVC] = 0.06, 23 °C, PhMe. The last data point for -OMe is not included in regression due to its high conversion.

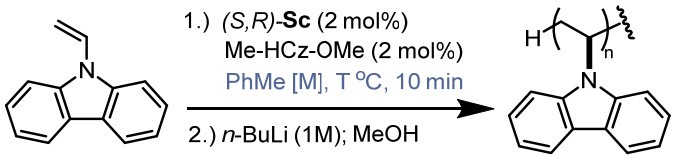
2.7. Eyring Data

Polymers were prepared under the conditions outlined in Figure 5B with various monomer concentrations and temperatures ranging from 0.06 to 0.24 M and -20 to 23 °C. The resulting polymer was precipitated twice from DCM into MeOH and dried overnight under vacuum. % *mm* was analyzed by VT-NMR at 100 °C (ethylene glycol temperature standard) in d_4-tetrachloroethane in the methine backbone region. This was done in triplicate and the summary of results are outlined below.

The % *mm* values were transformed to % *m* using the Bovey formalism—assuming chain-end control.

$$(eq\ 1.) \qquad \%\, m = \sqrt{(\%\, mm)}$$

Table S3: Tabulated Eyring Data



	[NVC]	% *m*	standard error
23 °C	0.24	93.9	0.2
	0.12	95.2	0.1
	0.06	95.7	0.1
0 °C	0.24	94.8	0.1
	0.12	96.2	0.2
	0.06	96.6	0.2
-20 °C	0.24	95.9	0.1
	0.12	96.9	0.1
	0.06	97.2	0.1

Representative stacked ^{1}H-NMR of methine region where triads are displayed for samples ran at 23 °C normalized by their % *mr/rr* peak.

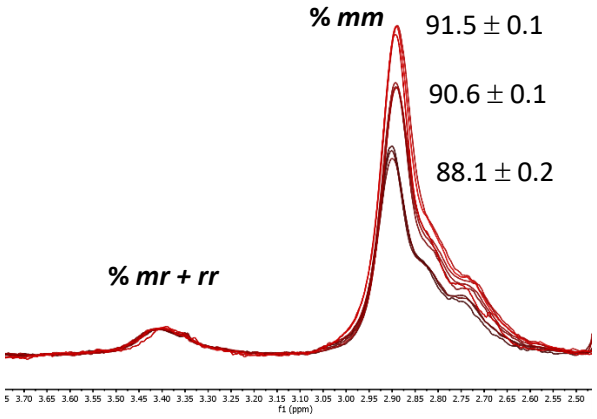


Figure S2: ^{1}H-NMR at 100 °C in $C_2D_2Cl_4$ of isotactic poly(NVC)

Extrapolating the Eyring data to effective zero monomer concentration presumably is the ΔG between pro-*meso* and pro-*racemo* conformations and illustrate the highly selectivity of this process.

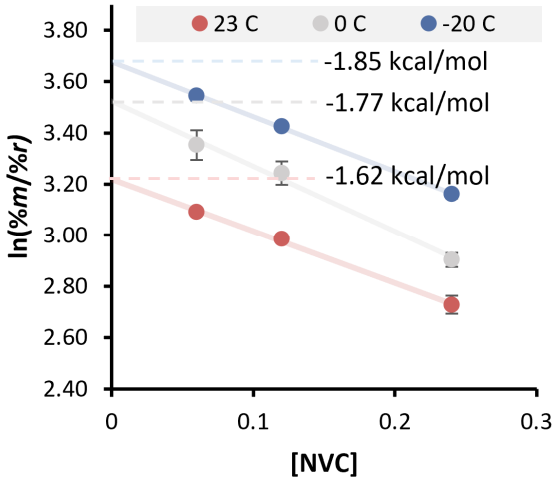


Figure S3: Concentration dependent Eyring plot with extrapolated energy differences at [0.00] effective monomer concentration.

For example, at -20 ºC and 0.06 M a selectivity of 97.2 %*m* is measured which correlated to a Gibbs free energy value of -1.78 kcal/mol which is 0.07 kcal/mol from the expected thermodynamic selectivity of -1.85 kcal/mol. Therefore at low monomer concentrations, the system is put under a Curtin-Hammett scenario where the thermodynamics of ground state energy between pro-meso and pro-racemo determine selectivity.

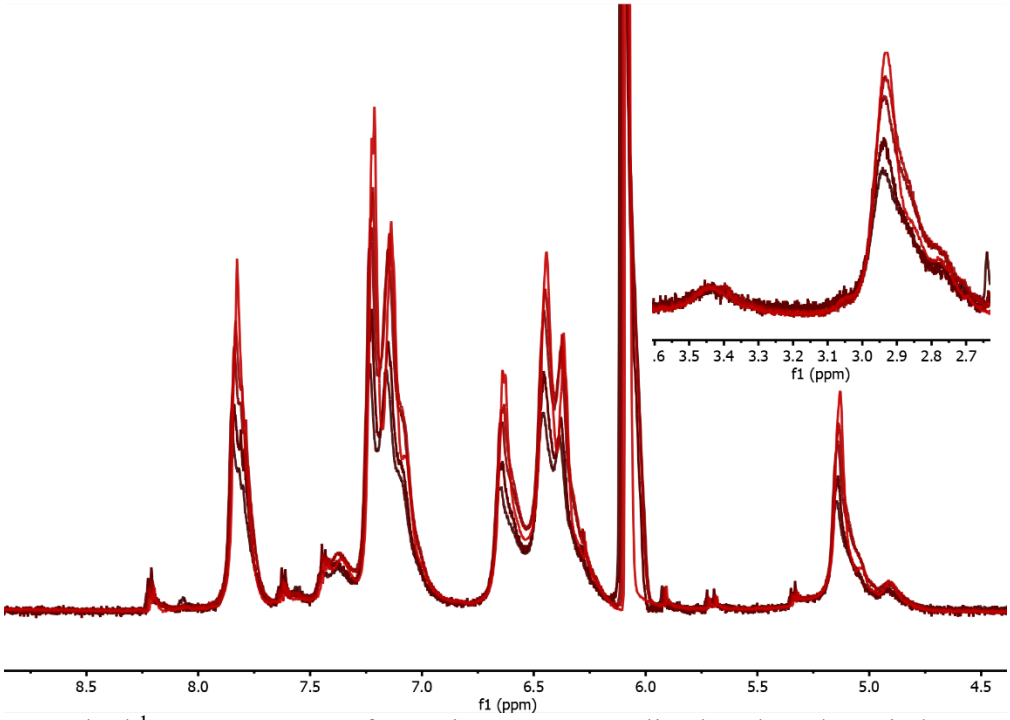


Figure S4: Stacked ^{1}H-NMR spectra from Figure 5a normalized to the rr/mr triad at 3.45.

2.8. Tri-deuteration Experimentation

d_3-*N*-vinylcarbazole was polymerized and purified under the standard conditions outlined in section 2.3. Due to the lack of backbone protons, VT-^{1}H-NMR could not be used to quantify tacticity; however, ^{13}C-NMR in $C_2D_2Cl_4$ can be used to resolve the triad sequences. Due to the significant chemical shift between *meso* and *racemo* triads and their broadness, no clear C-D coupling is observed and was assumed to be inconsequential to quantifying % *mm*. Qualitatively, the deuterated polymer was more soluble, less crystalline/brittle, and fluffier which is consistent with other lower isotactic samples. To achieve satisfactory SNR, 8192 scans were required.

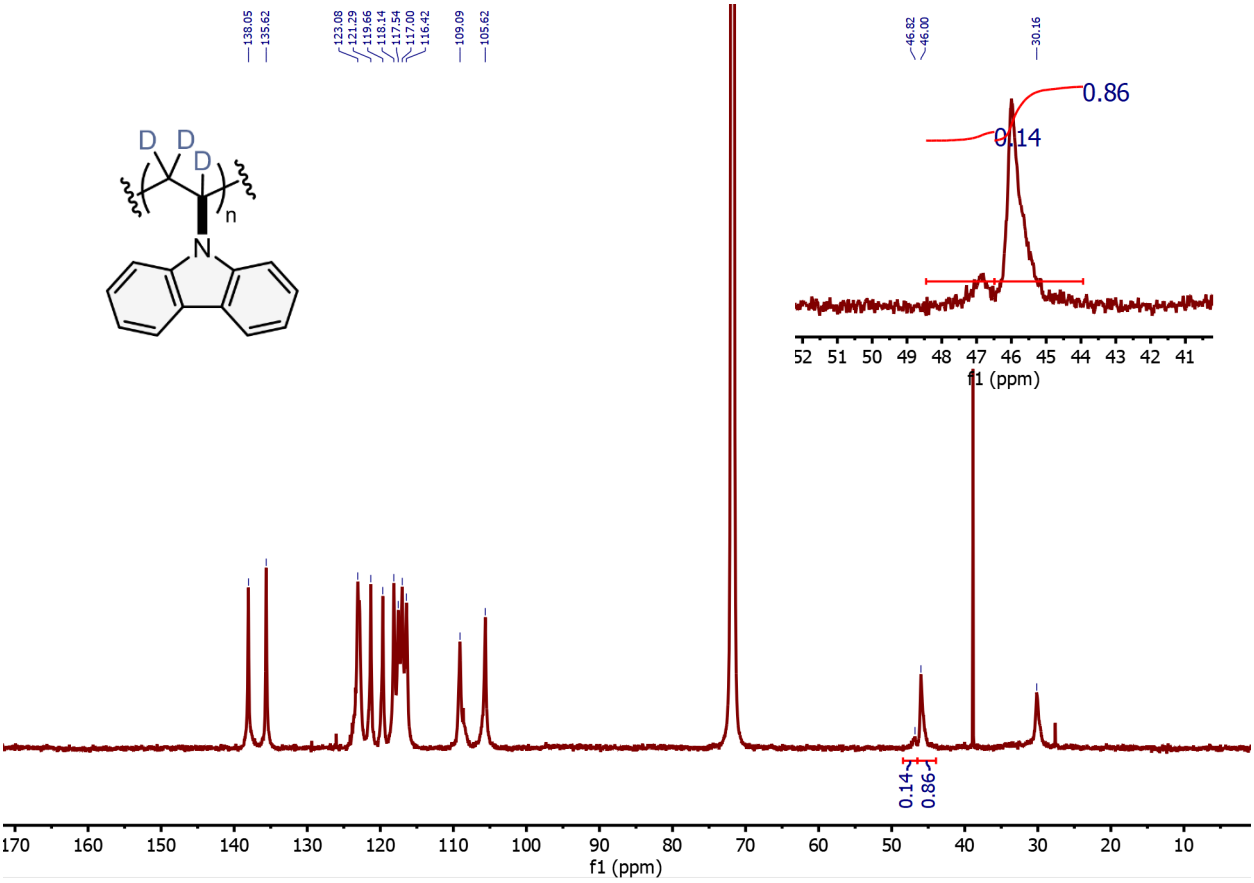


Figure S5: ^{13}C-NMR of poly(d_3-NVC) in $C_2D_2Cl_4$

A maximum KIE can be estimated for three inverse alpha and two inverse beta interacting deuteriums in the transition state based off known lower bounds[9]:

$$KIE \sim 2^{3(0.5)-2(0.38)} = 0.2$$

Since a KIE could not be measure from kinetic experiments due to its rapid rate (e.g. >90% at 5 seconds) we estimated it using the tacticity (selectivity) data measured. %*mm* values were

converted to %*m* using the Bovey relationship below, so that a two-state model could be approximated.

$$\% \boldsymbol{m} = \sqrt{(\% \boldsymbol{mm})}$$

$$\sqrt{(86\%\, mm)} = 92.7\%\, m$$

At [0.12]M of d_3-NVC and a reaction temperature of 23 °C a value of 92.7% *m* (vida supra) is obtained. Assuming pseudo-first order kinetics is maintained after deuteration and the rate of conformation is the same, we can claim under our hypothesis of competing stereoselectivity:

$$if, \qquad \%\boldsymbol{m_H} \propto \frac{\boldsymbol{k_{conf}}}{\boldsymbol{k_{p,H}[NVC]}}$$

$$then, \qquad \%\boldsymbol{m_D} \propto \frac{\boldsymbol{k_{conf}}}{\boldsymbol{k_{p,D}[d_3NVC]}}$$

Where $\%m_{H/D}$ is the percent meso diads and $k_{p,H/D}$ is the rate of polymerization for the protonated and deuterated monomers.

$$therefore, \qquad \%\boldsymbol{m_H} * \boldsymbol{k_{p,H}} * [\boldsymbol{NVC}] = \%\boldsymbol{m_D} * \boldsymbol{k_{p,D}} * [\boldsymbol{d_3NVC}]$$

$$if, \qquad \%\boldsymbol{m_H} = \%\boldsymbol{m_H}$$

$$then, \qquad \frac{\boldsymbol{k_{p,H}}}{\boldsymbol{k_{p,D}}} = \frac{[\boldsymbol{d_3NVC}]}{[\boldsymbol{NVC}]}$$

Therefore, since the value for the d_3-NVC monomer at [0.12] M is 92.7% *m* and a value of 93% *m* for the NVC monomer is found at [0.36] M:

$$\boldsymbol{KIE} \cong \frac{\boldsymbol{k_{p,H}}}{\boldsymbol{k_{p,D}}} \cong \frac{\boldsymbol{[0.12]}}{\boldsymbol{[0.36]}} = \boldsymbol{0.33}$$

An approximate KIE of 0.33 can be measured.

2.9. 3,6-di-tert-butyl-*N*-vinylcarbazole Experiments

3,6-di-tert-butyl-*N*-vinylcarbazole was utilized as a control monomer, and was synthesized using reported procedures,[10] where the tert-butyl groups function as a conformational lock and prevent facile chain-end conformer flipping. The monomer was polymerized using optimized condition in section 2.3, but substituting the monomer structure. While quantitative tacticity has not been assigned for this monomer, the atactic controls TfOH and $Sc(OTf)_3$ have the same stereomicrostructure as that disclosed by Aoshima and company[11] and matches that polymerized with (*S,R*)-**Sc**—indicating also an atactic structure.

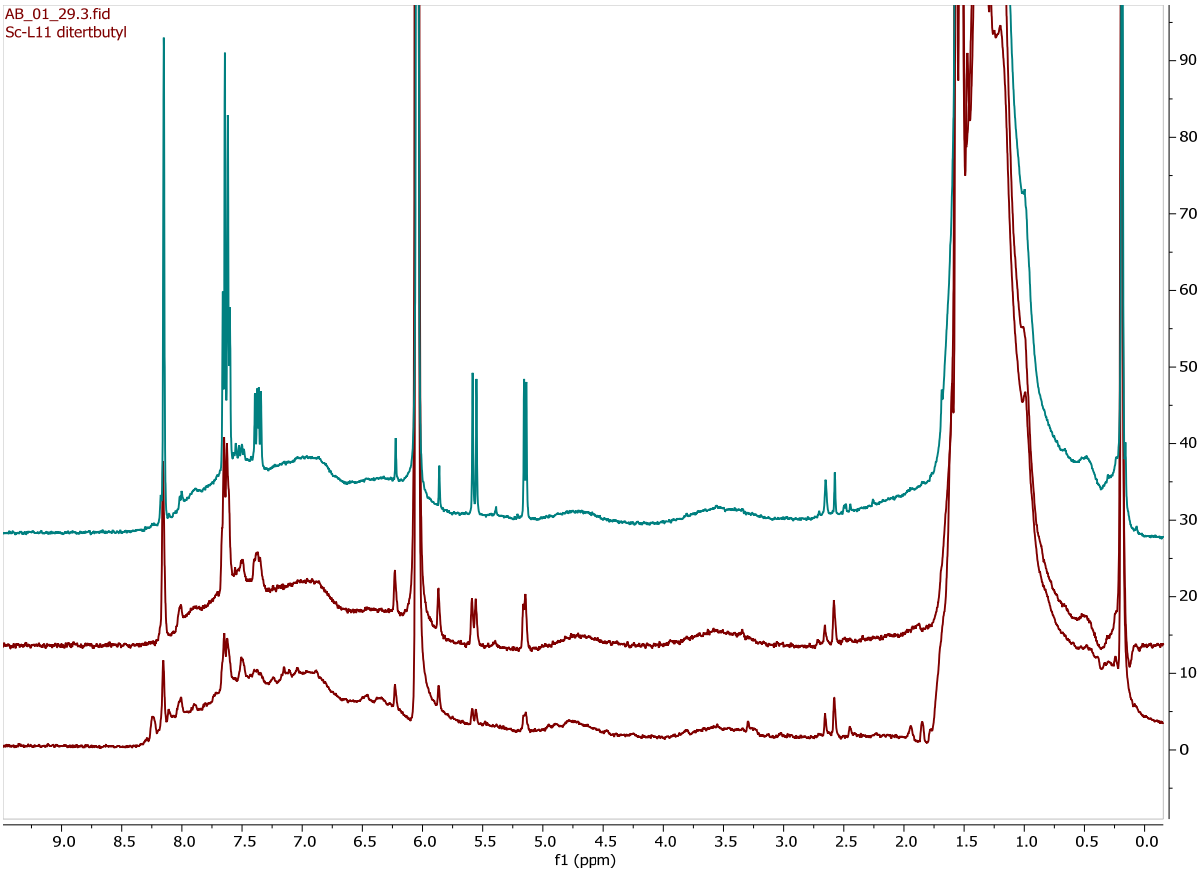
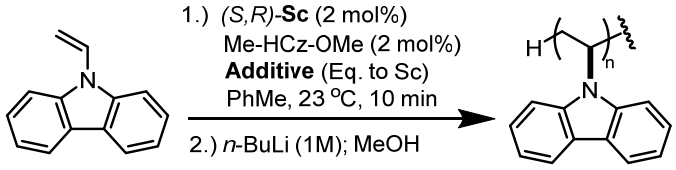


Figure S6: ^{1}H-NMR of poly(tBu-NVC) in $C_2D_2Cl_4$ prepared with TfOH, $Sc(OTf)_3$, and (S,R)-**Sc** from top to bottom respectively. Monomer is observed in each polymerization even though no additional conversion is observed after 1 minute. Residual monomer provided conversion.

2.10. Additive-Counterion Experiments

Additives were tested that are known to undergo anion exchange with M-Cl to yield M^+X^- of X with non-coordinating character. Exchanging for triflate harmed the isotaticty in every case. Interestingly, using three equivalents of $NaBArF_{24}$ with $Sc(OTf)_3$ led to a syndioselective polymerization with a % *mm* of 18%.

Table S4: Additive/Counter-ion effects on tacticity.



Sample # [a]	Additive	ScX_3	% *mm*	Conv. (%)
1	--	$ScCl_3$	**--**	< 1
2	$NaBArF_{24}$ (3 eq)	$Sc(OTf)_3$	**18**	>99
3	$NaBArF_{24}$ (3 eq)	$ScCl_3$	**33**	>99
4	$AgPF_6$ (3 eq)	$ScCl_3$	**54**	>99
5	$NaBArF_{24}$ (1 eq)	$Sc(OTf)_3$	**80**	>99
6	$NaBArF_{24}$ (1 eq)	$ScCl_3$	**24**	44[b]
7	TMSCl (3 eq)	$Sc(OTf)_3$	**91**	>99%

[a] 23 °C, S,R-Indane Box ligand, Toluene [0.12], 10 mins; [b] 24 hrs

2.11. Circular Dichroism

Samples were prepared in filtered tetrahydrofuran at 0.1 mg/mL and measured from 250 to 450 nm at a path length of 1 mm. mdeg values were converted to molar ellipticity using polymer molecular weight attained from high-temperature GPC—which ranged from 19 kDa to 23 kDa.

The mixing time of catalyst *(S,R)*-**Sc** and **Me-HCz-OMe** was changed from 0, 1, 5, 30, and 120 minutes before the addition of monomer solution and an enrichment of CD response was observed upon isolation of the resulting polymer, providing a temporal handle for the control of helicity. While the chirality of the initiator is ablated upon formation of the prochiral iminium species, we expect there may be memory effects that arise from the slow diffusion of the catalyst anion to the other enantioface of the initiator.

One rational for their reactivity digressing from that of Me-HCz-OMe, is due to the strong withdrawing nature of the 3,6-dibromo substitution of Me-BrCz-OMe destabilizing the proposed intermediate iminium promoting elimination and formation of MeOH and an enamine. Likewise, **iPr-HCz-OMe** can form a tertiary carbocation after 1,2-hydride shift that is primed for ring closure to a 5-membered ring and formation of MeOH—which can further initiate a helically unselective polymerization (Figure S6). These data highlight the importance of optimizing each initiator individually, as complex degradation, thermodynamic, and kinetic pathways possibly lead to a large temporal dependence on the pre-mixing phase and helical response.

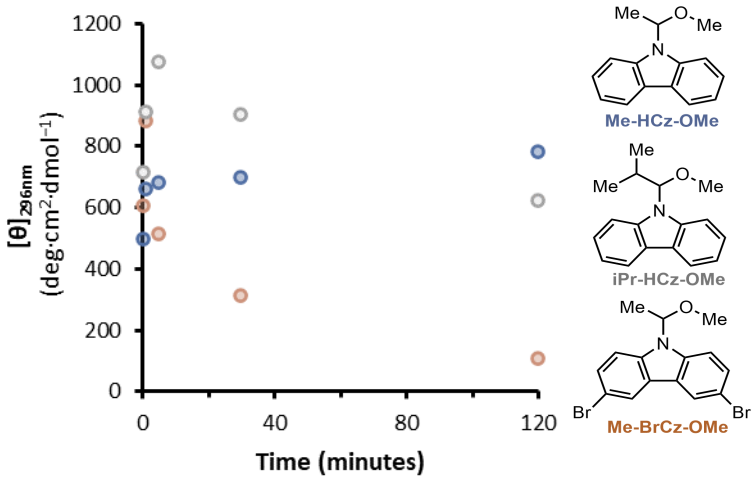


Figure S7: Relationship between catalyst-initiator pre-mix time and resulting polymer CD response. Polymerization was carried out at 23 ºC under optimized conditions ([NVC] = 0.06 M, [(S,R)-Sc] = 1.2 mM, [hemiaminal] = 1.2 mM), quenched, and polymer purified before being analyzed by CD in THF.

2.12. Initiation of Polymerization by Lewis Acid Activation of Brønsted Acids

During our investigation we found polymerization can be initiated by the addition of simple alcohols, carboxylic acids, and water. We hypothesize this occurs from the Lewis acid activation of the Brønsted acids and subsequent protonation of an equivalent of *N*-vinylcarbazole. When MeOH is used to quenched the reaction a low reaction time ~5 seconds there is >99% conversion of monomer and significant formation of **Me-HCz-OMe**—otherwise not observed when quenched with alkyl lithium.

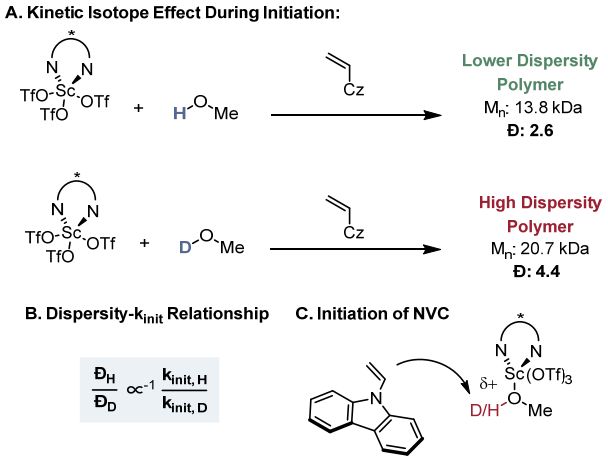


Figure S8: Overview of Lewis acid activation of Bronsted acids for in-situ initiator generation

When initiating with MeOH the same tacticity is observed as with **Me-HCz-OMe**, but a much lower dispersity is measured (~4 vs. ~2), which indicates protonation of NVC with [Sc]-HOMe is significantly faster than ionization of **Me-HCz-OMe.** To confirm the initiation is

occurring through a protic mechanism, the reaction was initiated with MeOD and a large increase in dispersity now observed when compared to initiation with MeOH. The dispersity increases since protonation is slower due to a positive KIE; this is due to the relative rate of initiation to propagation changing.

This mechanism was leveraged to generate [Sc]-O**R** for **R-**groups that were not synthetically accessible, e.g. R = -OPh.

3. Computational Work

3.1. Density Functional Theory Considerations and Experimentation

The calculations shown in this work were performed using the Gaussian 16 package.[12] All ground state structures were optimized using the B3LYP[13] approximate exchange-correlation energy density functionals with the basis set def2-SVP[14] and cpcm(toluene)[15] solvent model unless otherwise noted. Grimme's D3 correction was used.[9] All optimizations used the default ultrafine grid size unless otherwise stated. Vibrational analyses were performed to ensure intermediates had no imaginary frequencies. Grimme-type quasi-harmonic (150 cm-1) Gibb's free energies were estimated at 298 K using the Autoqchem and GoodVibes packages.[10] Renderings like in Figure 7C were done using Cylview.[16]

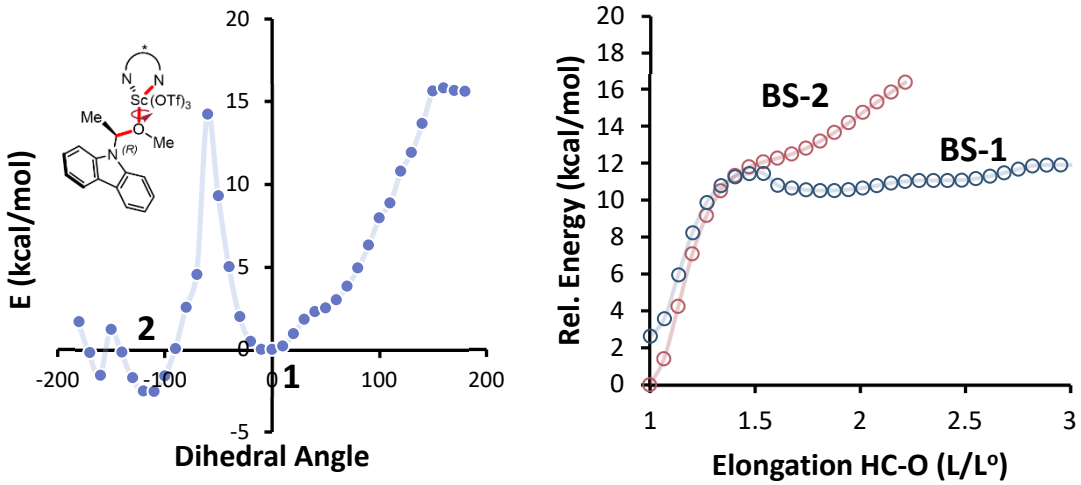


Figure S9: Conformational space of **Me-HCz-OMe –** *(S,R)*-**Sc** complex.

A dihedral scan of the tbu-NVC dimer shown in Figure 7B was carried out at the b3lyp-d3/def2-tzvp/cpcm(PhMe) level of theory with a integral=superfine in order to probe the relative conformer energies of the chain-end.[1] Discontinuities arise from -tBu group rotations required for full rotation. -H data is from a previous report.[1]

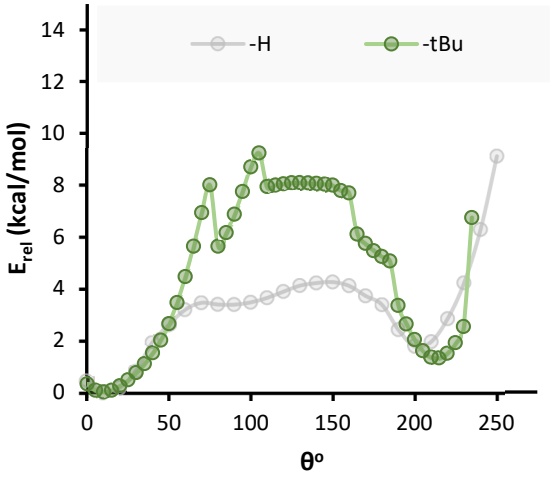


Figure S10: Difference in energy (kcal/mol) for the relaxed dihedral scan probing conformer flipping.

Additionally, ground state optimization with a truncated catalyst (substi. nPr groups for Me to reduce conformational freedom) of the pro-*meso* and pro-*racemo* conformers were carried out and a ΔG = 3.37 kcal/mol was measured which is 1 kcal/mol smaller, or 77%, than was reported for unsubstituted *N*-vinylcarbazole dimer with the same catalyze.[1]

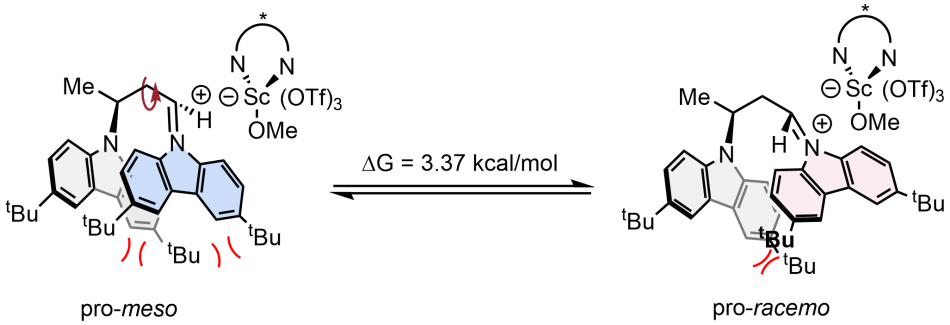


Figure S11: Delta Gibb's Free Energy between two chain-end conformers

Table S5: Tabulated DFT thermodynamic values for each diastereomeric pair of initiators with *(S,R)*-**Sc**.

Initiator	Structure	E	ZPE	H	T.S	T.qh-S	G(T)	qh-G(T)	qh-G(T) kcal/mol	ΔG(R-S) kcal/mol
Et-HCz-OMe	R-SR	-5546.7875	0.776019	-5545.9471	0.162588	0.147879	-5546.1097	-5546.095	-3480174.613	**1.506**
	S-SR	-5546.7903	0.776001	-5545.9499	0.161607	0.147524	-5546.1115	-5546.0974	-3480176.119	
Me-BrCz-OMe	R-SR	-10654.618	0.72791	-10653.824	0.166658	0.151055	-10653.991	-10653.976	-6685369.94	**1.882**
	S-SR	-10654.62	0.727941	-10653.826	0.169008	0.152923	-10653.995	-10653.979	-6685371.823	
Me-ClCz-OMe	R-SR	-6426.7086	0.729115	-6425.9146	0.163813	0.149068	-6426.0784	-6426.0636	-4032354.909	**1.945**

	S-SR	-6426.7108	0.729143	-6425.9158	0.166147	0.150929	-6426.0819	-6426.0667	-4032356.854	
Me-HCz-OMe	R-SR	-5507.4544	0.747903	-5506.6434	0.160973	0.146011	-5506.8043	-5506.7894	-3455510.349	**0.69**
	S-SR	-5507.4562	0.747909	-5506.6452	0.159212	0.145295	-5506.8044	-5506.7905	-3455511.039	
Me-OMeCz-OMe	R-SR	-5736.6003	0.81121	-5735.7217	0.168383	0.153264	-5735.8901	-5735.8749	-3599261.5	**1.129**
	S-SR	-5736.6016	0.811394	-5735.7221	0.169771	0.154579	-5735.8919	-5735.8767	-3599262.629	
Me-4-PyrCz-OMe	R-SR	-6737.0826	1.130893	-6735.8686	0.200884	0.181634	-6736.0694	-6736.0502	-4226871.501	**0.251**
	S-SR	-6737.0837	1.131314	-6735.8694	0.199929	0.18116	-6736.0694	-6736.0506	-4226871.752	
Me-tBuCz-OMe	R-SR	-5822.1054	0.968264	-5821.0637	0.182266	0.164557	-5821.246	-5821.2283	-3652820.758	**-0.251**
	S-SR	-5822.1068	0.96856	-5821.0651	0.178694	0.162837	-5821.2438	-5821.2279	-3652820.507	
Me-2-NaphCz-OMe	R-SR	-6277.1567	1.012482	-6276.0677	0.187844	0.170034	-6276.2555	-6276.2377	-3938339.157	**1.255**
	S-SR	-6277.1592	1.012687	-6276.0701	0.186996	0.169623	-6276.2571	-6276.2397	-3938340.412	
Me-2-NaphFCz-OMe	R-SR	-7667.004	0.898688	-7666.0152	0.218221	0.196154	-7666.2335	-7666.2114	-4810547.654	**1.443**
	S-SR	-7667.0066	0.898724	-7666.0179	0.217416	0.195816	-7666.2353	-7666.2137	-4810549.097	
S-sBu-HCz-OMe	R-SR	-5625.4393	0.845118	-5624.5285	0.16302	0.149295	-5624.6915	-5624.6778	-3529485.32	**-5.208**
	S-SR	-5625.4335	0.846625	-5624.5219	0.159854	0.147518	-5624.6818	-5624.6695	-3529480.111	
tBu-HCz-OMe	R-SR	-5625.4339	0.832028	-5624.5354	0.16606	0.151226	-5624.7015	-5624.6866	-3529490.842	**-4.644**
	S-SR	-5625.4284	0.832315	-5624.53	0.161863	0.149162	-5624.6919	-5624.6792	-3529486.198	
iPr-HCz-OMe	R-SR	-5586.10811	0.803557	-5585.238717	0.164947	0.150214	-5585.403664	-5585.388931	-3504831.554	**-6.169**
	S-SR	-5586.1138	0.816953	-5585.2326	0.159197	0.146556	-5585.3918	-5585.3791	-3504825.385	
Me-PhCz-OMe	R-SR	-5969.7517	0.905904	-5968.7743	0.177045	0.160753	-5968.9514	-5968.9351	-3745506.775	**1.508**
	S-SR	-5969.753628	0.905995	-5968.775348	0.178577	0.162155	-5968.953925	-5968.937503	-3745508.283	

4. NMR Spectra

(2a) 3,6-di-tert-butyl-9-(1-methoxyethyl)-9H-carbazole

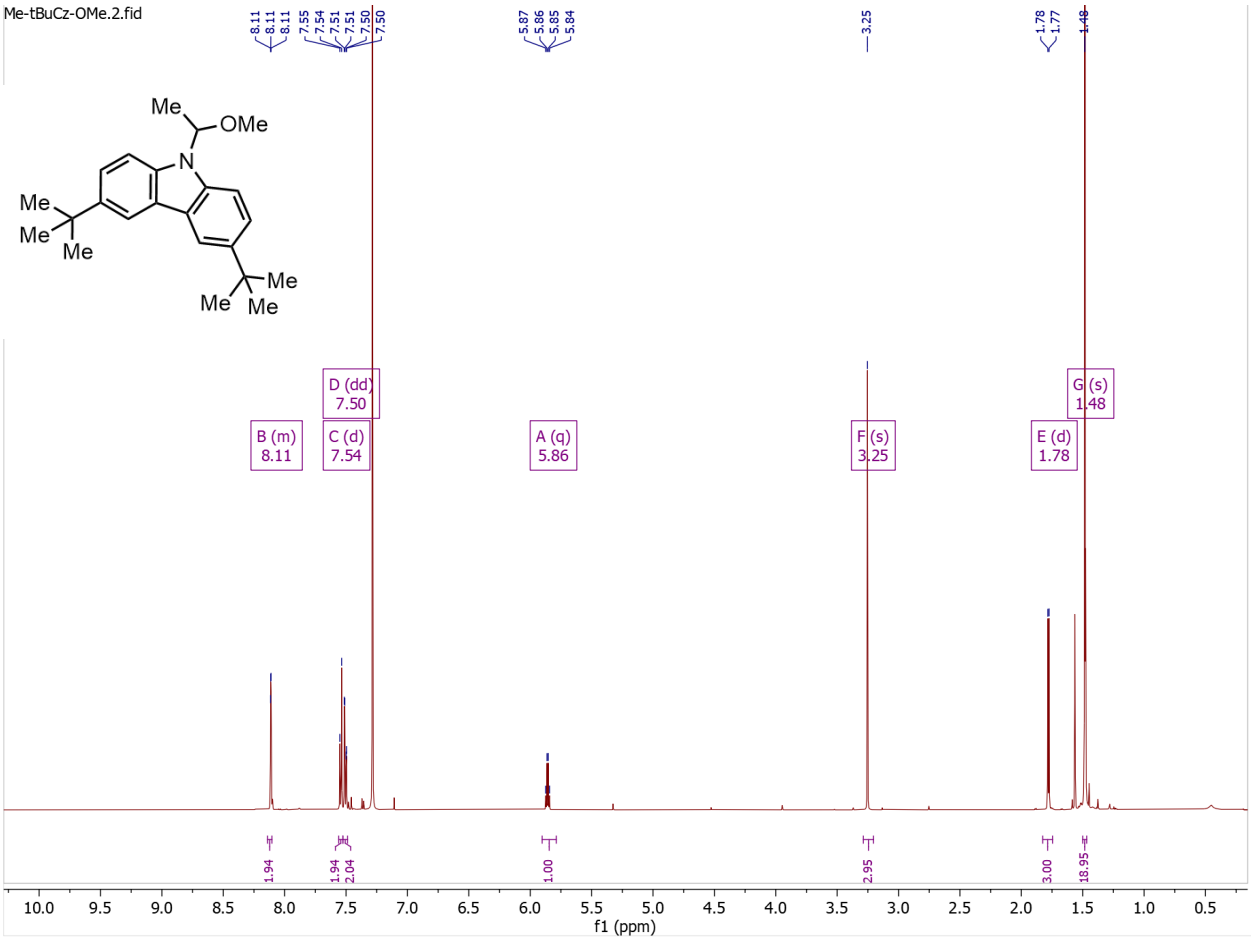


Figure S12: 3,6-di-tert-butyl-9-(1-methoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

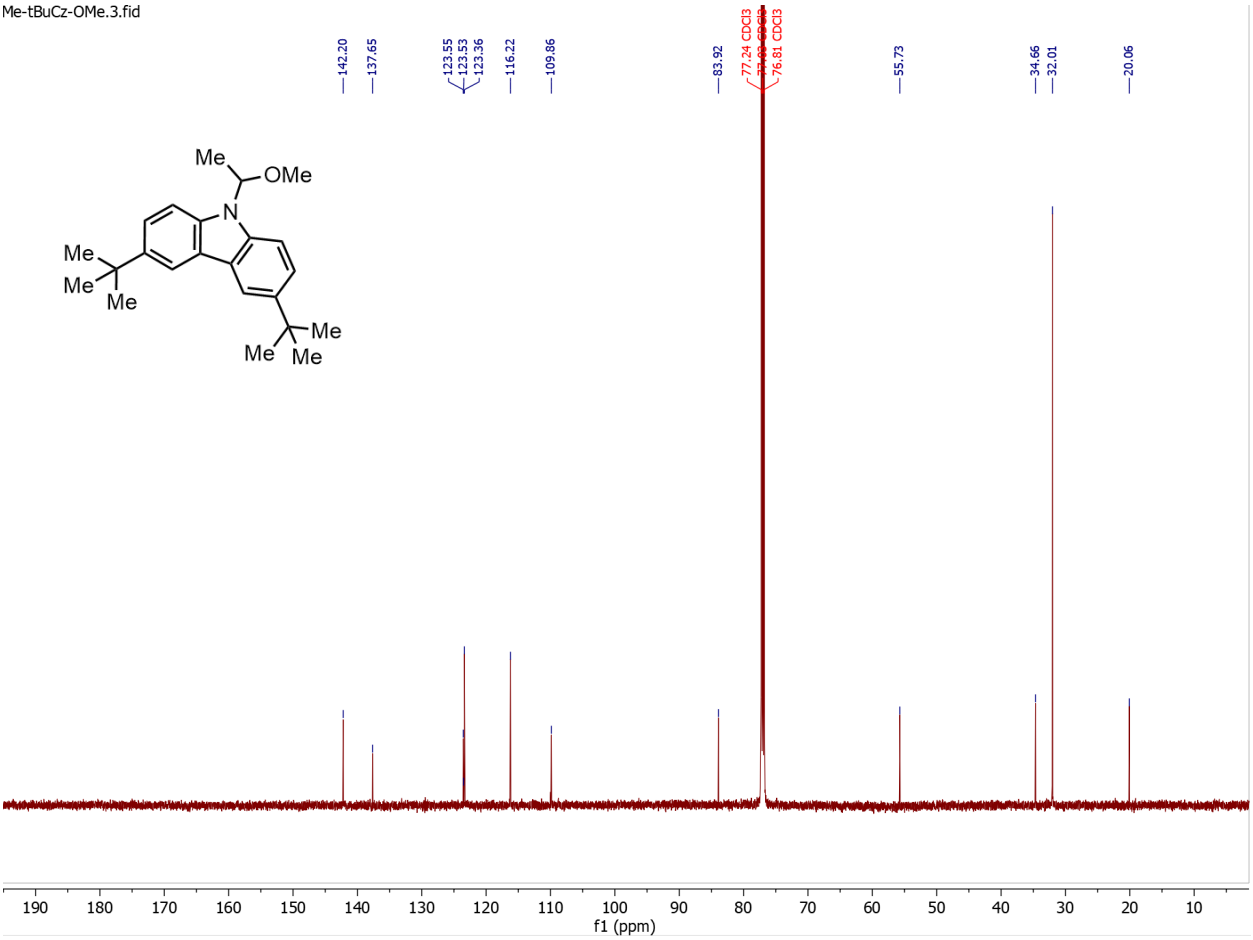


Figure S13: 3,6-di-tert-butyl-9-(1-methoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(2b) 3,6-dichloro-9-(1-methoxyethyl)-9H-carbazole:

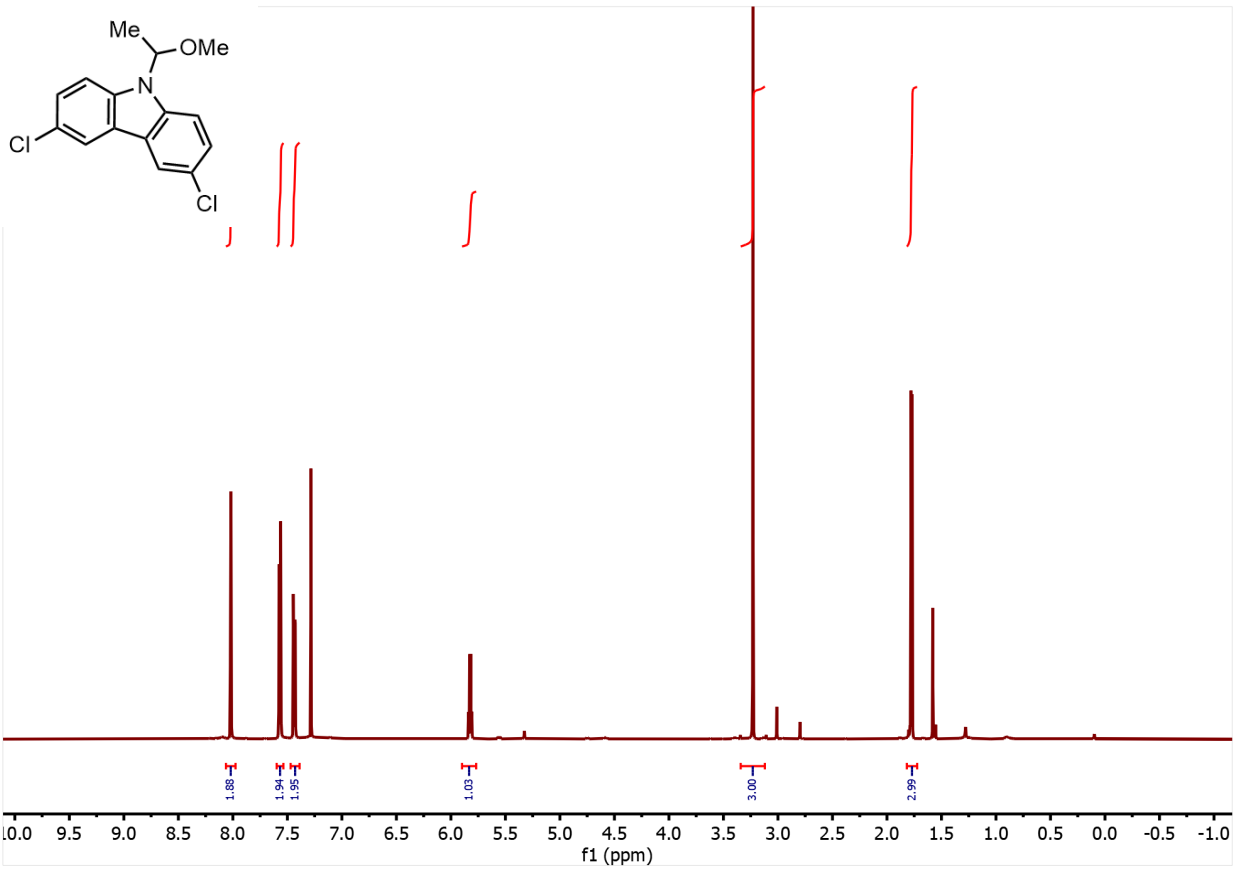


Figure S14: 3,6-dichloro-9-(1-methoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

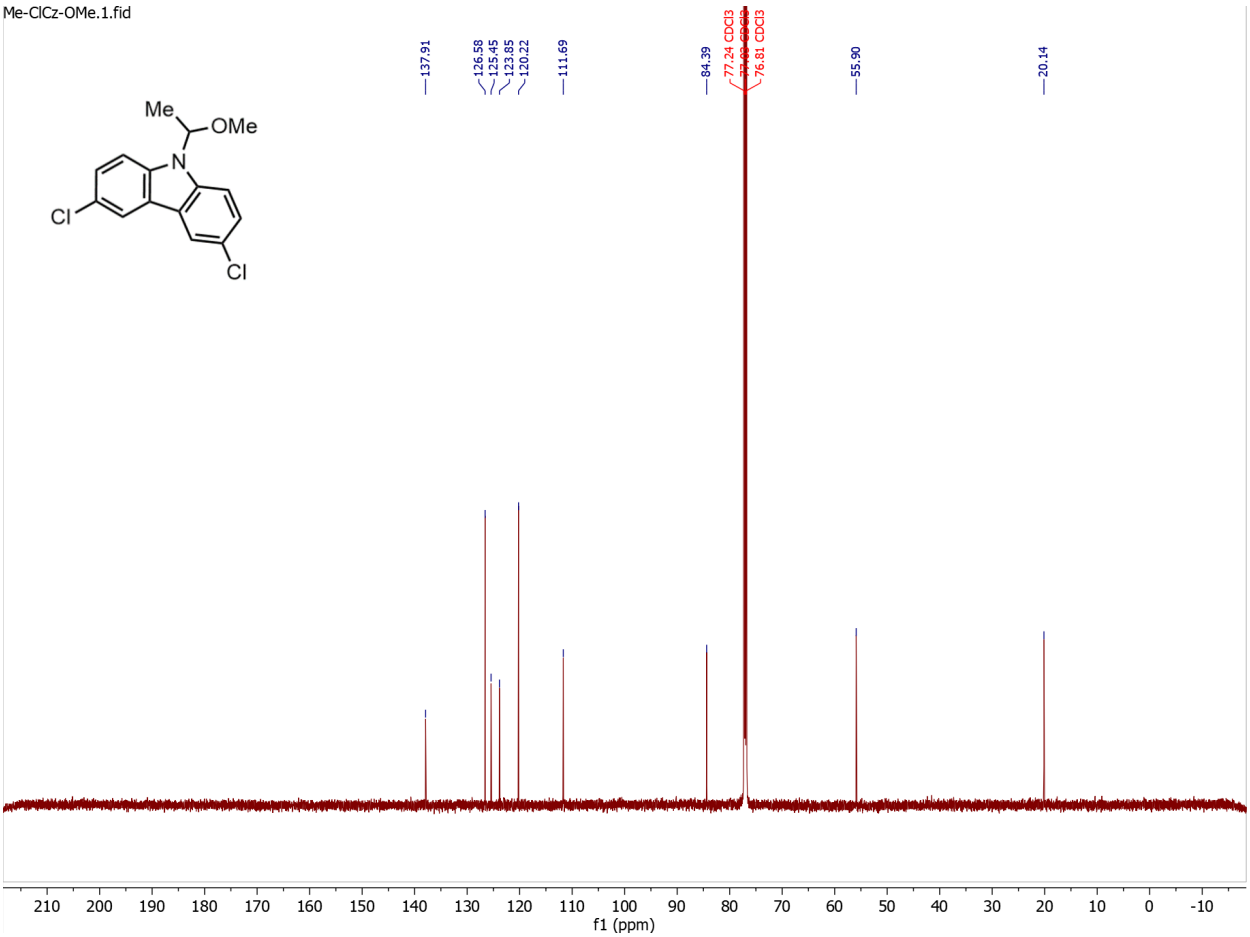


Figure S15: 3,6-dichloro-9-(1-methoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(2c) 3,6-dibromo-9-(1-methoxyethyl)-9H-carbazole:

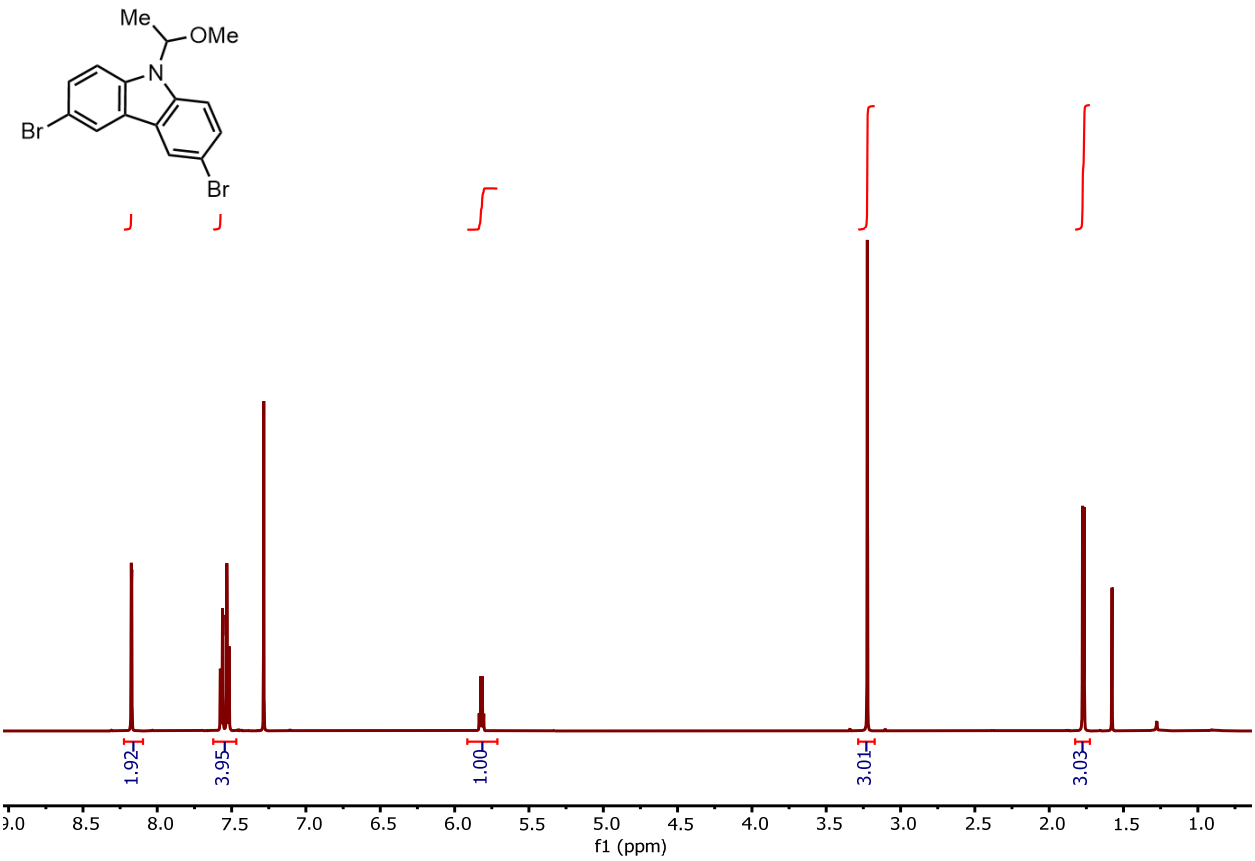


Figure S16: 3,6-dibromo-9-(1-methoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

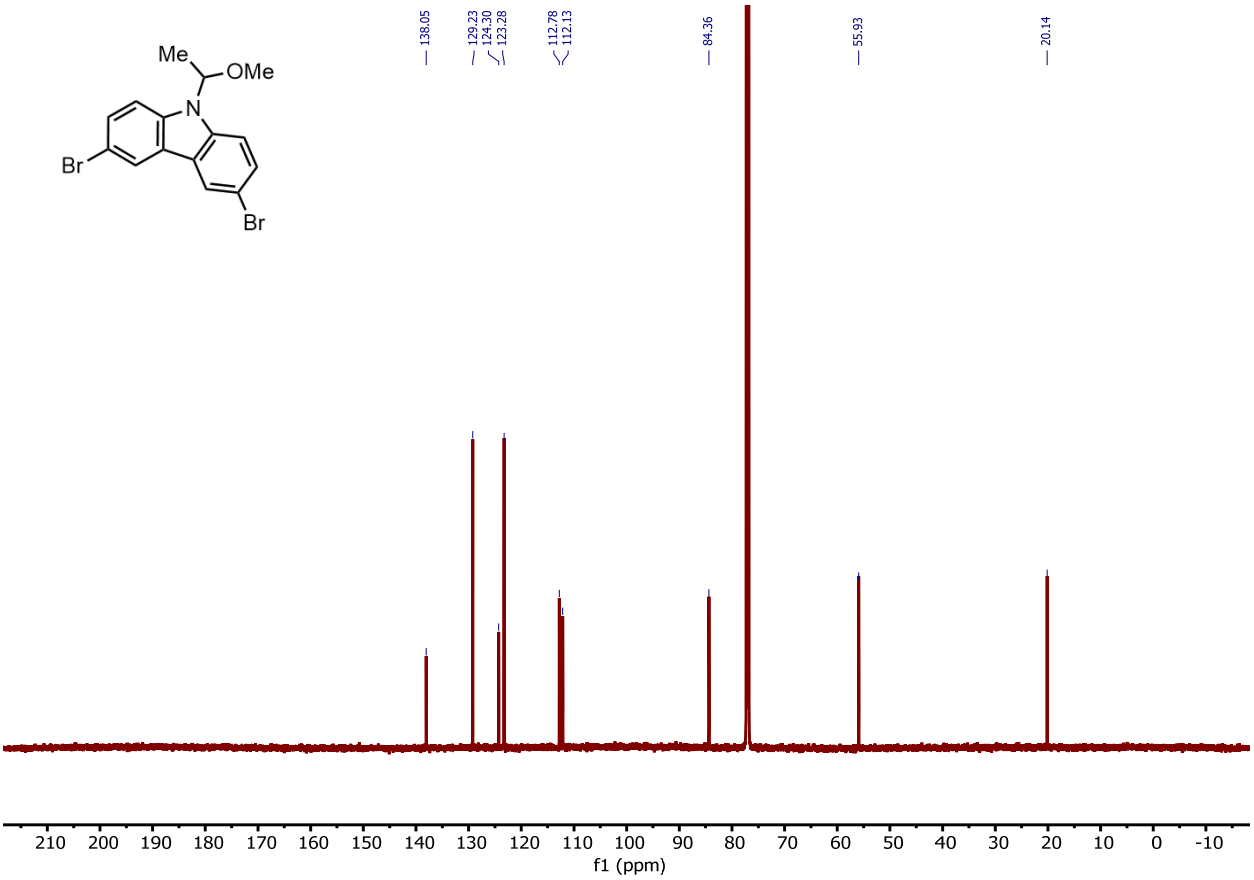


Figure S17: 3,6-dibromo-9-(1-methoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(2d) 9-(1-methoxyethyl)-3,6-diphenyl-9H-carbazole:

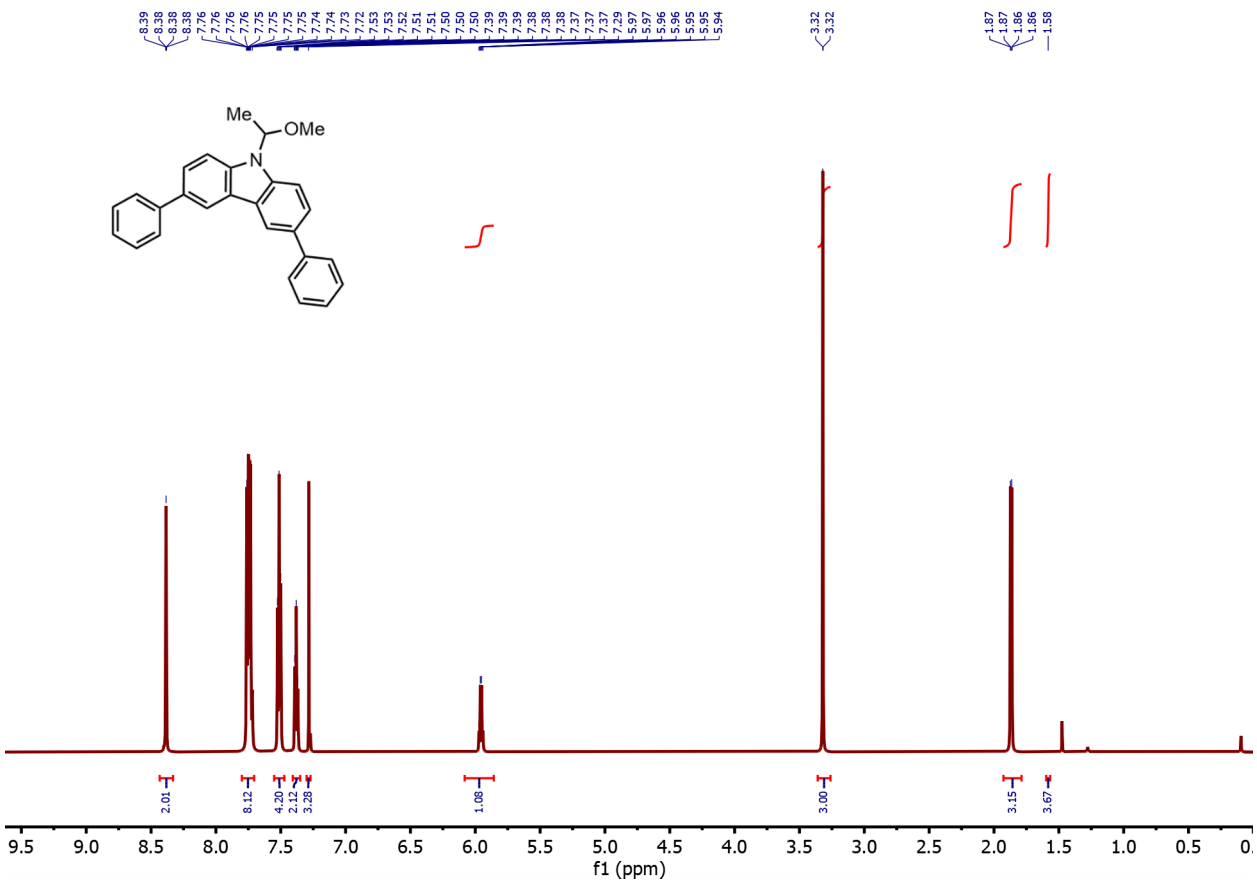


Figure S18: 9-(1-methoxyethyl)-3,6-diphenyl-9H-carbazole ^{1}H-NMR in $CDCl_3$

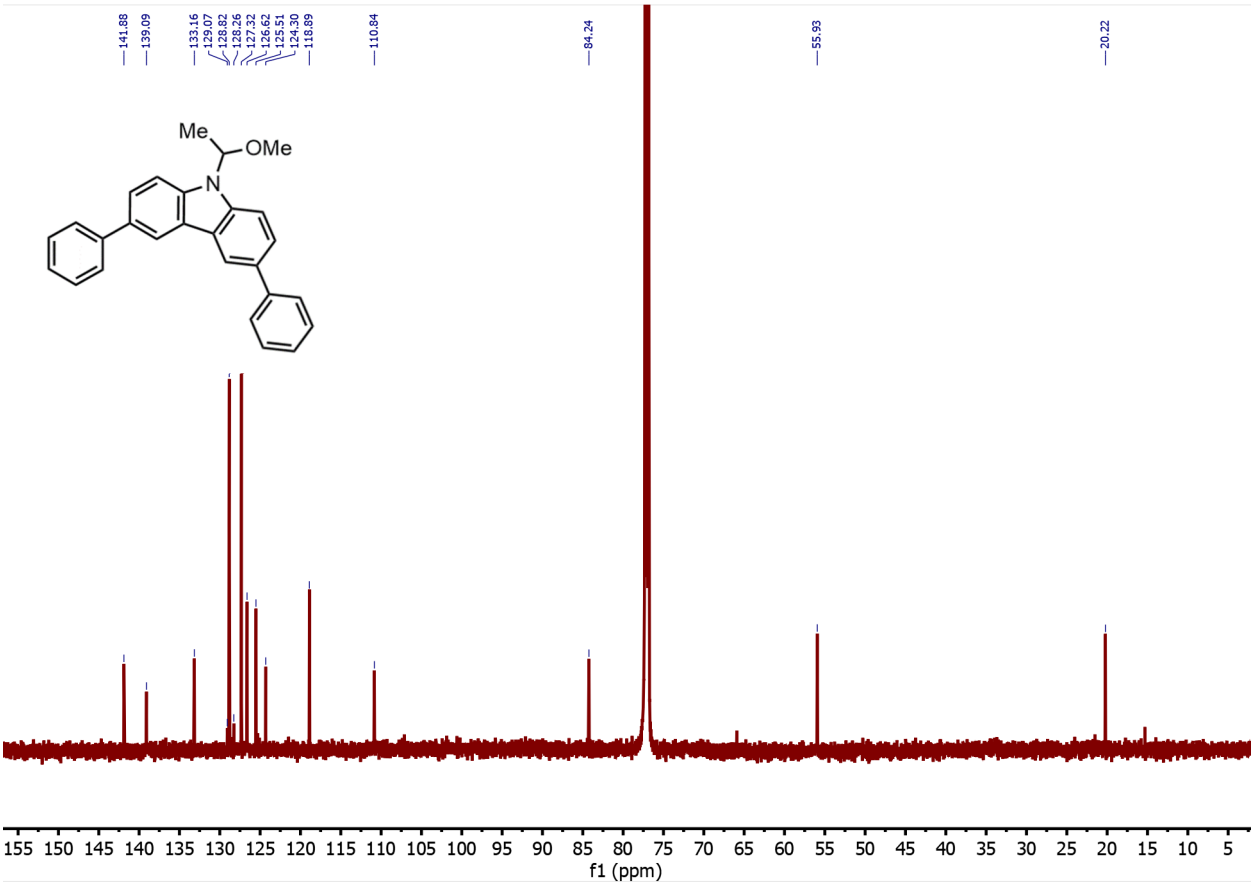


Figure S19: 9-(1-methoxyethyl)-3,6-diphenyl-9H-carbazole ^{13}C-NMR in $CDCl_3$

(2f) 9-(1-methoxyethyl)-3,6-di(phenanthren-9-yl)-9H-carbazole:

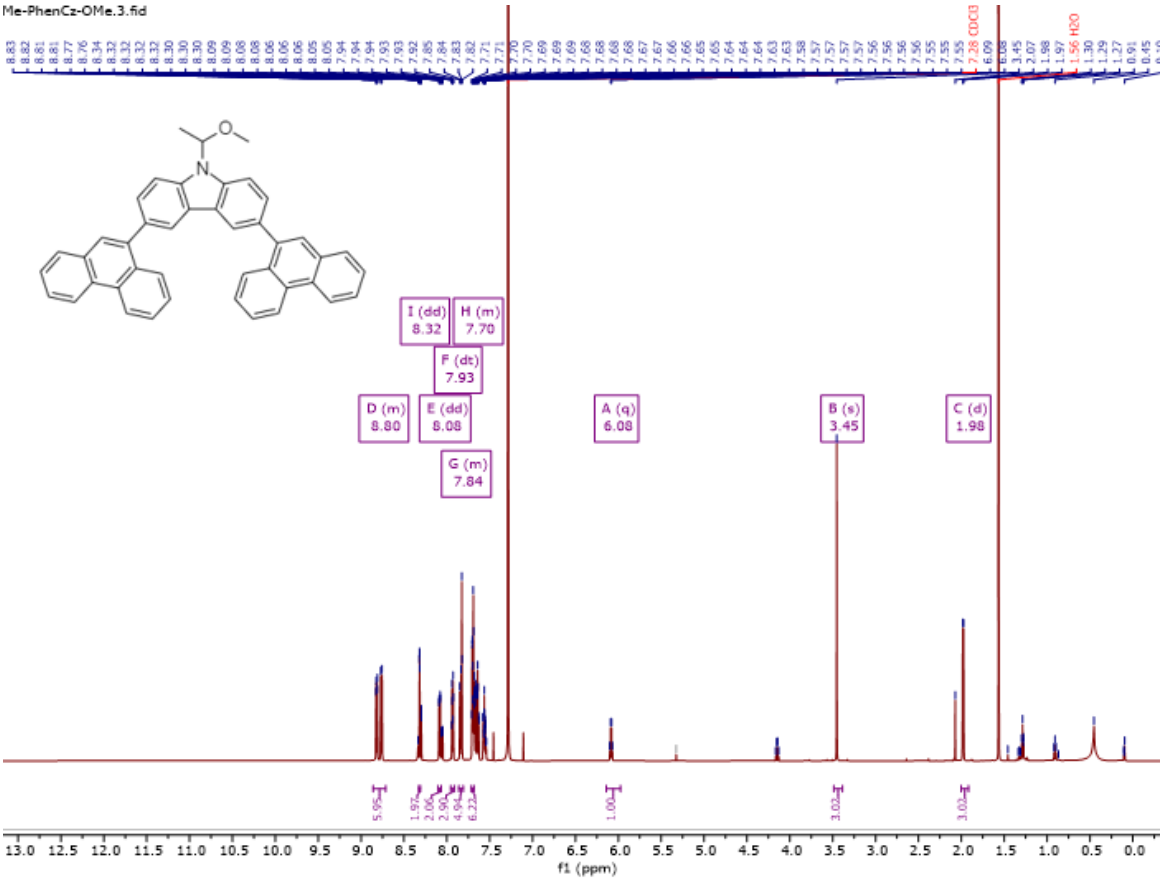


Figure S20: 9-(1-methoxyethyl)-3,6-di(phenanthren-9-yl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

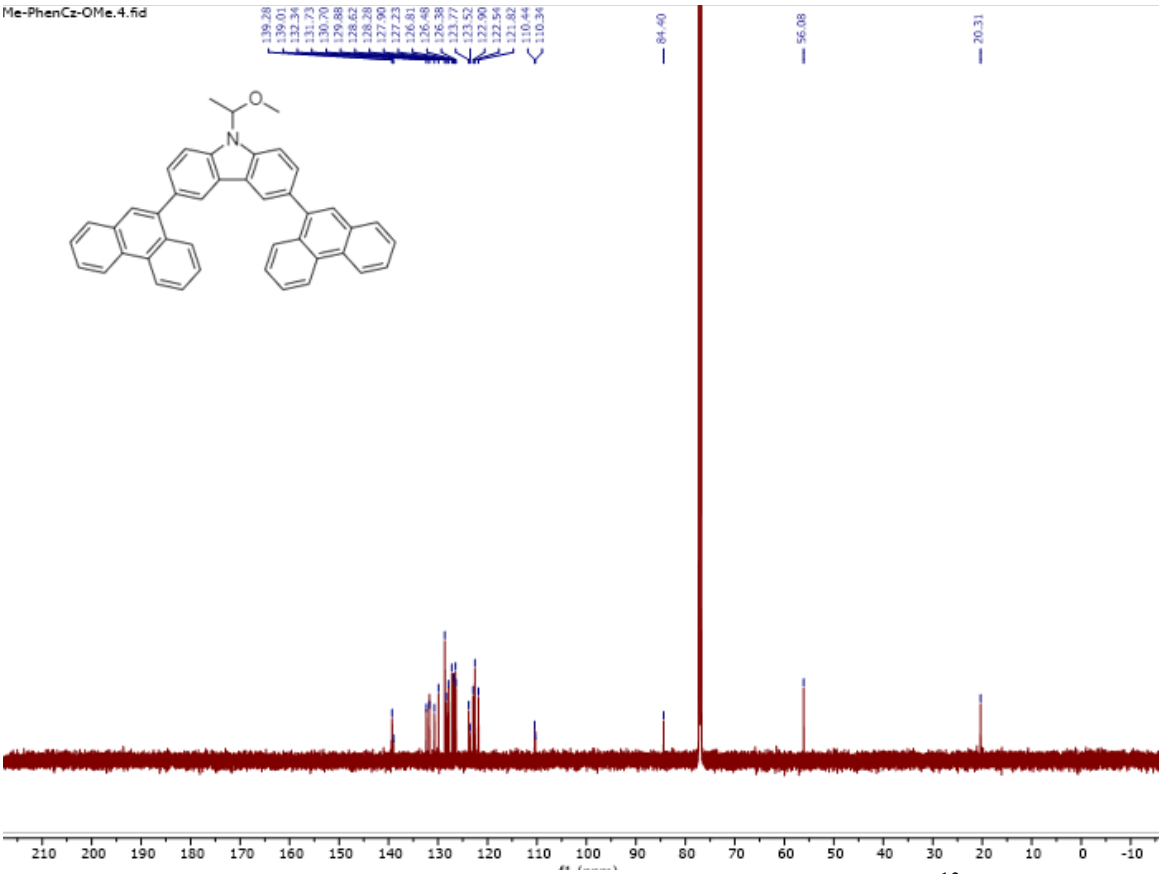


Figure S21: 9-(1-methoxyethyl)-3,6-di(phenanthren-9-yl)-9H-carbazole ^{13}C-NMR in $CDCl_3$. *Grease unable to be removed.

(2g) 9-(1-methoxyethyl)-3,6-di(pyren-1-yl)-9H-carbazole:

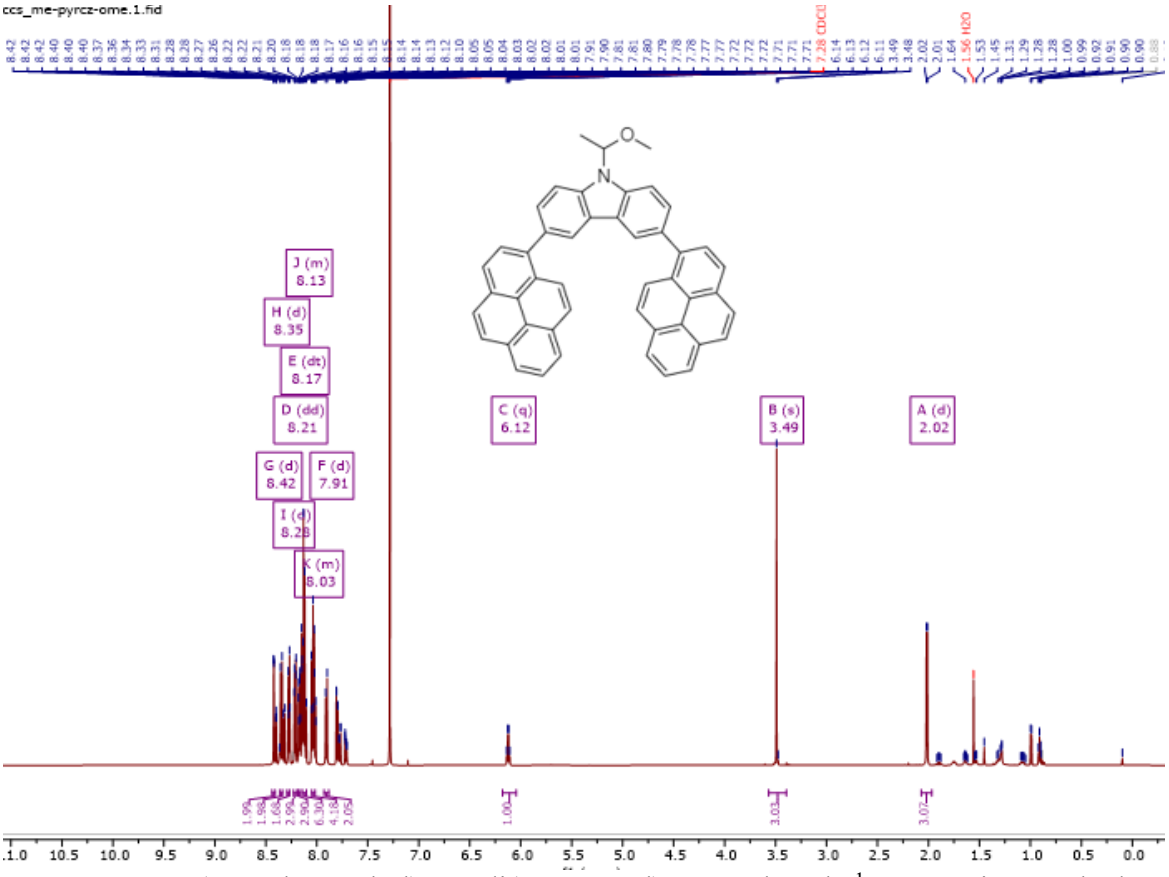


Figure S22: 9-(1-methoxyethyl)-3,6-di(pyren-1-yl)-9H-carbazole ^{1}H-NMR in $CDCl_3$. *Grease unable to be removed.

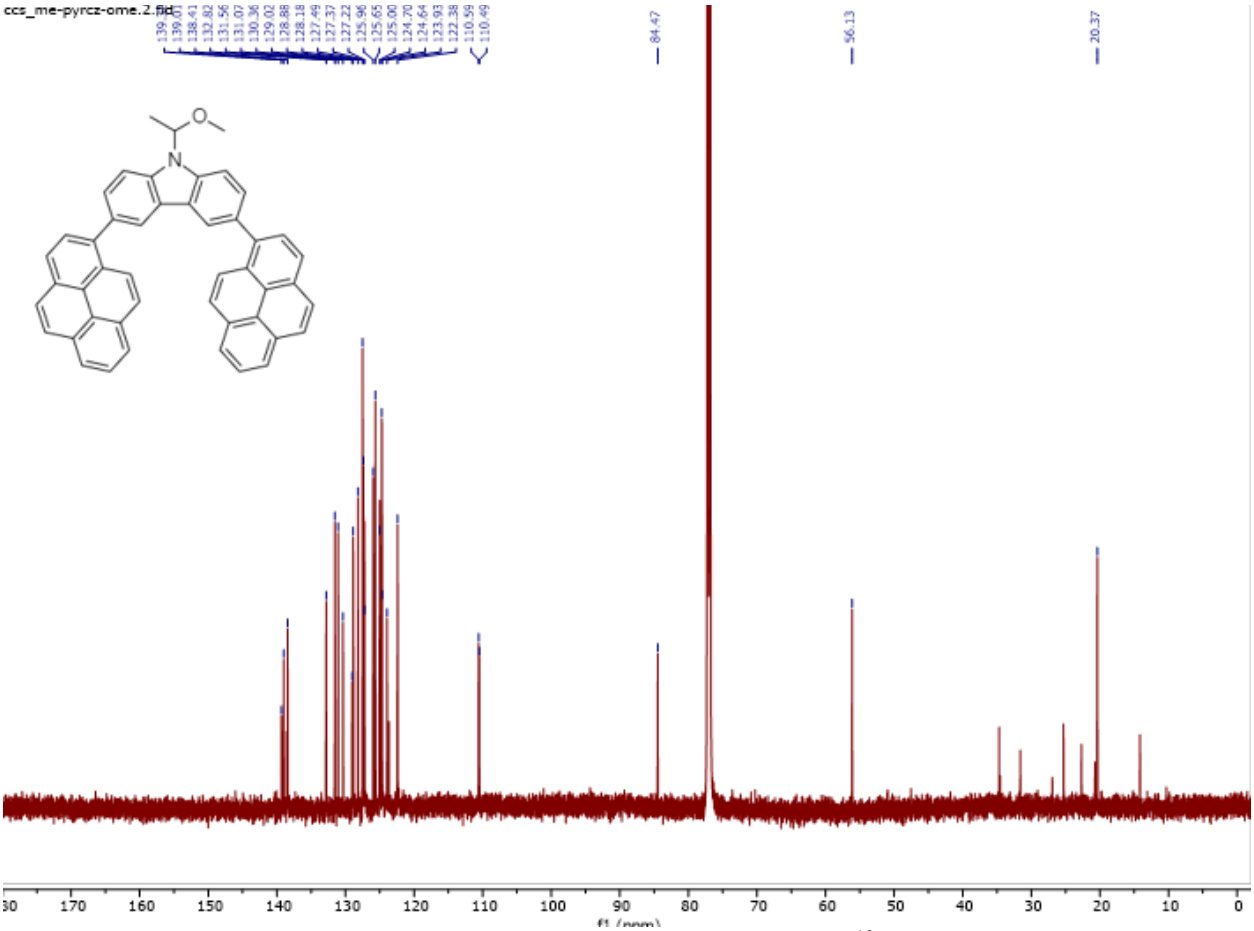


Figure S23: 9-(1-methoxyethyl)-3,6-di(pyren-1-yl)-9H-carbazole ^{13}C-NMR in $CDCl_3$. *Grease unable to be removed.

(2h) 3,6-dimethoxy-9-(1-methoxyethyl)-9H-carbazole

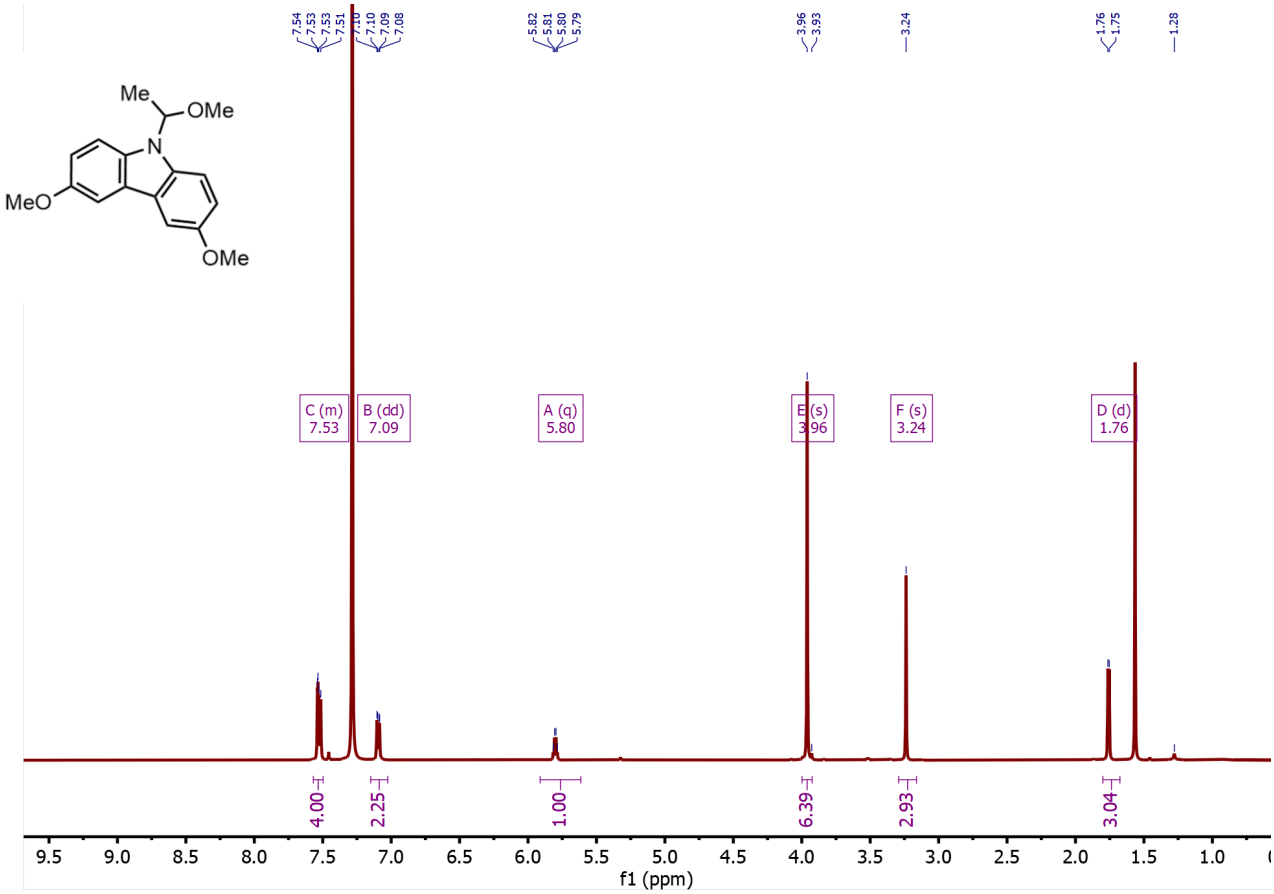


Figure S24: 3,6-dimethoxy-9-(1-methoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

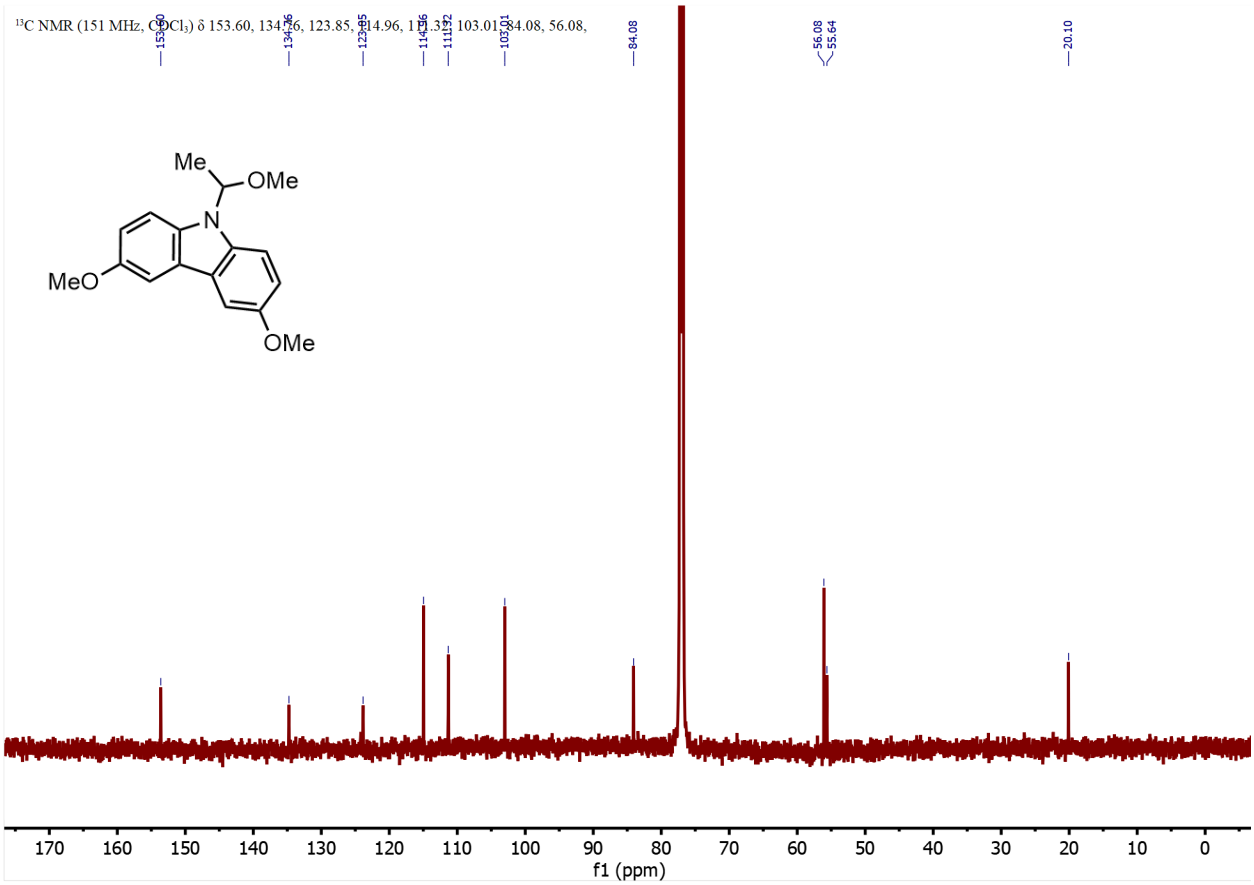


Figure S25: 3,6-dimethoxy-9-(1-methoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(3a) 9-(1-ethoxyethyl)-9H-carbazole:

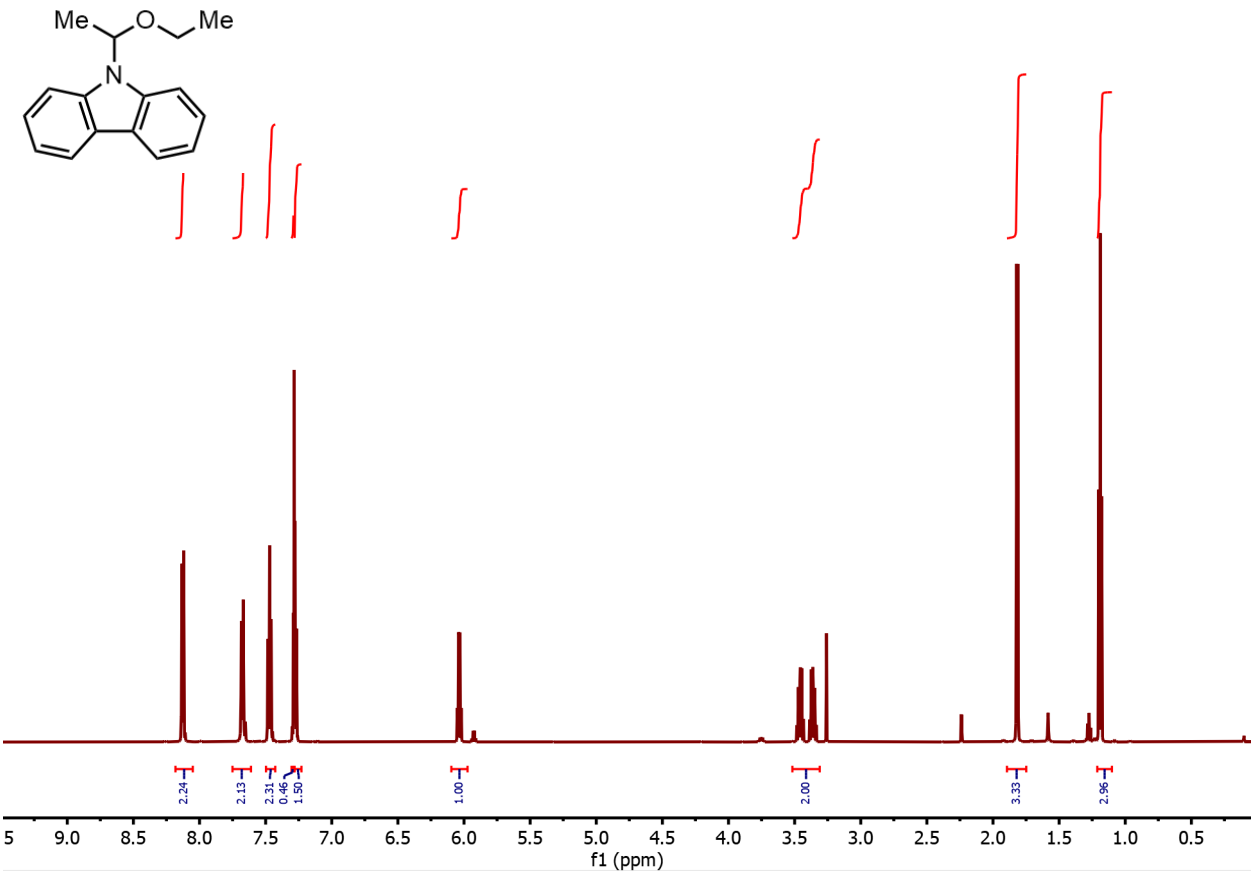


Figure S26: 9-(1-ethoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

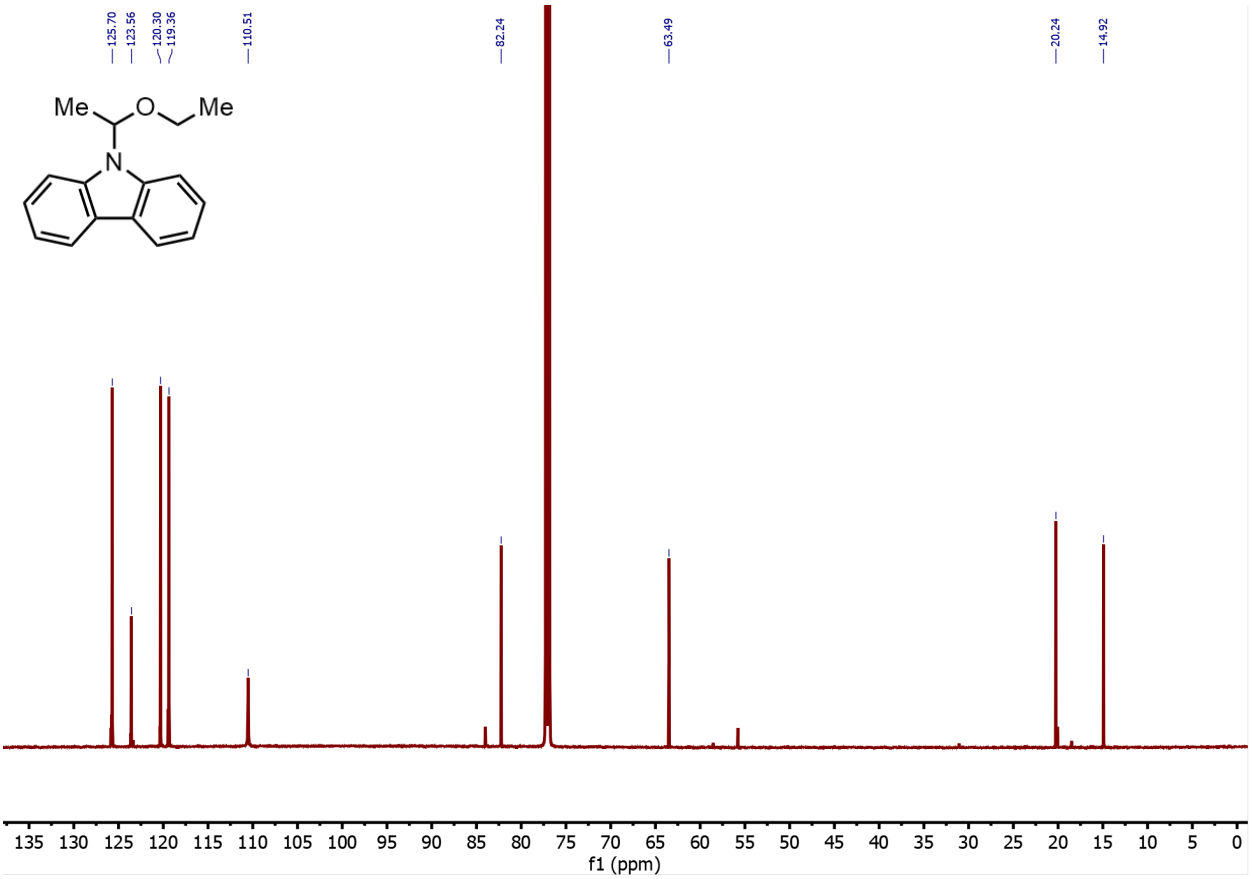


Figure S27: 9-(1-ethoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(3b) 9-(1-isopropoxyethyl)-9H-carbazole

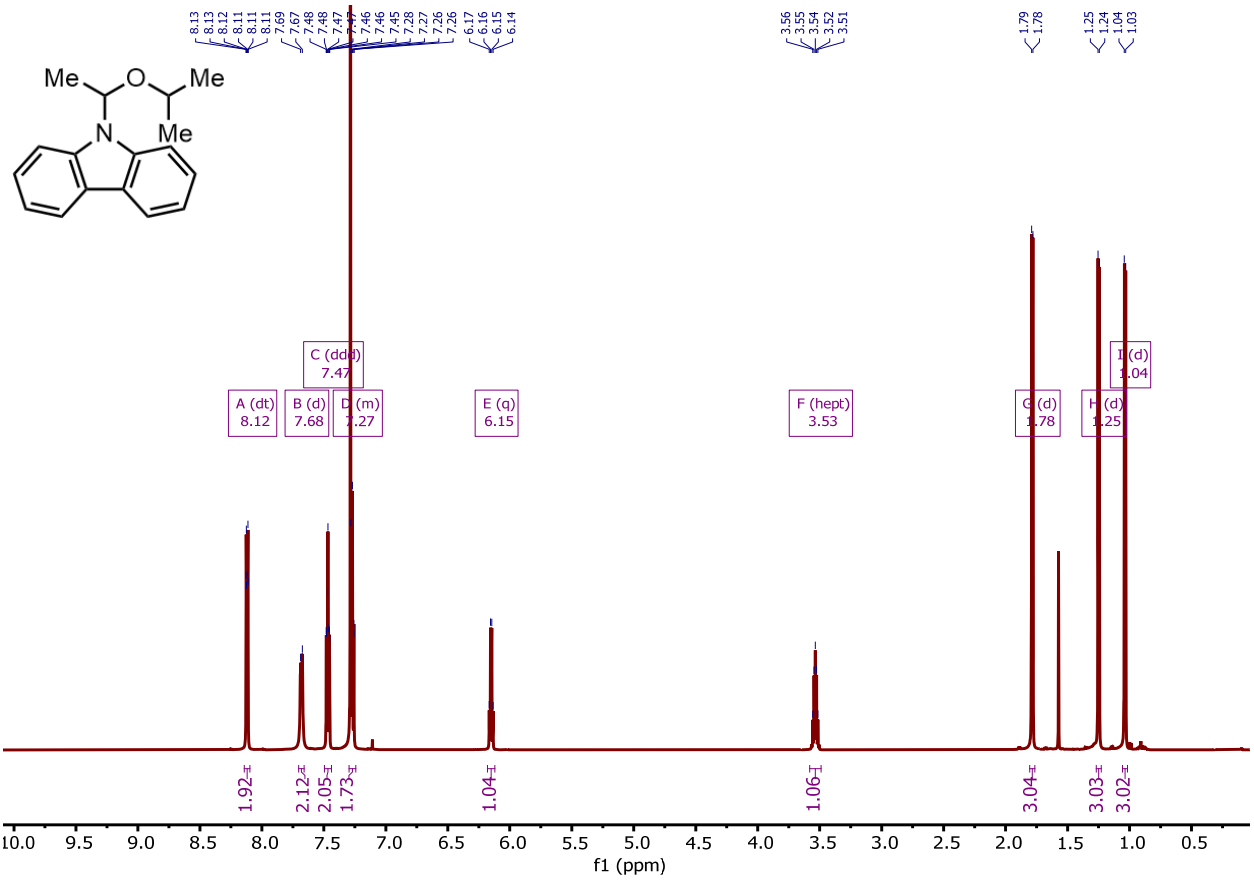


Figure S28: 9-(1-isopropoxyethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

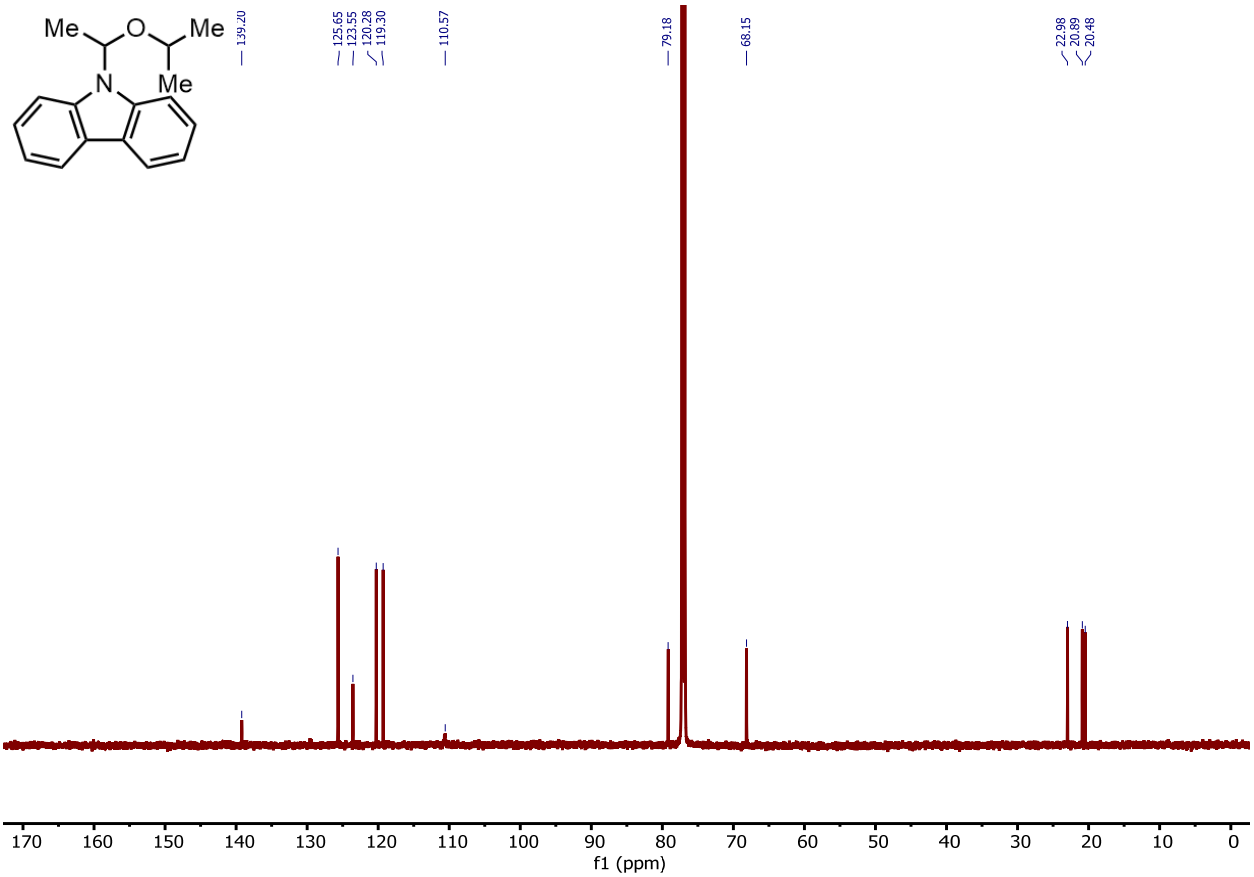


Figure S29: 9-(1-isopropoxyethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(3c) 9-(1-((S)-2-methylbutoxy)ethyl)-9H-carbazole

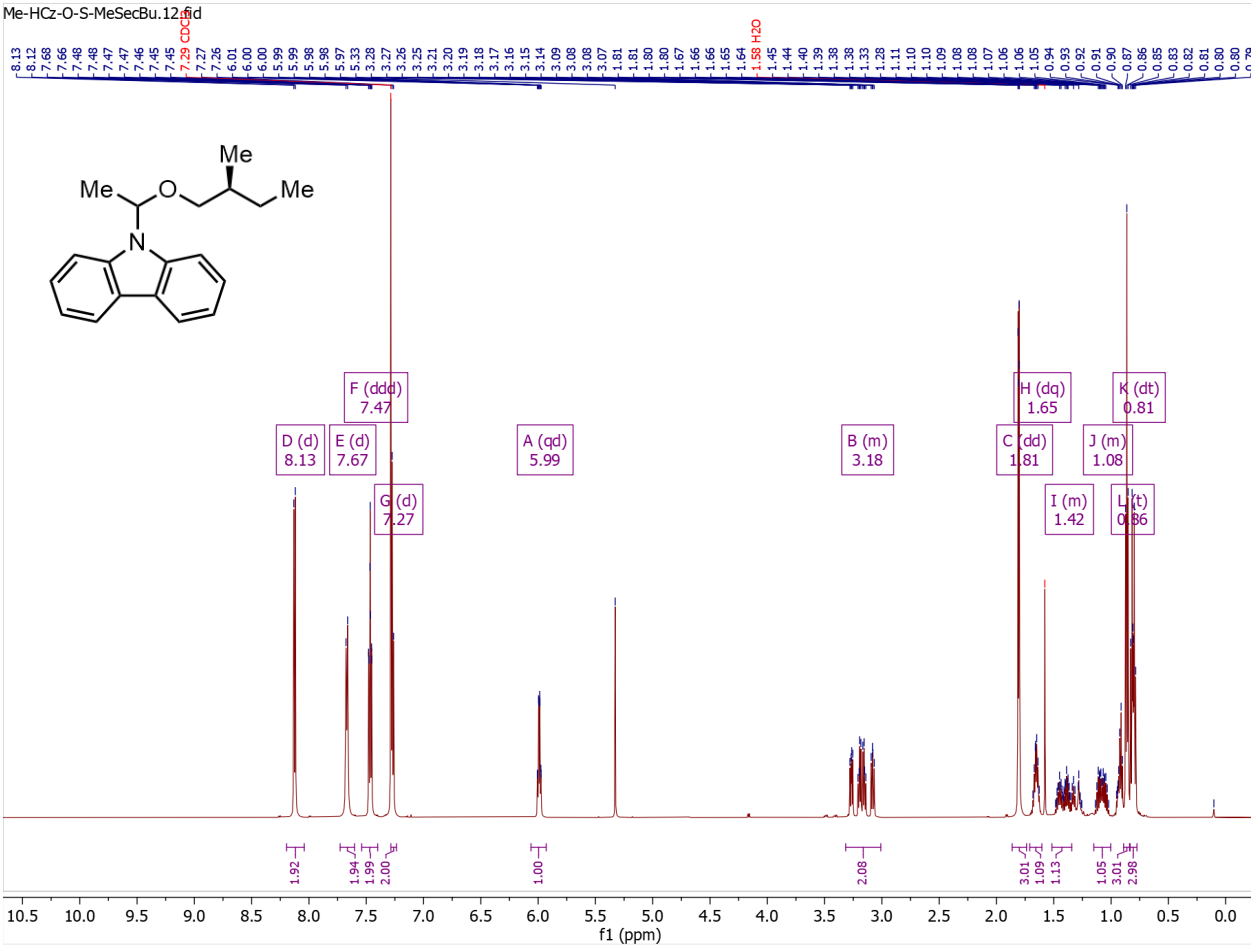


Figure S30: 9-(1-((S)-2-methylbutoxy)ethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

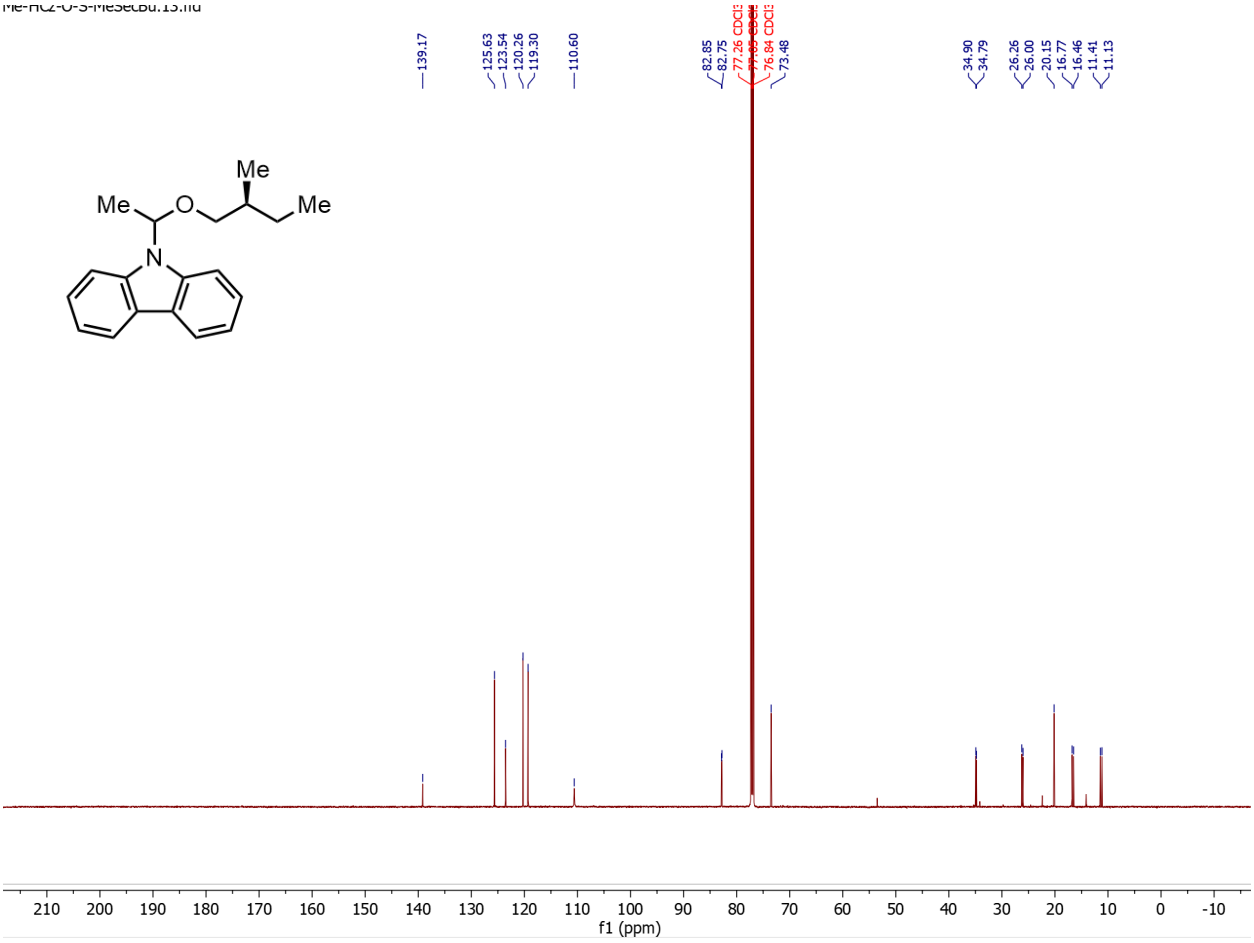


Figure S31: 9-(1-((S)-2-methylbutoxy)ethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(3d) 9-(1-(tert-butoxy)ethyl)-9H-carbazole:

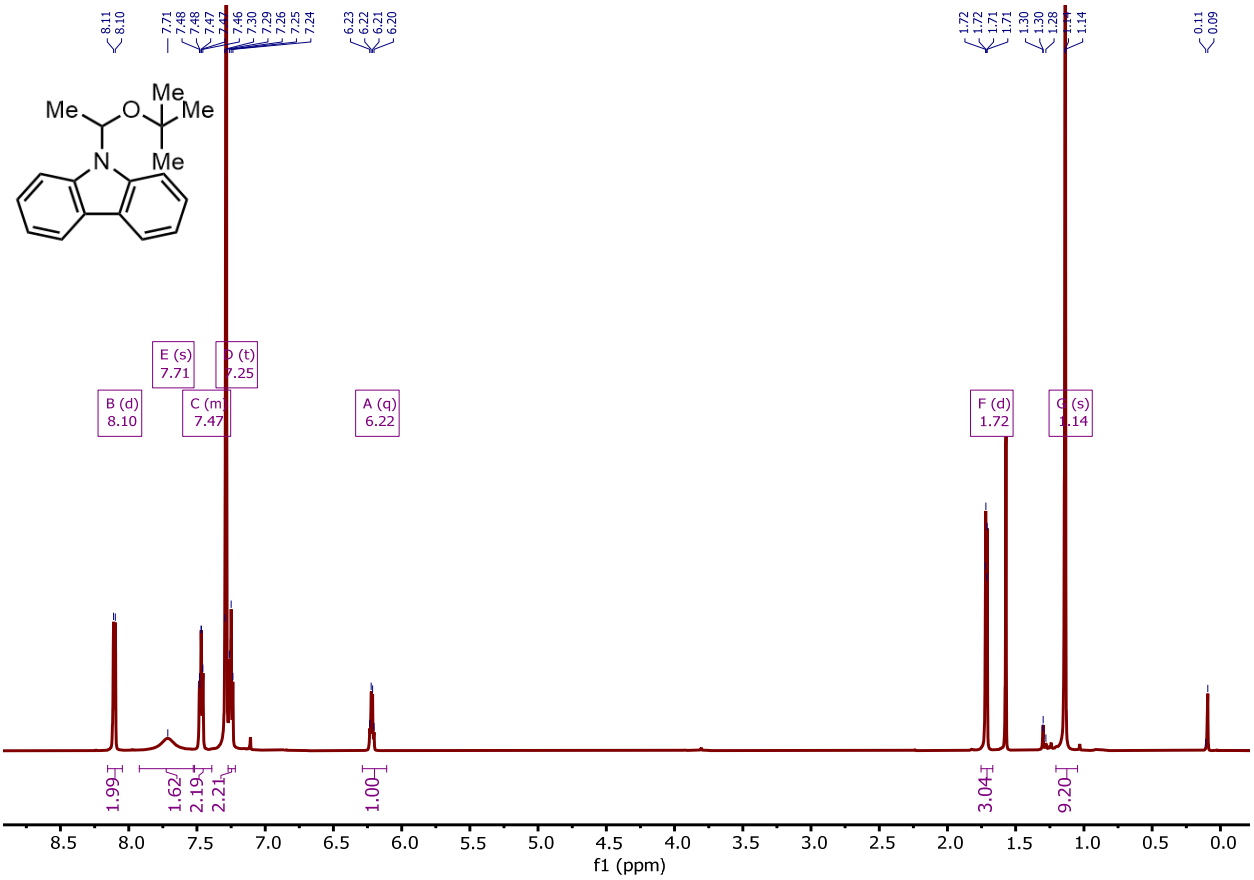


Figure S32: 9-(1-(tert-butoxy)ethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

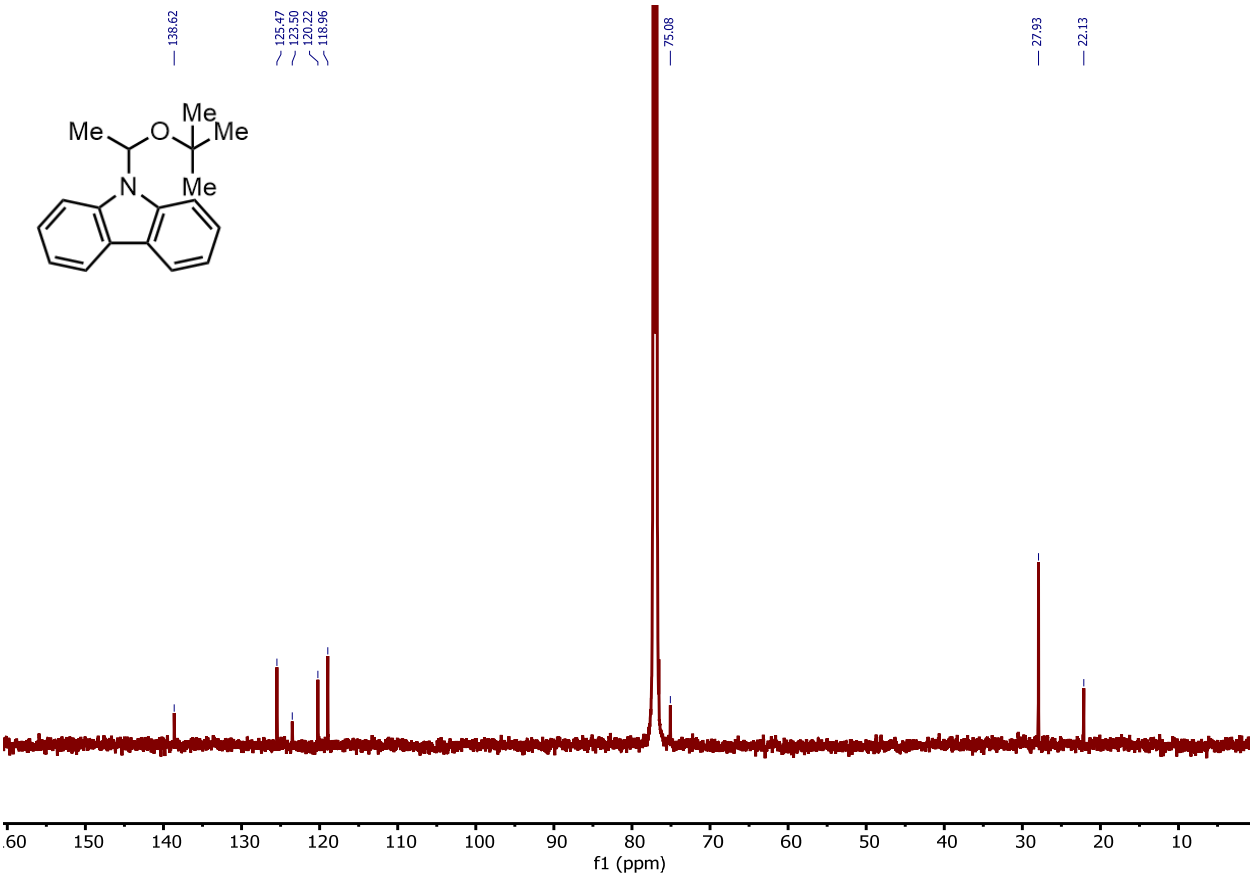


Figure S33: 9-(1-(tert-butoxy)ethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4a) 9-(1-methoxypropyl)-9H-carbazole

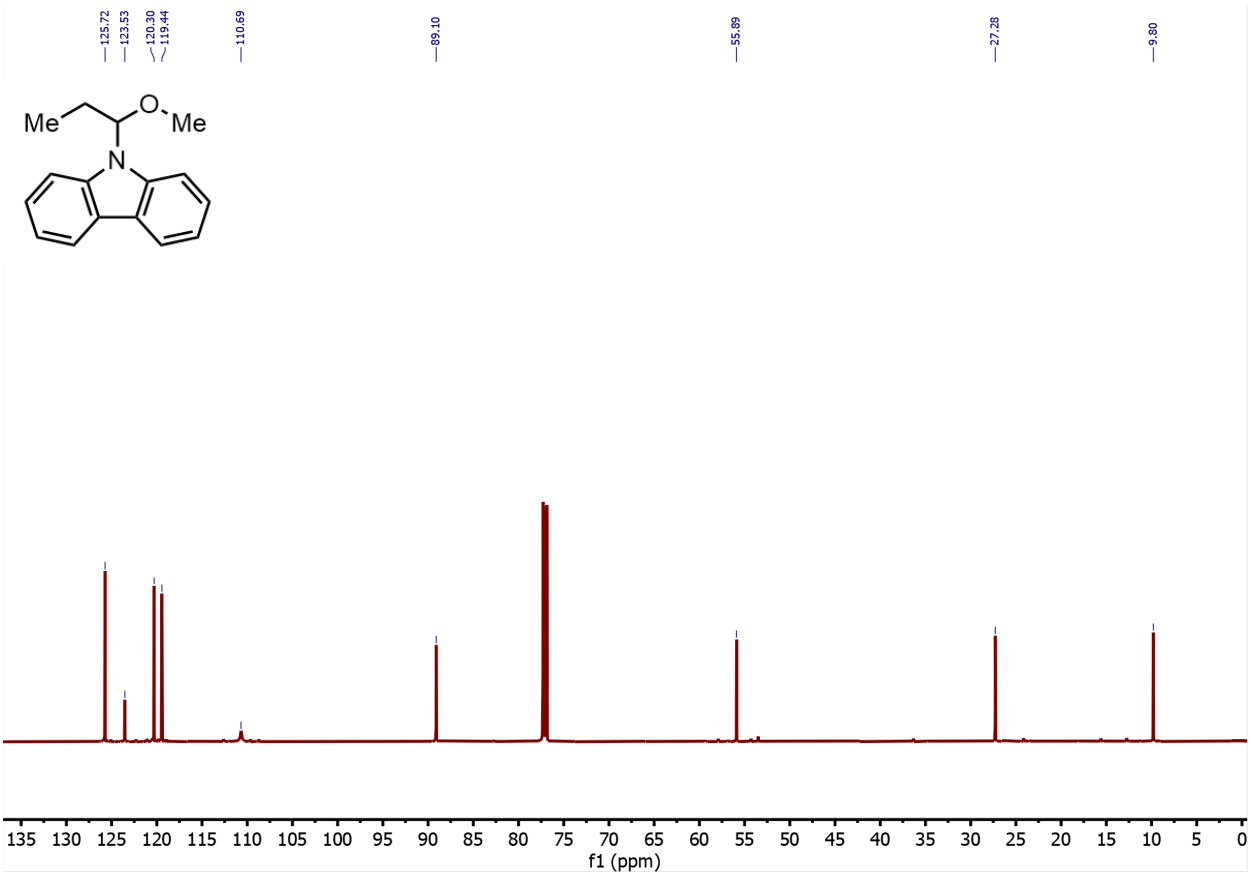


Figure S34: 9-(1-methoxypropyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

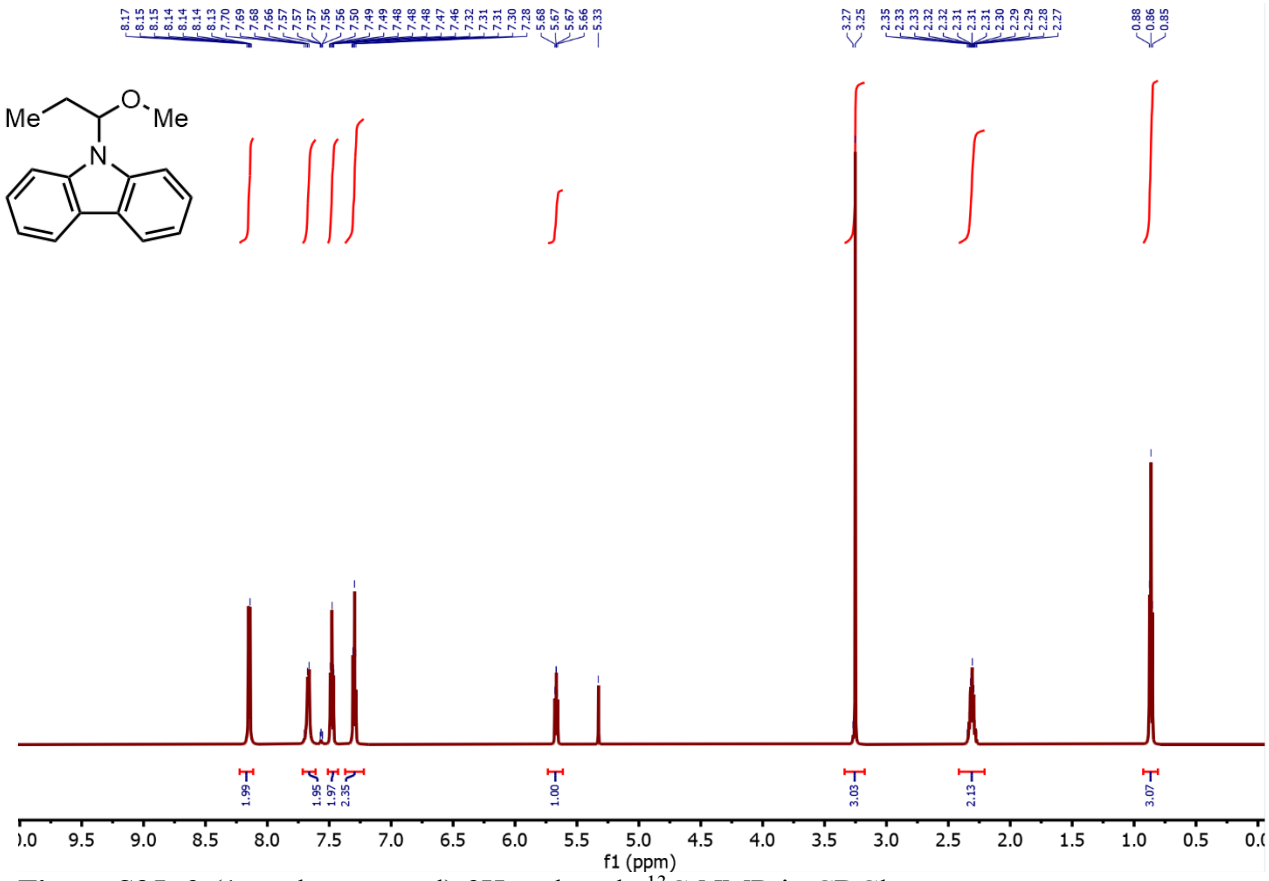


Figure S35: 9-(1-methoxypropyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4b) 9-(1-methoxy-2-methylpropyl)-9H-carbazole

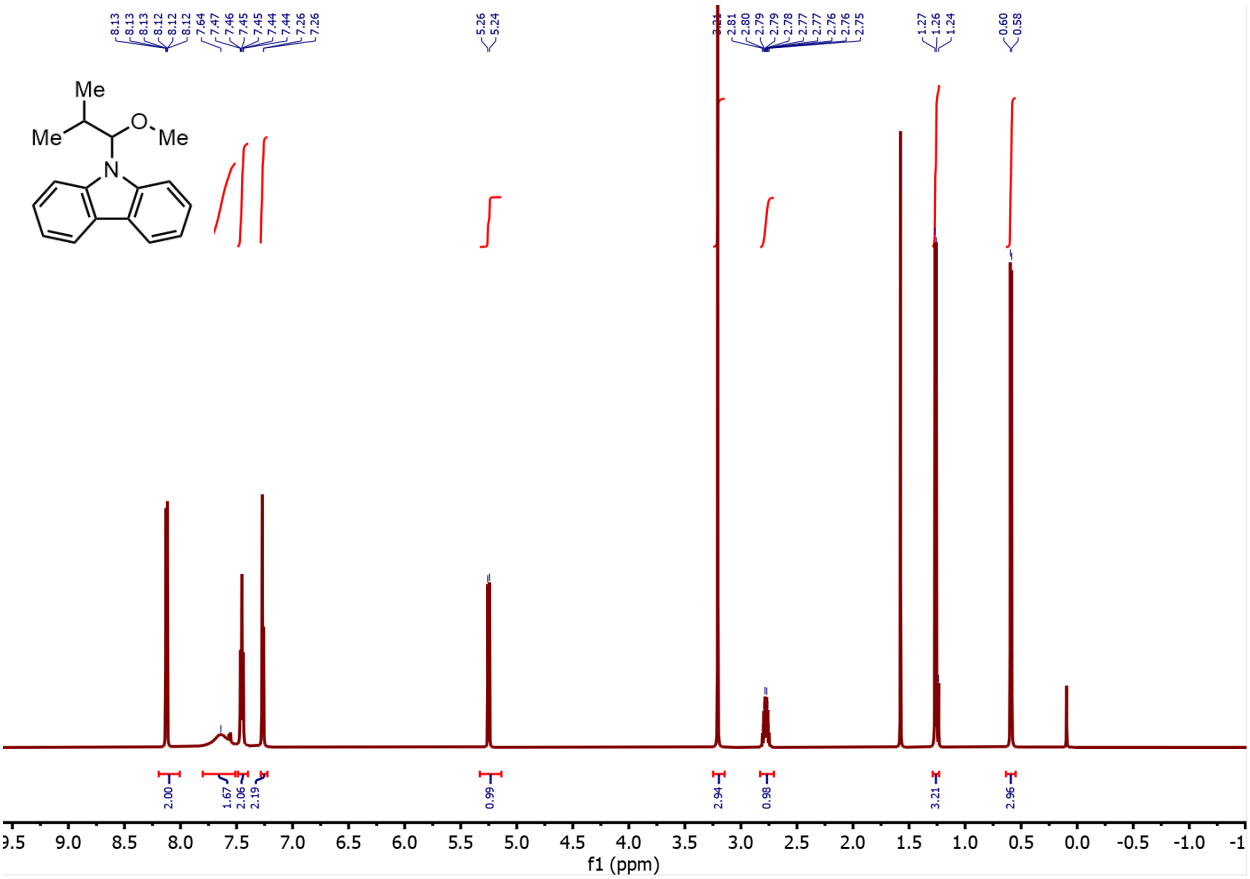


Figure S36: 9-(1-methoxy-2-methylpropyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

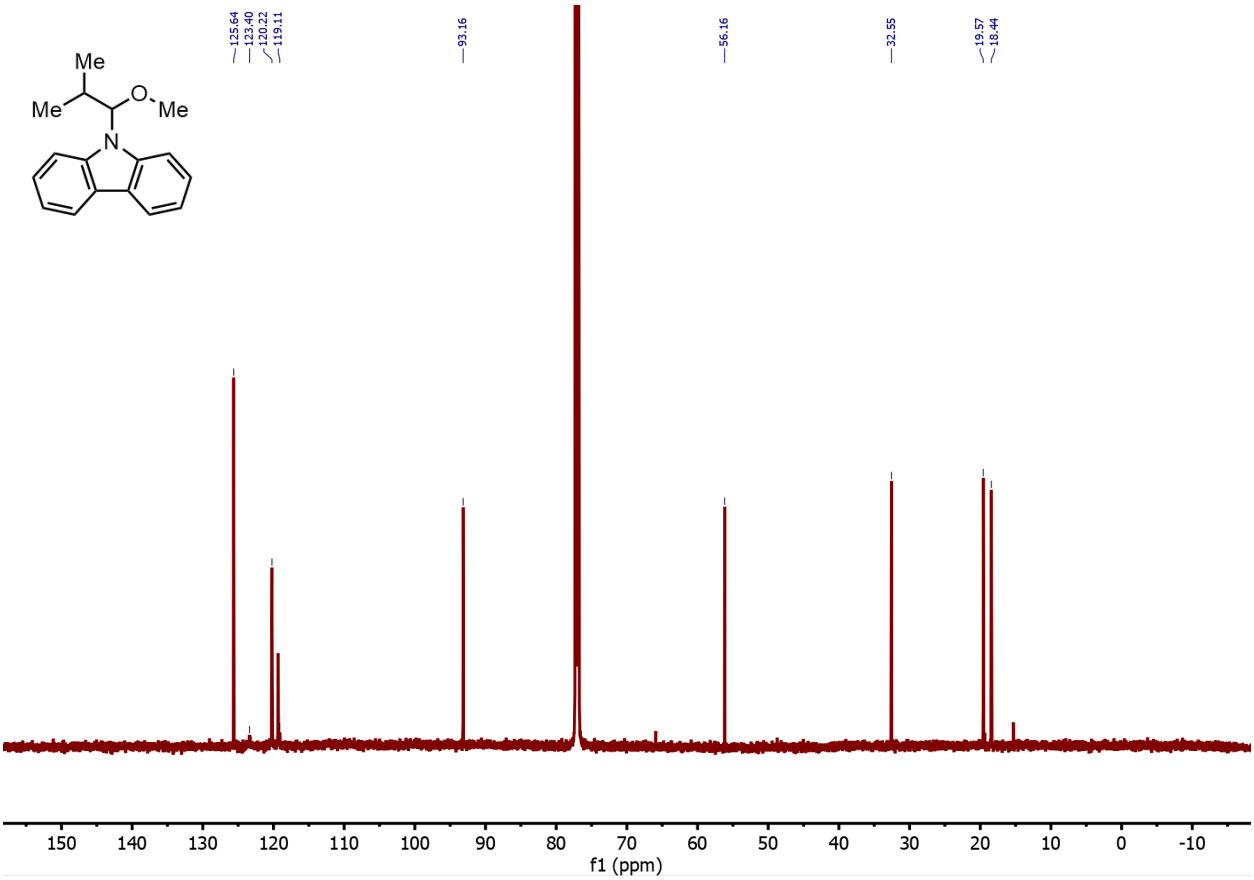


Figure S37: 9-(1-methoxy-2-methylpropyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4c) 9-(1-methoxy-2-phenylethyl)-9H-carbazole

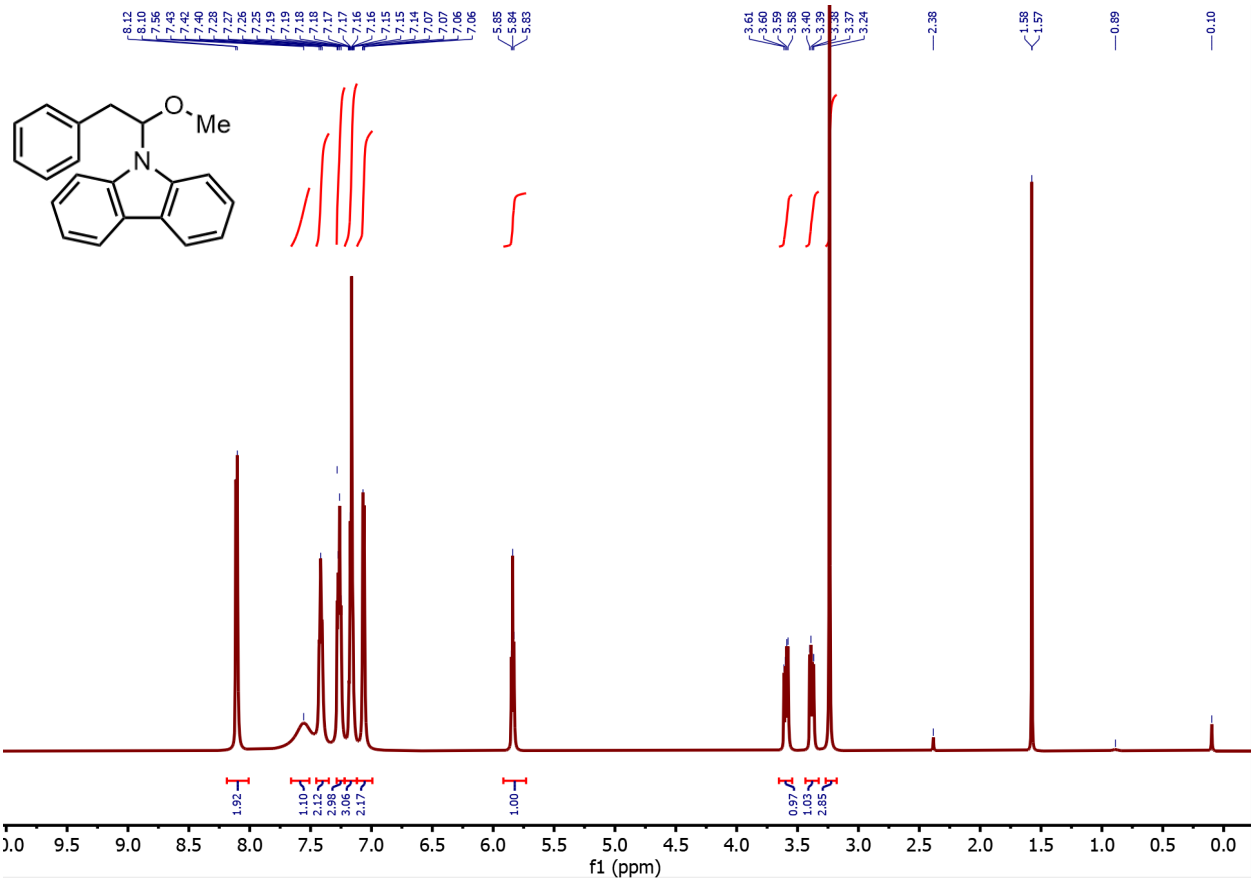


Figure S38: 9-(1-methoxy-2-phenylethyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

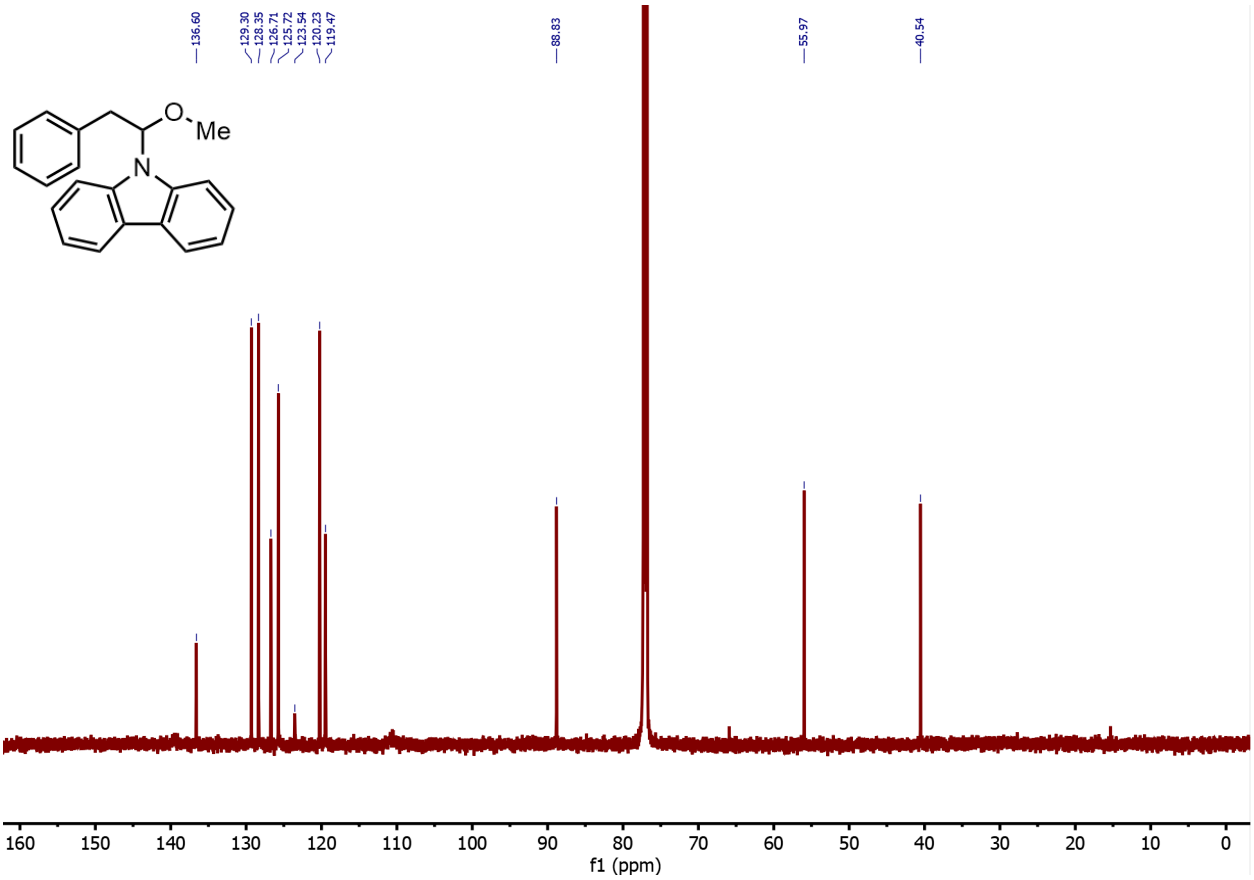


Figure S39: 9-(1-methoxy-2-phenylethyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4d) 9-(cyclopropyl(methoxy)methyl)-9H-carbazole:

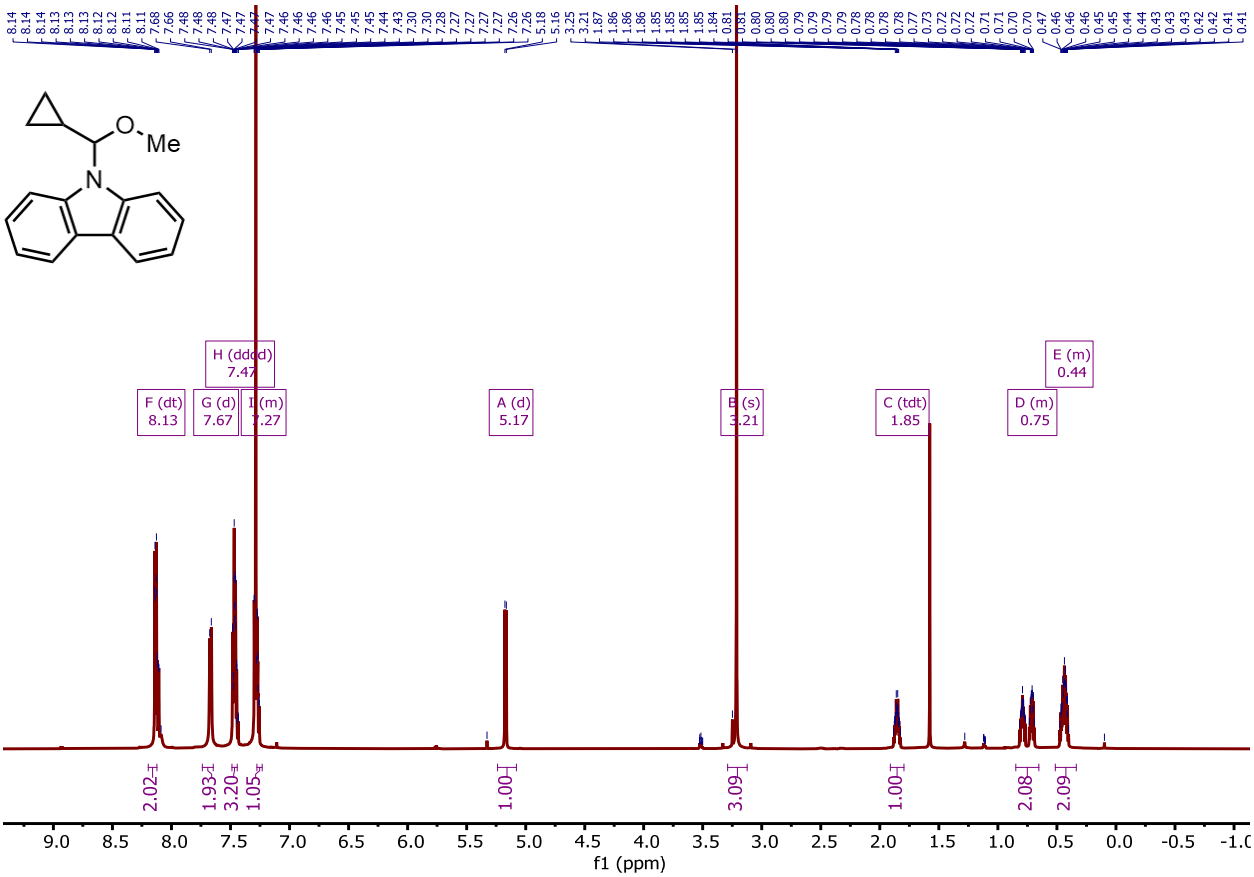


Figure S40: 9-(cyclopropyl(methoxy)methyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

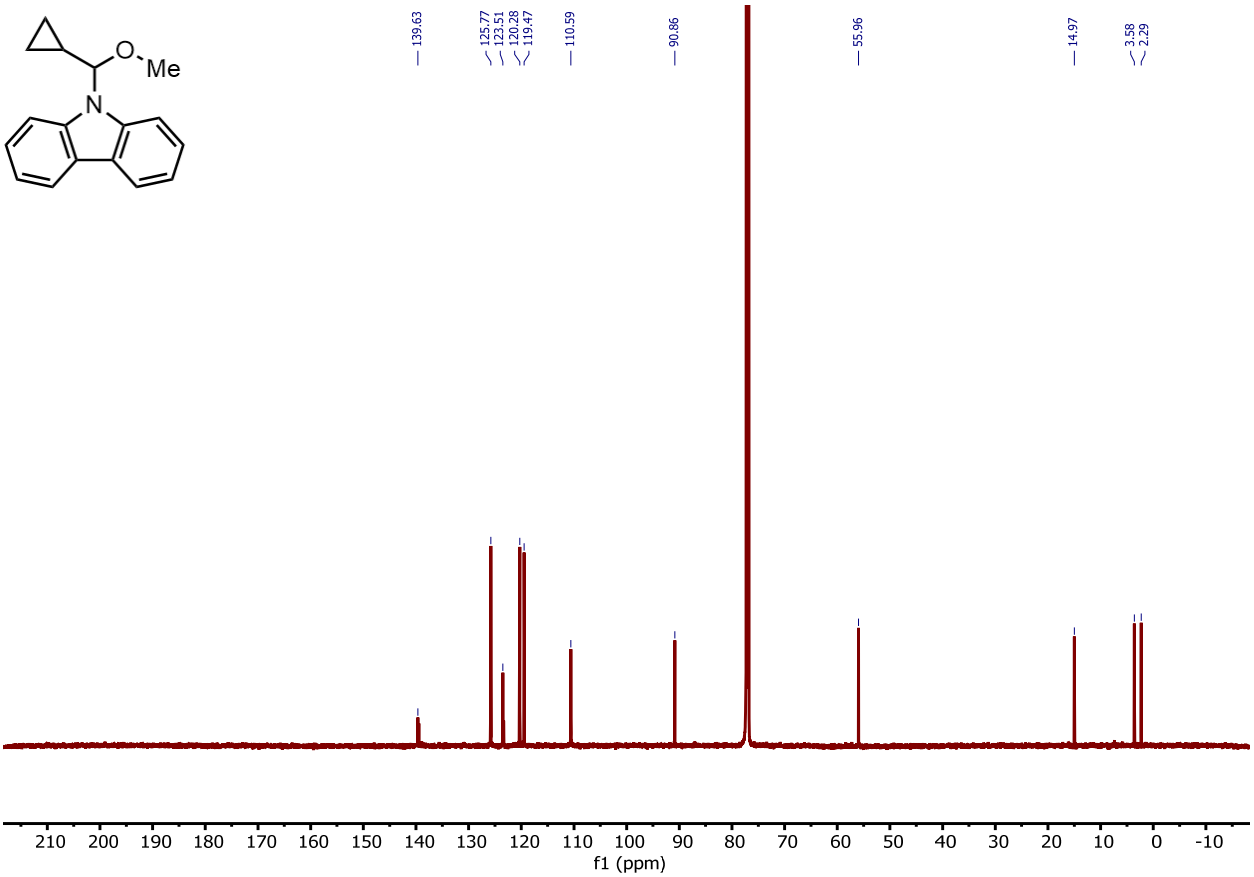


Figure S41: 9-(cyclopropyl(methoxy)methyl)-9H-carbazole ^{13}C-NMR in CDCl3

(4e) 9-(cyclobutyl(methoxy)methyl)-9H-carbazole:

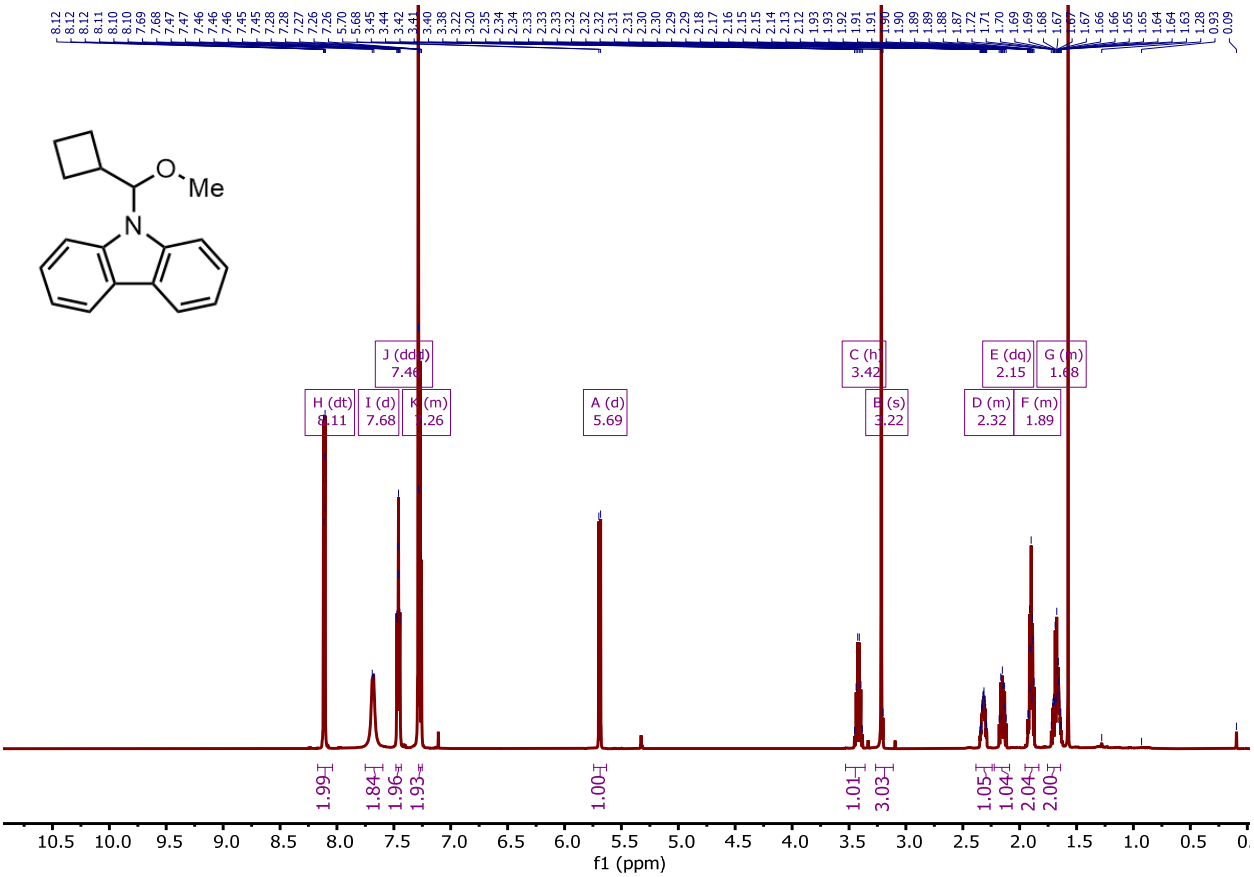


Figure S42: 9-(cyclobutyl(methoxy)methyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

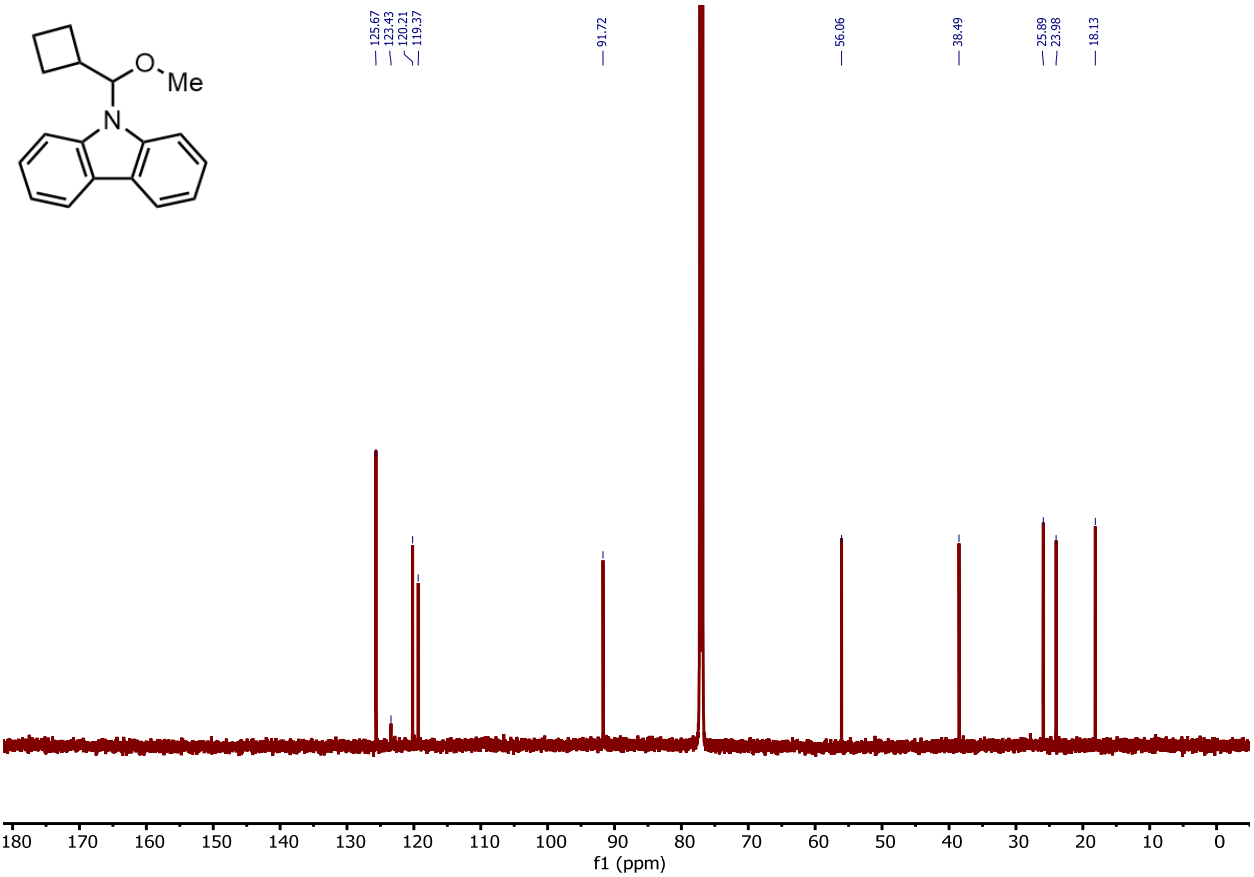


Figure S43: 9-(cyclobutyl(methoxy)methyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4f) 9-(cyclopentyl(methoxy)methyl)-9H-carbazole

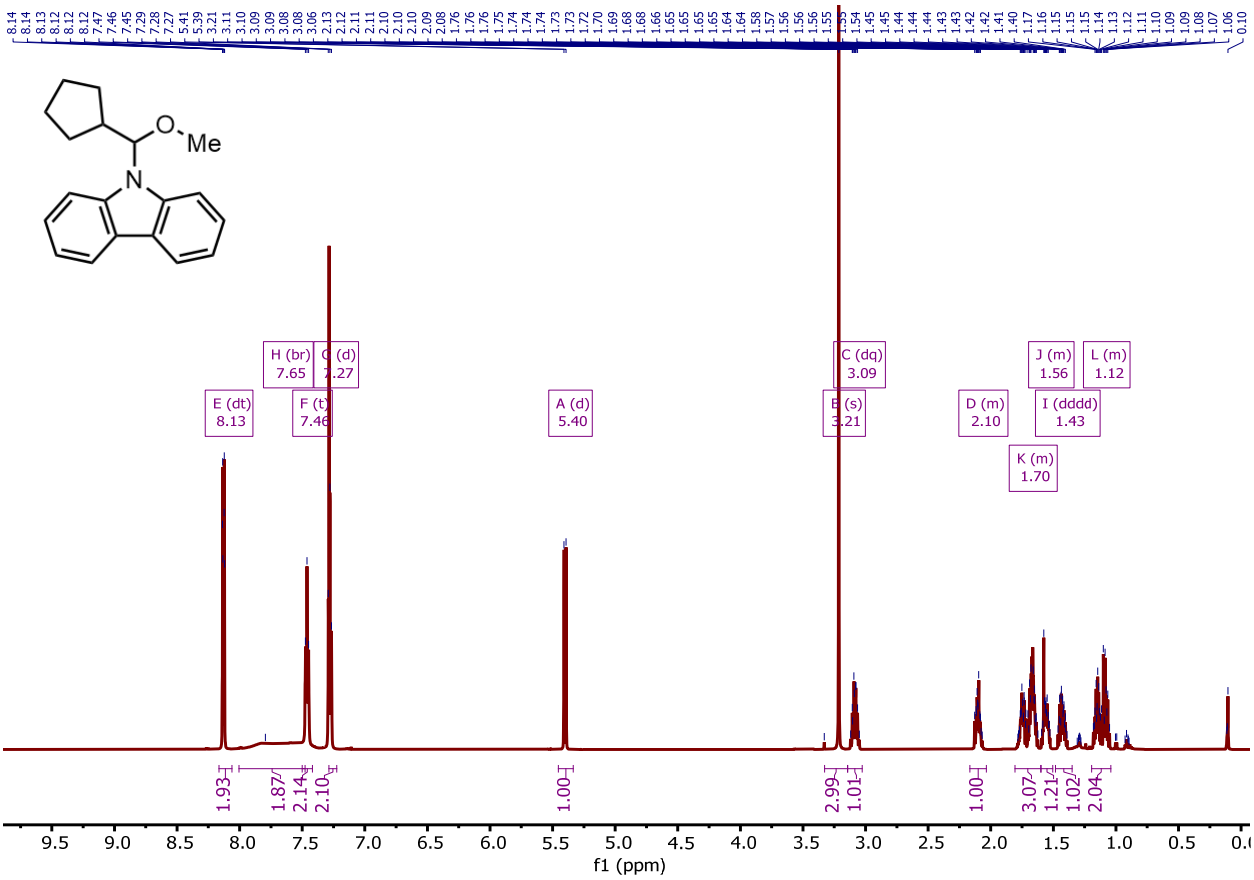


Figure S44: 9-(cyclopentyl(methoxy)methyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

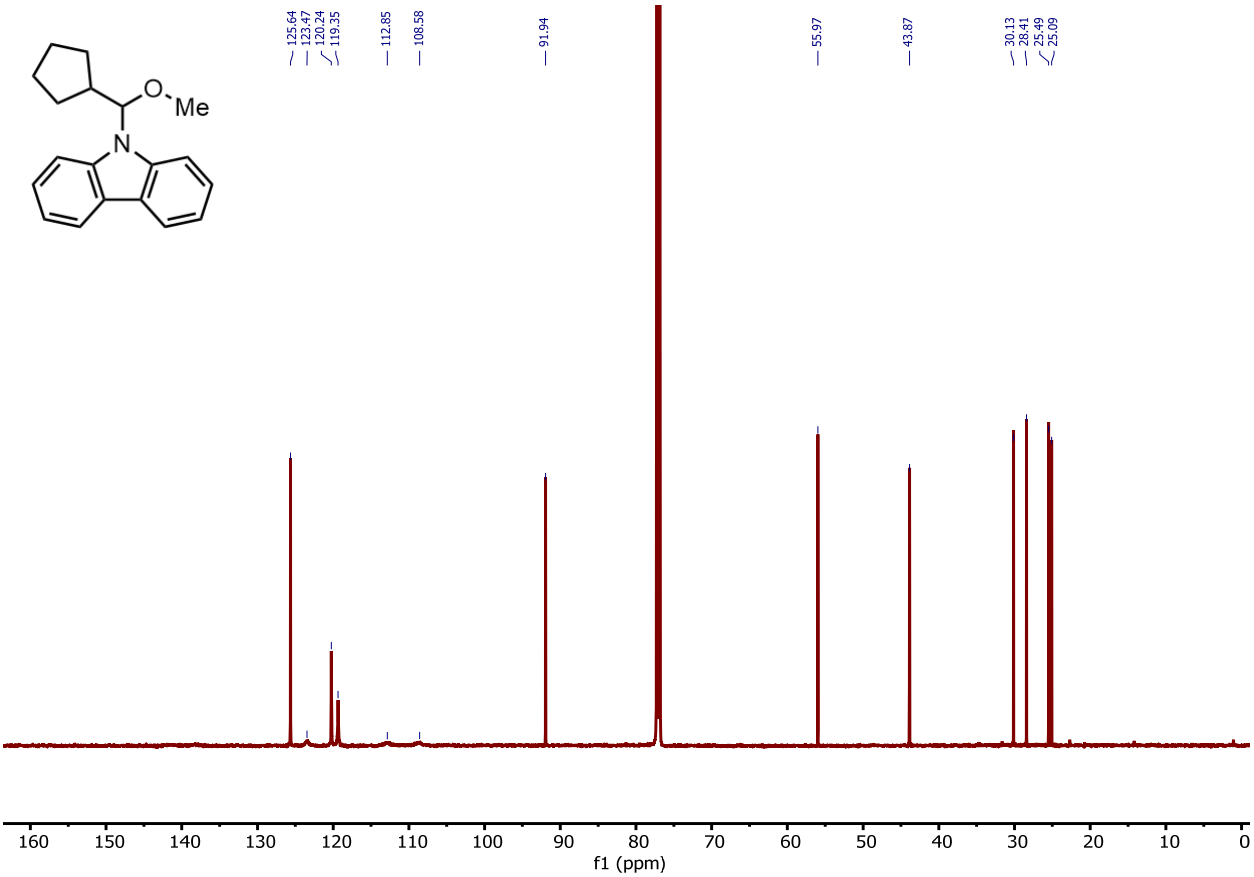


Figure S45: 9-(cyclopentyl(methoxy)methyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

(4g) 9-(cyclohexyl(methoxy)methyl)-9H-carbazole:

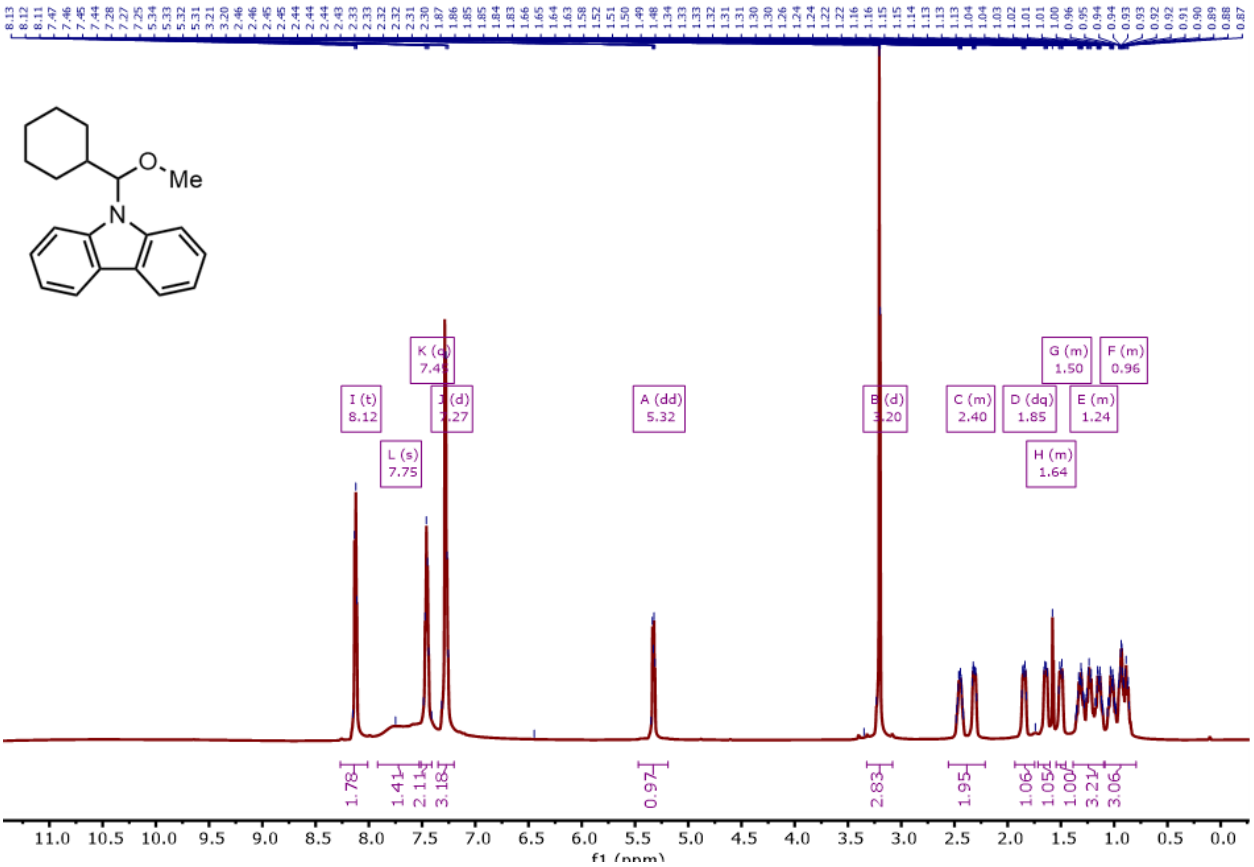


Figure S46: 9-(cyclohexyl(methoxy)methyl)-9H-carbazole ^{1}H-NMR in $CDCl_3$

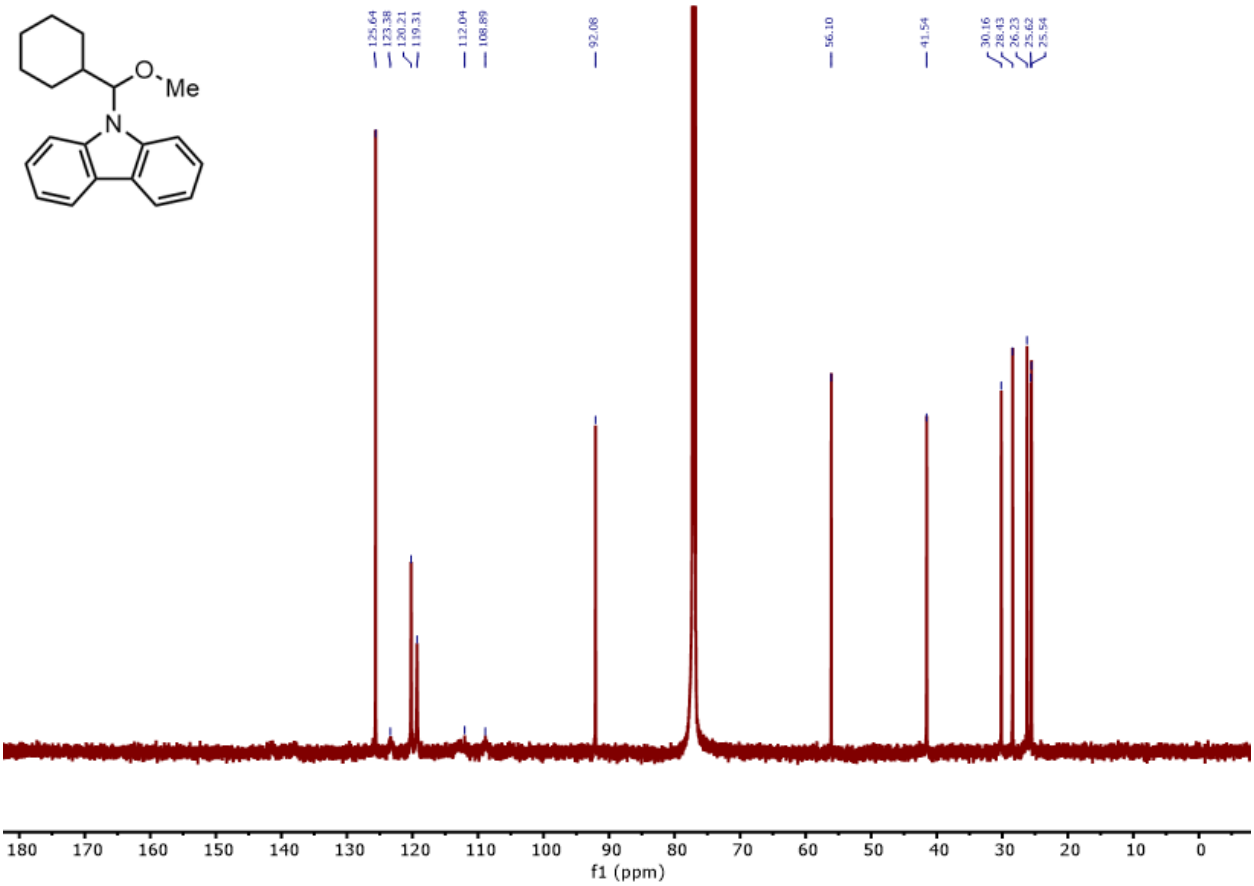


Figure S47: 9-(cyclohexyl(methoxy)methyl)-9H-carbazole ^{13}C-NMR in $CDCl_3$

9-(1-methoxy-2,2-dimethylpropyl)-9H-carbazole (4h)

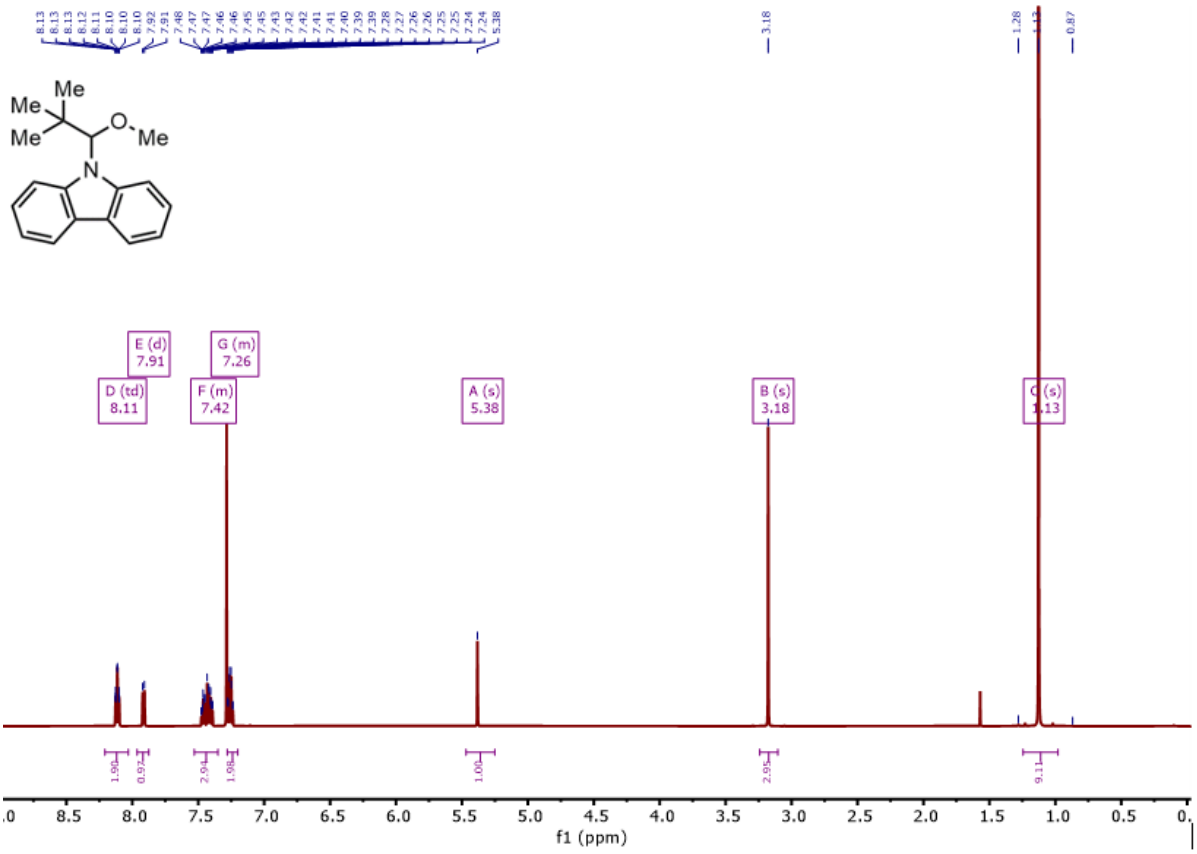


Figure S48: 9-(1-methoxy-2,2-dimethylpropyl)-9H-carbazole ^{1}H-NMR $CDCl_3$

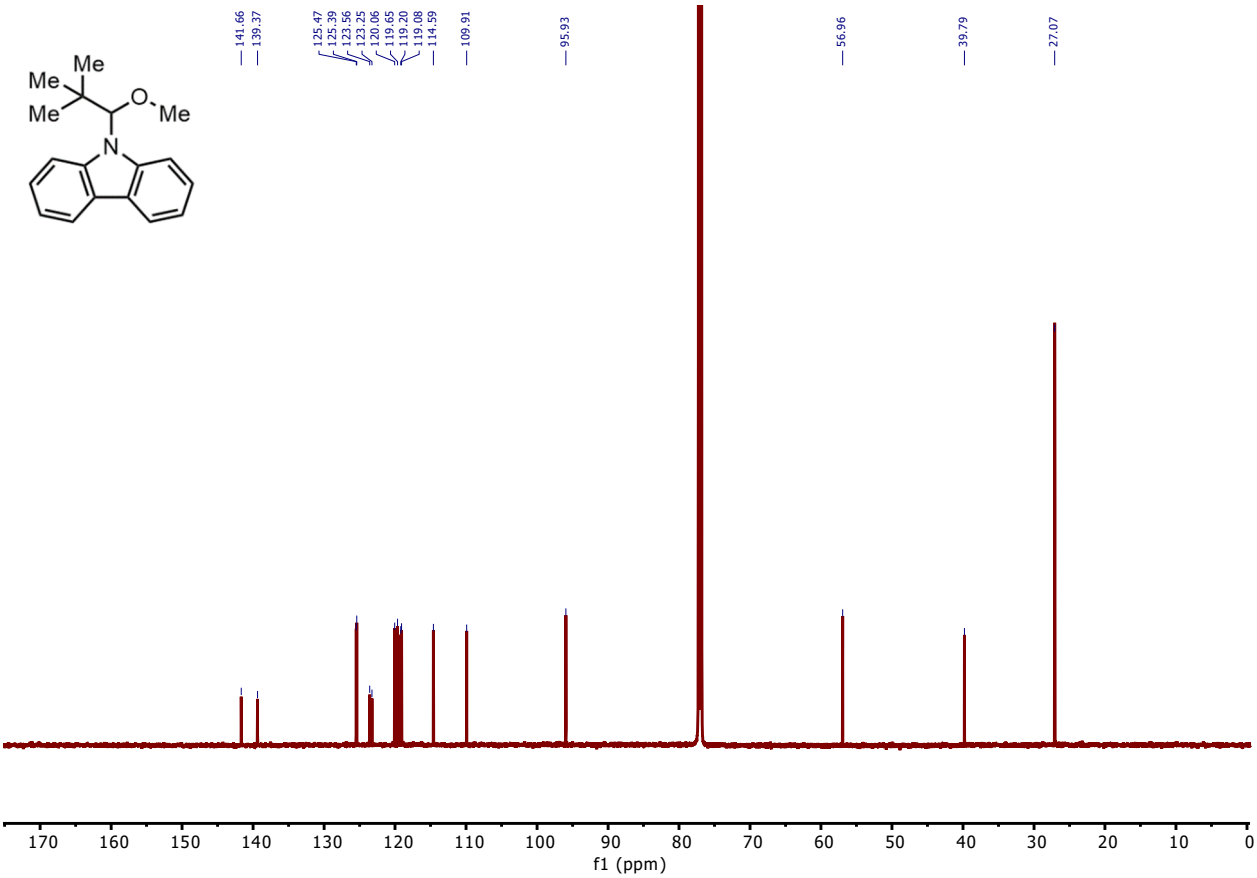


Figure S49: 9-(1-methoxy-2,2-dimethylpropyl)-9H-carbazole ^{13}C-NMR $CDCl_3$

Poly(d3-NVC):

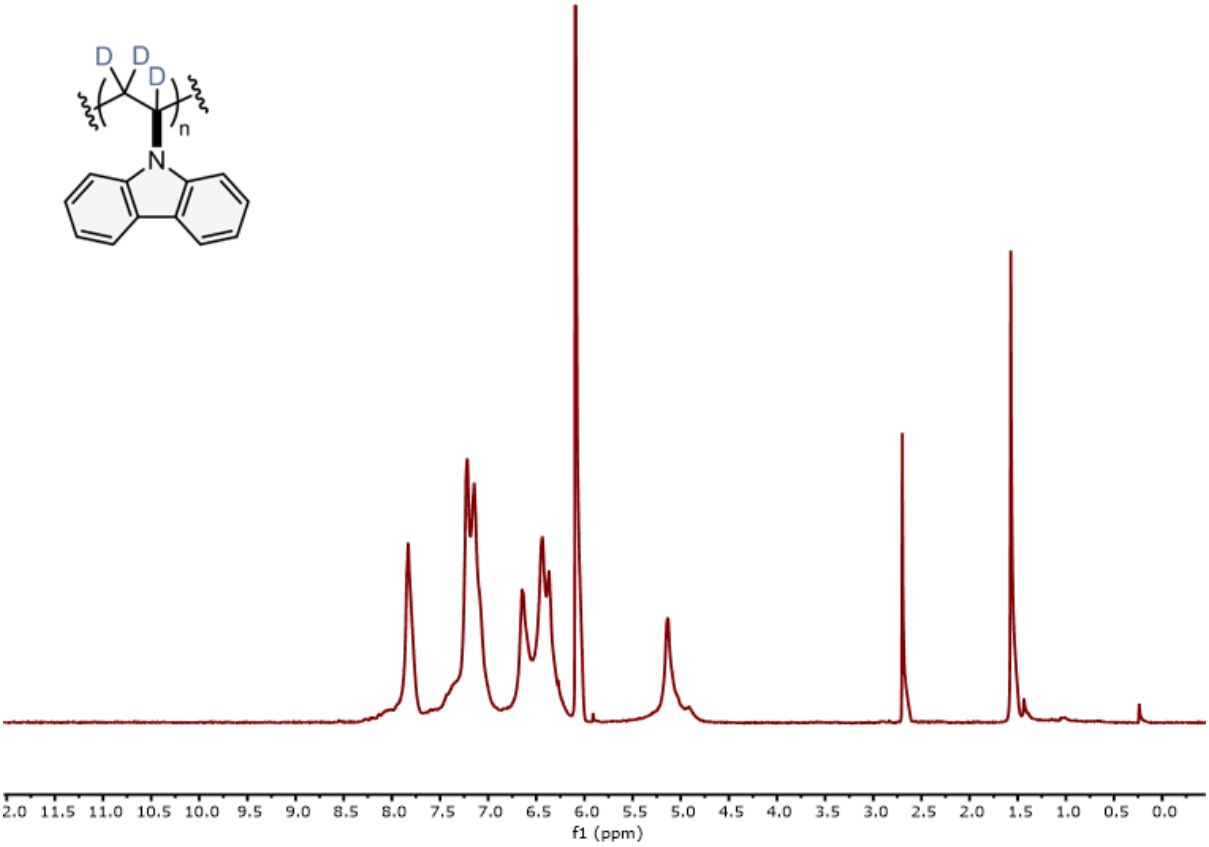


Figure S50: poly(d3-NVC) ^{1}H-NMR showing lack of methine proton in the 3.5-4.0 ppm range and methylene in the 1.0-2.0 ppm range.

5. Density Functional Theory Geometry Coordinates

Et-HCz-OMe-R-SR

0 1

C	-0.99372600	1.94876600	-1.94506400
C	-1.35829300	1.58961900	-3.37882000
N	-0.30691800	1.65021800	-4.34773100
C	-0.34671700	0.88281500	-5.52510300
C	0.70994700	1.27390500	-6.38137400
C	1.42200000	2.33702300	-5.70273000
C	0.76786400	2.55944200	-4.45910500
C	1.22929500	3.56154100	-3.59198500
C	2.34135200	4.31376000	-3.97783500
C	2.99752500	4.09012000	-5.20068800
C	2.53835000	3.10108400	-6.06827600
C	0.87869900	0.63969800	-7.62054100
C	-0.01015200	-0.37049000	-7.99034400
C	-1.05639200	-0.75001700	-7.12901600
C	-1.23690500	-0.12992200	-5.89083200
H	-1.88957500	1.77359900	-1.34222500
H	-0.79766800	3.02230000	-1.84797300
H	-1.75678900	0.56817300	-3.38504800
H	0.74856800	3.77346000	-2.64144200
H	2.70372800	5.09529800	-3.30561300
H	3.86539900	4.69619600	-5.47024800
H	3.03441200	2.92052000	-7.02493200
H	1.69405400	0.93649800	-8.28454900
H	0.10606300	-0.87201800	-8.95389700
H	-1.74572900	-1.54518000	-7.42429400
H	-2.04389300	-0.44910300	-5.23887500
Sc	-4.55345400	2.26431700	-2.88380900
S	-3.39678000	4.36511900	-0.30093400
O	-2.29673500	3.63463800	0.32320900
O	-4.48034300	4.88220300	0.53138900
C	-2.61882100	5.86013500	-1.12439800
F	-2.25254200	6.73886300	-0.20119300
F	-1.53687000	5.48513400	-1.81987800
F	-3.48384800	6.43143400	-1.96046500
S	-4.55809200	-0.19507200	-0.66753700
O	-5.42292800	-1.22620600	-1.24219000
O	-5.05216400	0.59856300	0.45914100
C	-3.02411100	-1.07937700	-0.05333800
F	-3.36749000	-1.99384000	0.84379200
F	-2.40247600	-1.67938800	-1.07466800
F	-2.18956300	-0.20448200	0.49984000
S	-5.81181100	3.72988900	-5.62851100
O	-7.19206300	3.24727300	-5.72727600
O	-4.82678100	3.22577700	-6.59287400
C	-5.88190100	5.58423800	-5.86854000
F	-6.29213500	5.85340000	-7.10248100
F	-6.72510000	6.12407000	-4.99417300
F	-4.66886500	6.10411000	-5.68475600
O	-3.93458000	3.65904500	-1.55770400
O	-3.89661400	0.67737200	-1.75105200
O	-5.26897900	3.69618000	-4.19337900
C	-9.17488600	1.36327800	-3.98875100
C	-7.94705000	0.64382900	-3.37021300
C	-6.83425700	0.55318100	-4.38326100
N	-5.57584300	0.79268200	-4.21580500
C	-4.88738200	0.20991700	-5.39324300
C	-4.48940600	-1.23549400	-5.14923800
C	-3.76491900	-1.76730600	-4.08242800
C	-3.52879600	-3.14507300	-4.04791300
C	-4.02210600	-3.97358200	-5.06524700
C	-4.77651100	-3.43954500	-6.11792300
C	-5.01624400	-2.06399700	-6.15002200
C	-5.83156700	-1.26197700	-7.14057100
C	-6.01386100	0.08125900	-6.43743800
O	-7.19008800	0.04967400	-5.55730100
C	-8.29973900	-0.81927800	-2.97898900
C	-7.56523000	1.41468100	-2.12773000
N	-6.53277700	2.15793500	-1.90516300
C	-6.81092300	2.91920200	-0.65591200
C	-8.00097300	2.15807000	-0.03183900
C	-9.04527300	3.19366300	0.38713400
C	-8.65718400	4.42813800	-0.39625200
C	-7.37905600	4.29302900	-0.95587200
C	-6.80818200	5.32375600	-1.70473800
C	-7.54106100	6.49896800	-1.89451800
C	-8.81963400	6.64014000	-1.33607800
C	-9.38469300	5.60646100	-0.58021400
O	-8.48735100	1.38070400	-1.17637500
H	-9.49486200	0.82180300	-4.88838500
H	-9.99617800	1.37355500	-3.26077400
H	-8.91465900	2.39113300	-4.27337800
H	-4.05769300	0.85507100	-5.71714100
H	-3.42007600	-1.12797400	-3.27272500
H	-2.96914300	-3.57314700	-3.21317400
H	-3.83342200	-5.04937700	-5.02662400
H	-5.18476800	-4.09302300	-6.89322000
H	-5.28695400	-1.10628600	-8.08728000
H	-6.79918900	-1.72192900	-7.39167900
H	-8.59782400	-1.37510300	-3.87777300
H	-7.43499300	-1.30925700	-2.51077700
H	-9.13566300	-0.80994500	-2.26742000
H	-5.92311900	2.93970000	-0.01780700
H	-7.71895200	1.43244400	0.74149600
H	-10.06627500	2.83734300	0.18158700
H	-8.97476900	3.37144800	1.47350700
H	-5.81614900	5.21294900	-2.13820500
H	-7.11376300	7.30928500	-2.48951000
H	-9.38100600	7.56456400	-1.49463400
H	-10.38178800	5.71783800	-0.14603900
H	-6.13342300	0.95241200	-7.09370900
C	-2.18587100	3.64049800	-4.48422000
H	-3.10514600	4.21848100	-4.58909600
H	-1.46809800	4.20748800	-3.88048400
H	-1.77305800	3.43227900	-5.47981900
O	-2.52821700	2.39863900	-3.82434700
C	0.15220900	1.10346000	-1.39419200
H	1.09628500	1.27703400	-1.93161000
H	0.31181200	1.34140200	-0.33237100
H	-0.08777000	0.03037500	-1.46241000

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C	-1.30858000	1.11589200	-2.15844000
C	-1.30063200	2.13344700	-3.29210500
N	-0.22334000	1.95907800	-4.21913200
C	0.01895200	0.82609000	-5.00064600
C	1.23777100	1.00556800	-5.70752400
C	1.74954200	2.31130500	-5.33483100
C	0.81680100	2.87341400	-4.42180200
C	1.01074800	4.14541700	-3.86912500
C	2.15481500	4.85049200	-4.24955600
C	3.08854600	4.30706000	-5.15270500
C	2.89186100	3.03842300	-5.69848000

C	1.68452900	0.00388100	-6.58158000
C	0.91094200	-1.14612500	-6.74805600
C	-0.30869100	-1.29621700	-6.06022000
C	-0.77258700	-0.31276000	-5.18494700
H	-2.09475400	1.40134900	-1.45285400
H	-1.56125000	0.11916400	-2.54293700
H	-1.20599500	3.13660000	-2.86267200
H	0.29946600	4.58385300	-3.16865400
H	2.32569300	5.84613400	-3.83285300
H	3.97363400	4.88611000	-5.42614200
H	3.61445100	2.61402200	-6.39975200
H	2.62201300	0.12873700	-7.12892900
H	1.24792300	-1.93346500	-7.42641700
H	-0.91433200	-2.19329200	-6.21276600
H	-1.72723900	-0.42648300	-4.67958600
Sc	-4.59084100	2.08064000	-2.93043500
S	-3.00937100	4.30245400	-0.67166300
O	-1.66417300	3.78936800	-0.40619100
O	-3.82745200	4.82119300	0.41781500
C	-2.72480700	5.73902800	-1.85609300
F	-1.88679300	6.60000200	-1.29399100
F	-2.17499800	5.28536200	-2.99413100
F	-3.85885800	6.36051300	-2.15713300
S	-4.84292900	-0.62394200	-0.91451300
O	-5.66192100	-1.61718400	-1.60907400
O	-5.38124500	0.03613600	0.27649300
C	-3.29811900	-1.52848800	-0.36084300
F	-3.63059900	-2.51608400	0.45963700
F	-2.66327300	-2.03589300	-1.42239000
F	-2.47864900	-0.68774700	0.26636600
S	-6.11987800	4.11114900	-5.14352200
O	-7.50147400	4.18889200	-4.67402500
O	-5.83746600	3.38273000	-6.38888100
C	-5.55073400	5.86902100	-5.43954500
F	-6.25059000	6.39871900	-6.43570000
F	-5.72712700	6.59758100	-4.34056500
F	-4.25765900	5.86987500	-5.76028800
O	-3.80634200	3.34145300	-1.56376400
O	-4.19167300	0.37228200	-1.88422000
O	-5.13200600	3.73119300	-4.03453700
C	-9.32171800	1.52803200	-3.98471000
C	-8.09855700	0.73575400	-3.45132800
C	-7.02354900	0.66446400	-4.51027900
N	-5.74947000	0.85039900	-4.39129100
C	-5.13365400	0.29484700	-5.62201200
C	-4.73632000	-1.16136700	-5.45175200
C	-3.94001800	-1.73478300	-4.46086600
C	-3.72044600	-3.11553500	-4.48521600
C	-4.30195300	-3.90722400	-5.48528100
C	-5.12760400	-3.33226400	-6.45959700
C	-5.34953100	-1.95364600	-6.43259800
C	-6.21868300	-1.11601900	-7.34403400
C	-6.31091500	0.22503300	-6.61696800
O	-7.45060000	0.23644200	-5.69115100
C	-8.49651500	-0.73512500	-3.13625600
C	-7.64210500	1.40734700	-2.17674000
N	-6.56405300	2.07884900	-1.94826400
C	-6.73482100	2.73155000	-0.62154600
C	-7.92271400	1.96524200	0.00300900
C	-8.88065300	2.99837800	0.59688400
C	-8.48420400	4.28669100	-0.08893800
C	-7.26137300	4.14615000	-0.75876000
C	-6.70525500	5.20395600	-1.47485400
C	-7.38300500	6.42579900	-1.50360400
C	-8.59960600	6.57849300	-0.82365300
C	-9.15921600	5.50927100	-0.11327100
O	-8.51839800	1.33780300	-1.18482200
H	-9.70883800	1.03025400	-4.88335900
H	-10.10622000	1.54251400	-3.21693000
H	-9.03452100	2.55682000	-4.23743800
H	-4.30862100	0.93029600	-5.96655100
H	-3.53340700	-1.12906800	-3.65421100
H	-3.10771200	-3.57476700	-3.70639300
H	-4.12666000	-4.98595300	-5.49240400
H	-5.60252100	-3.95650100	-7.22090300
H	-5.74963600	-0.96667900	-8.33132200
H	-7.21610200	-1.54653200	-7.52034400
H	-8.84422000	-1.22273100	-4.05640400
H	-7.64090300	-1.28765600	-2.72530700
H	-9.31046100	-0.73445200	-2.39963100
H	-5.80305400	2.66100900	-0.04736400
H	-7.63258400	1.14699900	0.67272900
H	-9.93039000	2.71152400	0.43133100
H	-8.72791700	3.05826600	1.68776300
H	-5.77635400	5.07021700	-2.02025300
H	-6.96360400	7.25955100	-2.07081700
H	-9.12144100	7.53842500	-0.85608800
H	-10.11390400	5.62810400	0.40589700
H	-6.42099700	1.10809800	-7.25748000
C	-2.56136900	2.87739600	-5.24127600
H	-3.56802600	2.87476500	-5.66512400
H	-2.27033200	3.91533500	-5.02985100
H	-1.86478800	2.41757900	-5.95233000
O	-2.59250500	2.10894100	-4.01155300
C	0.02852400	1.09092400	-1.42043000
H	0.85222900	0.77040900	-2.07653800
H	0.26639500	2.08599000	-1.01551400
H	-0.03175000	0.38818800	-0.57655300

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C	-0.86587100	2.50702300	-1.63101000
C	-1.13460800	1.83000200	-2.95830100
N	-0.03588500	1.71405500	-3.86608400
C	-0.11178200	0.80730400	-4.93344500
C	0.84813800	1.13402600	-5.91711800
C	1.57044800	2.28840300	-5.41203000
C	0.99479500	2.63043400	-4.15637200
C	1.48289700	3.72941000	-3.43828300
C	2.53267200	4.46632900	-3.98642000
C	3.12496100	4.14296900	-5.23035600
C	2.62548900	3.03911500	-5.93801600
C	0.90879000	0.39249300	-7.10408200
C	0.01474800	-0.67260000	-7.30989000
C	-0.90203400	-1.00024000	-6.28067300
C	-0.97698000	-0.27241200	-5.09834700
H	-1.68303300	2.26830500	-0.94253400
H	0.07608000	2.13550700	-1.20415300
H	-0.82484800	3.59841200	-1.71501600
H	-1.51625000	0.82283300	-2.76883200
H	1.07650200	4.01750500	-2.47252400
H	2.92477100	5.30893100	-3.41318300
H	3.03993500	2.77689700	-6.91372900
H	1.62154100	0.67467900	-7.88176800
H	-1.57112100	-1.85277500	-6.40492100

H	-1.69205200	-0.55139300	-4.33001700
Sc	-4.38278500	2.31596200	-2.86468900
S	-3.63297800	4.57152500	-0.23743800
O	-2.38998600	4.26690400	0.46642200
O	-4.81864700	4.95560600	0.52223000
C	-3.21609900	6.02480200	-1.35227600
F	-2.84952900	7.06100100	-0.60917900
F	-2.20358600	5.69148700	-2.16329700
F	-4.26092900	6.37044300	-2.10151200
S	-4.36062300	-0.32778700	-0.89637300
O	-5.33027500	-1.23552200	-1.51439400
O	-4.73283300	0.37072800	0.33507500
C	-2.85540400	-1.36416100	-0.48640600
F	-3.15895700	-2.24582500	0.45568600
F	-2.44311600	-2.01266800	-1.57996000
F	-1.87057600	-0.57694500	-0.05986600
S	-5.67405400	4.25550300	-5.29197100
O	-7.08315900	3.86100900	-5.28819700
O	-4.83736700	3.87542000	-6.43758000
C	-5.62885900	6.12592600	-5.23833300
F	-6.16124200	6.60747800	-6.35540500
F	-6.31958000	6.57355200	-4.19342600
F	-4.36698000	6.53603900	-5.13774600
O	-3.96233400	3.51148100	-1.30049200
O	-3.70402900	0.60805400	-1.92805000
O	-4.97244200	3.95498100	-3.96114000
C	-8.94405300	1.37228900	-4.34725300
C	-7.67287600	0.66365400	-3.81724000
C	-6.51767700	0.83349500	-4.76884300
N	-5.27432200	1.02416600	-4.46216100
C	-4.51201400	0.59144300	-5.65507800
C	-4.27722200	-0.91255900	-5.64060100
C	-3.83156700	-1.71227000	-4.59001200
C	-3.68987800	-3.08741600	-4.80420200
C	-4.01646200	-3.64909400	-6.04677300
C	-4.53459900	-2.85075500	-7.07513700
C	-4.68071600	-1.47914300	-6.85801500
C	-5.30250400	-0.43080600	-7.75412500
C	-5.52455600	0.74188300	-6.80269300
O	-6.78040400	0.57302400	-6.04219200
C	-7.89584300	-0.87303000	-3.70912700
C	-7.38333500	1.22085800	-2.44387200
N	-6.42231200	1.99853700	-2.06443300
C	-6.81971800	2.52770700	-0.73037100
C	-7.89707100	1.53127000	-0.25986900
C	-9.04398800	2.34405400	0.33836100
C	-8.85653700	3.71219000	-0.28032800
C	-7.59003200	3.82616900	-0.86920400
C	-7.20245900	4.98994600	-1.53128200
C	-8.09993700	6.06045200	-1.58324500
C	-9.36157400	5.96116200	-0.97878300
C	-9.74959100	4.78516900	-0.32522600
O	-8.31205700	0.94238300	-1.54192000
H	-9.18485900	0.98057100	-5.34433000
H	-9.78322800	1.17273800	-3.66850300
H	-8.77724200	2.45421500	-4.42437900
H	-3.59039200	1.17743100	-5.77920600
H	-3.62441500	-1.27922900	-3.61406000
H	-3.33170000	-3.72347300	-3.99148400
H	-3.89649200	-4.72371500	-6.20438300
H	-4.84042400	-3.30038900	-8.02330600
H	-4.62030600	-0.11417600	-8.56189700
H	-6.24035900	-0.75839200	-8.22726400
H	-8.11314100	-1.28234700	-4.70457900
H	-7.00442900	-1.36229900	-3.29299700
H	-8.74890200	-1.06438000	-3.04508600
H	-5.95034600	2.59430500	-0.06869100
H	-7.52060200	0.70624800	0.35882800
H	-10.02010600	1.88510200	0.11953200
H	-8.93605400	2.37676800	1.43587800
H	-6.22951000	5.05556400	-2.01136900
H	-7.81470600	6.97607000	-2.10575100
H	-10.05318200	6.80622000	-1.02793100
H	-10.73970300	4.70503000	0.13120100
H	-5.56402800	1.73597400	-7.26379100
C	-1.93360000	3.57530800	-4.52385500
H	-2.85777800	4.06295700	-4.83537500
H	-1.29542300	4.29928300	-4.00211800
H	-1.41703600	3.18017800	-5.40872800
O	-2.29539300	2.49071600	-3.63701500
C	4.25039800	4.95049100	-5.76835400
C	5.29935400	4.35557400	-6.45622600
C	4.27643000	6.36806000	-5.58905000
C	6.38022800	5.11440300	-6.98066900
H	5.32069500	3.27032200	-6.58419000
C	5.30894800	7.13255600	-6.08451600
H	3.44794300	6.85507900	-5.07008800
C	7.46155100	4.50768100	-7.68230700
C	6.39048000	6.53738700	-6.79265100
H	5.30307200	8.21707900	-5.94491500
C	8.49861400	5.27081100	-8.17803100
H	7.45591000	3.42324800	-7.82309000
C	7.47377600	7.29621500	-7.31681600
C	8.50524300	6.67842900	-7.99458500
H	9.32156000	4.79281600	-8.71549700
H	7.47618200	8.38017100	-7.17253000
H	9.33279500	7.27121500	-8.39232700
C	-0.01004600	-1.43023900	-8.58754600
C	-1.20551400	-1.92132500	-9.09754900
C	1.18801200	-1.66632700	-9.32910000
C	-1.26148400	-2.64270200	-10.31922400
H	-2.14240800	-1.74227700	-8.56474500
C	1.16789500	-2.36149500	-10.51792500
H	2.14074500	-1.30936100	-8.93190900
C	-2.48717300	-3.14363400	-10.84512000
C	-0.04908300	-2.87073400	-11.05252800
H	2.09857900	-2.53939700	-11.06371200
C	-2.51222700	-3.83997200	-12.03586500
H	-3.41006300	-2.96715700	-10.28572800
C	-0.10833300	-3.59295700	-12.27681600
C	-1.31169800	-4.06745100	-12.75880500
H	-3.45871900	-4.22040600	-12.42833600
H	0.81772500	-3.76609400	-12.83201800
H	-1.34519400	-4.62044200	-13.70086400

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C	-1.21266900	1.33871000	-1.42105500
C	-1.03179300	2.25405200	-2.61584700
N	0.09784500	1.92540100	-3.43808300
C	0.19513300	0.78016500	-4.23538800
C	1.25991400	0.93902200	-5.15888900
C	1.83590000	2.24864800	-4.90558400
C	1.07969800	2.83333000	-3.85559300
C	1.36498200	4.12233400	-3.39387300

C	2.41921900	4.81158400	-3.99218800
C	3.19793700	4.25273800	-5.03624200
C	2.89255500	2.95797800	-5.48508200
C	1.50816800	-0.05310500	-6.11607000
C	0.69326300	-1.19659500	-6.16971500
C	-0.35216300	-1.32913300	-5.22339100
C	-0.61369500	-0.35792200	-4.26336200
H	-0.27616400	1.36368200	-0.84685300
H	-2.01067100	1.70484600	-0.76950400
H	-1.42541900	0.30370100	-1.70569500
H	-0.90103300	3.28169700	-2.25655200
H	0.78156500	4.59379600	-2.60151300
H	2.63364800	5.82763000	-3.65457600
H	3.48927800	2.49424100	-6.27333100
H	2.30487900	0.09316200	-6.84847400
H	-0.97728800	-2.22279500	-5.23274600
H	-1.43456000	-0.49038200	-3.56705000
Sc	-4.36729700	2.08709200	-2.68926600
S	-3.31100100	4.42486000	-0.25923700
O	-2.02749400	3.96629300	0.27332300
O	-4.32085900	4.98656000	0.62898700
C	-2.84834300	5.80432200	-1.45284800
F	-2.32118600	6.80821700	-0.76534300
F	-1.93649900	5.36107500	-2.33412000
F	-3.90486200	6.24209400	-2.12991600
S	-4.89122400	-0.50822300	-0.61459300
O	-5.64057800	-1.50043100	-1.38669900
O	-5.57100100	0.20617700	0.46794400
C	-3.47186100	-1.43209900	0.18613600
F	-3.94941800	-2.35120000	1.01455500
F	-2.73129800	-2.03166400	-0.75263600
F	-2.70189000	-0.58266000	0.85960300
S	-5.67087300	4.06053200	-5.10734000
O	-7.10795300	4.10601000	-4.84462000
O	-5.19362900	3.32794800	-6.28970700
C	-5.12118200	5.83242500	-5.35413500
F	-5.62001200	6.29007700	-6.49672000
F	-5.55199200	6.59083300	-4.35114100
F	-3.79015700	5.88613400	-5.40388700
O	-3.92066400	3.39010700	-1.21632900
O	-4.07332500	0.43067100	-1.51504700
O	-4.84415800	3.71649200	-3.86505800
C	-8.65922900	1.22244800	-4.87366100
C	-7.54147300	0.53621400	-4.04915500
C	-6.23400100	0.54339100	-4.80475500
N	-5.04226500	0.73970800	-4.33927400
C	-4.12267000	0.17146900	-5.35282400
C	-3.87527000	-1.31087400	-5.12361600
C	-3.50222400	-1.95658100	-3.94661400
C	-3.31591100	-3.34242600	-3.96851400
C	-3.51807700	-4.06579900	-5.15258700
C	-3.94645300	-3.41856200	-6.31907700
C	-4.13827000	-2.03531100	-6.29451400
C	-4.65176500	-1.12411600	-7.38723500
C	-4.96167200	0.17363900	-6.64357300
O	-6.31623200	0.13815400	-6.06513900
C	-7.87710500	-0.96849000	-3.82168100
C	-7.45848900	1.22063700	-2.70246700
N	-6.50806000	1.93798100	-2.20453100
C	-7.03144800	2.55144000	-0.95176700
C	-8.29737900	1.71415000	-0.65620800
C	-9.42666300	2.68408300	-0.30833500
C	-8.93181600	4.01220500	-0.83653400
C	-7.57253500	3.94959300	-1.17235800
C	-6.89868300	5.06673600	-1.66191200
C	-7.60482400	6.26244800	-1.81728200
C	-8.96429700	6.33302000	-1.48233000
C	-9.63651400	5.20855800	-0.98795800
O	-8.54844000	1.08814500	-1.96111400
H	-8.76889500	0.70169300	-5.83388500
H	-9.60652300	1.15979200	-4.32242300
H	-8.41284000	2.27565100	-5.05809400
H	-3.18975200	0.74476500	-5.41727400
H	-3.38454400	-1.39621400	-3.02257900
H	-3.02082700	-3.85883900	-3.05235900
H	-3.36456000	-5.14765500	-5.15990100
H	-4.14627200	-3.99211600	-7.22789700
H	-3.88349500	-0.92754900	-8.15443900
H	-5.53869700	-1.51666700	-7.90711400
H	-7.94258700	-1.47704400	-4.79258700
H	-7.10675600	-1.44740000	-3.20246500
H	-8.84505200	-1.04346200	-3.30916900
H	-6.26751000	2.49360600	-0.16682900
H	-8.13860500	0.89477300	0.05623600
H	-10.38157100	2.35746200	-0.74777300
H	-9.56527500	2.71397700	0.78556500
H	-5.85019700	5.00016600	-1.93365200
H	-7.09167500	7.14166500	-2.21279500
H	-9.50606700	7.27351800	-1.61186400
H	-10.69723600	5.26580300	-0.72976700
H	-4.90338100	1.09249100	-7.23872300
C	-2.09016300	3.04820700	-4.66528300
H	-3.02148200	2.98840500	-5.23203600
H	-1.89241400	4.09652400	-4.40582900
H	-1.27553000	2.63910900	-5.27465100
O	-2.25068000	2.26247400	-3.45562700
C	4.30893200	5.02783300	-5.64825200
C	4.57194200	4.95695400	-7.00966900
C	5.13787000	5.86794700	-4.84241100
C	5.63347400	5.68675400	-7.60926600
H	3.93746100	4.34488500	-7.65576500
C	6.17429500	6.58908600	-5.39201100
H	4.95943200	5.91805200	-3.76602400
C	5.90404300	5.62016500	-9.00645000
C	6.45727600	6.52498100	-6.78525500
H	6.80257700	7.21732100	-4.75459900
C	6.94106600	6.34227900	-9.56027200
H	5.27488600	4.98398600	-9.63518900
C	7.51926700	7.25623300	-7.38663000
C	7.75726900	7.16780900	-8.74329300
H	7.13867200	6.28109700	-10.63350300
H	8.14526600	7.89201700	-6.75439800
H	8.57555600	7.73446000	-9.19469000
C	0.88123700	-2.23783700	-7.21266700
C	-0.20667500	-2.92699000	-7.73442400
C	2.18275500	-2.55553200	-7.70909100
C	-0.05471300	-3.92735600	-8.73061400
H	-1.21812000	-2.69533400	-7.39191800
C	2.36390800	-3.51849400	-8.67700700
H	3.05246600	-2.04195500	-7.29347600
C	-1.16921800	-4.63551300	-9.26561500
C	1.25944900	-4.23440800	-9.21885500
H	3.37045200	-3.75263700	-9.03448000
C	-0.99251000	-5.60277400	-10.23334000

H	-2.16924800	-4.40000900	-8.89155300
C	1.40826100	-5.23730800	-10.21688100
C	0.30832400	-5.90707100	-10.71390800
H	-1.85536700	-6.14061100	-10.63440400
H	2.41136000	-5.46969600	-10.58510600
H	0.43469300	-6.67554600	-11.48064800

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C	-0.86138100	2.52814200	-1.63031200
C	-1.12801300	1.84725000	-2.95584100
N	-0.02377500	1.72926400	-3.86511700
C	-0.10682400	0.82846600	-4.93306500
C	0.86199300	1.14537800	-5.91251000
C	1.59558100	2.28848300	-5.39987500
C	1.01707000	2.63290800	-4.14546500
C	1.51462500	3.72134700	-3.41723600
C	2.57428800	4.44889300	-3.95485400
C	3.16223900	4.12072400	-5.19881000
C	2.66124800	3.02648700	-5.91828600
C	0.91427600	0.41165800	-7.10349400
C	-0.00562100	-0.62928300	-7.30767400
C	-0.92962600	-0.95599300	-6.28606000
C	-0.99062500	-0.23595400	-5.10045500
H	-1.68518400	2.29586100	-0.94751600
H	0.07515900	2.15203800	-1.19557100
H	-0.81484000	3.61920600	-1.71626800
H	-1.50300100	0.83851700	-2.76111800
H	1.10433000	4.01147900	-2.45406300
H	2.96230800	5.29590700	-3.38821900
H	3.09365400	2.75160900	-6.88092700
H	1.64395800	0.66462000	-7.87392500
H	-1.62373500	-1.78408300	-6.42806200
H	-1.71501200	-0.50341200	-4.33708800
Sc	-4.39221000	2.30240600	-2.90657900
S	-3.65252600	4.62504700	-0.32837100
O	-2.41496500	4.32918400	0.38885100
O	-4.84461200	5.01245100	0.41954300
C	-3.23159800	6.07054900	-1.45110800
F	-2.94334400	7.13480200	-0.71374000
F	-2.16614600	5.75878000	-2.20042300
F	-4.24734500	6.36014300	-2.26201900
S	-4.35100500	-0.29119500	-0.88500800
O	-5.30934700	-1.21683500	-1.49318200
O	-4.73782200	0.43150000	0.32793000
C	-2.84344900	-1.30904900	-0.43867300
F	-3.15118500	-2.17322500	0.51795200
F	-2.41466800	-1.97649900	-1.51413600
F	-1.86841000	-0.50629100	-0.01772700
S	-5.62420600	4.13935400	-5.44342100
O	-7.02400600	3.71727600	-5.51006200
O	-4.71557100	3.74273000	-6.52662100
C	-5.61827500	6.01119900	-5.43447700
F	-6.11310400	6.45676200	-6.58302800
F	-6.35992700	6.46672500	-4.42872500
F	-4.36960200	6.44958900	-5.29163100
O	-3.96971000	3.55698700	-1.38739500
O	-3.68934900	0.62826000	-1.92931000
O	-4.99494100	3.89181100	-4.06545400
C	-8.94151200	1.35718700	-4.33203700
C	-7.68725400	0.62770800	-3.78763100
C	-6.53401300	0.75335600	-4.74812800
N	-5.28876300	0.95428800	-4.45622300
C	-4.53521800	0.49158900	-5.64453100
C	-4.28574500	-1.00890100	-5.59612100
C	-3.80093300	-1.77860200	-4.53954300
C	-3.62947000	-3.15313700	-4.73337800
C	-3.95759500	-3.74240900	-5.96377000
C	-4.50899300	-2.97506500	-6.99750100
C	-4.69426000	-1.60638900	-6.79592200
C	-5.33886200	-0.58933700	-7.70910900
C	-5.55881100	0.60587000	-6.78670000
O	-6.80653400	0.45273900	-6.00977800
C	-7.94669500	-0.89908800	-3.64128700
C	-7.38438300	1.21524800	-2.43016900
N	-6.41956500	2.00170200	-2.07818700
C	-6.81386300	2.57684000	-0.76258600
C	-7.89213000	1.59953800	-0.25610200
C	-9.03662300	2.43510800	0.31494800
C	-8.84874500	3.77952500	-0.35360200
C	-7.58296500	3.87050000	-0.94789100
C	-7.19651600	5.00783200	-1.65546000
C	-8.09387100	6.07572800	-1.74730700
C	-9.35440500	6.00032800	-1.13696000
C	-9.74153000	4.85041100	-0.43809900
O	-8.31005500	0.96762500	-1.51657300
H	-9.19763700	0.94524900	-5.31701200
H	-9.78279500	1.20136300	-3.64448000
H	-8.74366700	2.43143800	-4.44120300
H	-3.61981800	1.08164900	-5.79509100
H	-3.58636900	-1.32336900	-3.57509900
H	-3.24362700	-3.76721700	-3.91630600
H	-3.80833000	-4.81570000	-6.10622300
H	-4.79638300	-3.43720900	-7.94498800
H	-4.66778000	-0.29984200	-8.53383300
H	-6.28064100	-0.93845100	-8.15858000
H	-8.17370600	-1.32811000	-4.62615200
H	-7.06610100	-1.39822500	-3.21364100
H	-8.80350200	-1.05445900	-2.97273500
H	-5.94429200	2.66494200	-0.10416400
H	-7.51662000	0.79578200	0.39042200
H	-10.01390000	1.96997800	0.11519800
H	-8.92600200	2.50733600	1.41031300
H	-6.22490300	5.05462300	-2.14075400
H	-7.80943000	6.97023900	-2.30571800
H	-10.04595700	6.84301400	-1.21741500
H	-10.73102100	4.78801000	0.02240200
H	-5.60729300	1.58707700	-7.27405000
C	-1.91683500	3.60334000	-4.50201700
H	-2.83949100	4.10956500	-4.78629900
H	-1.26514700	4.30589700	-3.96847000
H	-1.41683100	3.22852000	-5.40532900
O	-2.27827600	2.49655400	-3.64267700
C	4.29247500	4.92351600	-5.72922100
C	5.41939200	4.34209500	-6.29227800
C	4.27165600	6.34359100	-5.68352300
C	6.51674700	5.08612200	-6.80507900
C	5.30599900	7.11896100	-6.15942300
C	7.67014900	4.48045100	-7.37851700
C	6.45997900	6.52425500	-6.73252900
C	8.71132400	5.24827700	-7.85631400
C	7.55124500	7.28218900	-7.23498400
C	8.65200300	6.65857300	-7.78402400
C	-0.06005400	-1.38139300	-8.58461800
C	-1.26747100	-1.65679000	-9.20947800

C	1.10759900	-1.86848300	-9.22759800
C	-1.38686300	-2.42624200	-10.39540000
C	1.06085100	-2.59584900	-10.39790600
C	-2.63733800	-2.74433200	-10.99538800
C	-0.17888700	-2.90552300	-11.01744900
C	-2.69793900	-3.48820900	-12.15421000
C	-0.28055000	-3.66670400	-12.21290500
C	-1.51078100	-3.94894500	-12.76943800
F	3.20521700	6.96518000	-5.17311000
F	5.48688900	3.00620600	-6.34580100
F	7.77734200	3.15656900	-7.47321400
F	9.78527600	4.67763700	-8.39185700
F	9.67114600	7.36917700	-8.25299200
F	7.53866300	8.61327900	-7.18720800
F	5.19499900	8.44616400	-6.08201900
F	2.30017400	-1.62617700	-8.67882400
F	2.20760100	-3.01868200	-10.93181000
F	0.80886300	-4.12738300	-12.82411600
F	-1.60280600	-4.66225400	-13.88565400
F	-3.86718400	-3.78956400	-12.70838400
F	-3.78818700	-2.34949100	-10.44421400
F	-2.39092200	-1.16143900	-8.67142900

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C	-1.14042300	1.41740100	-1.51259700
C	-1.02774300	2.31617000	-2.72777900
N	0.09251000	2.00360700	-3.57804500
C	0.17285400	0.86855000	-4.38690200
C	1.20305700	1.04538400	-5.34658700
C	1.78724400	2.34981800	-5.08738100
C	1.05713700	2.91924800	-4.00968000
C	1.34415600	4.20605000	-3.54175700
C	2.37159800	4.91164200	-4.16379300
C	3.12211500	4.36186100	-5.23194100
C	2.81976200	3.07091400	-5.69093700
C	1.40689000	0.07773600	-6.33741200
C	0.57182400	-1.04944900	-6.37903700
C	-0.42473100	-1.21673300	-5.38817100
C	-0.63408800	-0.27103800	-4.39339200
H	-0.18694900	1.47986300	-0.97010700
H	-1.92769400	1.77128700	-0.84165900
H	-1.33141000	0.37155400	-1.77407700
H	-0.91629300	3.35413000	-2.39205500
H	0.78842600	4.65910000	-2.71970500
H	2.60593400	5.91598600	-3.80951600
H	3.38028000	2.63308600	-6.51768400
H	2.18221100	0.21998000	-7.09170400
H	-1.06192700	-2.10067500	-5.40608500
H	-1.42291500	-0.41629700	-3.66385100
Sc	-4.36216500	2.05958600	-2.69182400
S	-3.26509900	4.49124600	-0.37142300
O	-1.95305300	4.07154400	0.12304600
O	-4.25580300	5.04681500	0.54164200
C	-2.87597900	5.85793600	-1.60565900
F	-2.38627900	6.90144700	-0.95066200
F	-1.95409200	5.43130600	-2.48538100
F	-3.95691800	6.23074700	-2.28290800
S	-4.74796800	-0.46143400	-0.50355400
O	-5.49586200	-1.50283600	-1.20880400
O	-5.41063500	0.28268600	0.56945000
C	-3.28093300	-1.31510800	0.28928500
F	-3.70870500	-2.20989600	1.16970900
F	-2.55314800	-1.93488600	-0.64631600
F	-2.51356100	-0.41858400	0.90246700
S	-5.77862100	3.91178100	-5.13854500
O	-7.20877500	3.92931400	-4.83786800
O	-5.31243700	3.15021100	-6.30681000
C	-5.28284800	5.68749600	-5.46037200
F	-5.83634600	6.09819900	-6.59533100
F	-5.69176200	6.46637600	-4.46403600
F	-3.95603700	5.77023500	-5.56462200
O	-3.88325000	3.42542600	-1.28756800
O	-3.98268800	0.45816500	-1.46877400
O	-4.91056200	3.63399900	-3.90756200
C	-8.69589200	1.01279000	-4.70559400
C	-7.53595000	0.38952100	-3.88963600
C	-6.25319100	0.39615200	-4.68671800
N	-5.05271000	0.63847300	-4.26653800
C	-4.15146000	0.04722000	-5.28345300
C	-3.86152600	-1.41796400	-5.00043600
C	-3.41804700	-2.00378000	-3.81557600
C	-3.18211600	-3.38171000	-3.79465600
C	-3.39749800	-4.15506000	-4.94550100
C	-3.88991300	-3.56885900	-6.11793600
C	-4.14109800	-2.19559300	-6.13142200
C	-4.70820700	-1.34523700	-7.24435400
C	-5.02733300	-0.02430200	-6.54737600
O	-6.36387900	-0.06283600	-5.92563200
C	-7.82491900	-1.11232400	-3.58939100
C	-7.42875300	1.12981200	-2.57451200
N	-6.47876700	1.88349300	-2.13173900
C	-6.97737800	2.53374800	-0.88724400
C	-8.21716000	1.68413500	-0.52363700
C	-9.35526600	2.64456200	-0.17820800
C	-8.90228500	3.96164300	-0.76794900
C	-7.55235200	3.91248400	-1.14156000
C	-6.91473400	5.02432800	-1.68851800
C	-7.64836900	6.20058300	-1.86394600
C	-8.99888700	6.25739800	-1.49211900
C	-9.63443200	5.13858600	-0.93987000
O	-8.49344400	1.00513400	-1.79641600
H	-8.82198700	0.44883700	-5.63902000
H	-9.62382400	0.95114200	-4.12228200
H	-8.48196700	2.06268500	-4.94214200
H	-3.23473600	0.63853900	-5.40201900
H	-3.28336500	-1.40455200	-2.91833400
H	-2.83475400	-3.85305500	-2.87244200
H	-3.19903600	-5.22953300	-4.91971500
H	-4.07356800	-4.17231400	-7.00986800
H	-3.96220700	-1.17450700	-8.03758400
H	-5.59988600	-1.77984700	-7.72083200
H	-7.90533500	-1.66298500	-4.53586400
H	-7.02380600	-1.54499200	-2.97509900
H	-8.77492600	-1.18995100	-3.04470900
H	-6.18991200	2.51938100	-0.12379200
H	-8.02152200	0.89507100	0.21347800
H	-10.31545700	2.28390300	-0.57768600
H	-9.46348100	2.71190100	0.91743800
H	-5.87303600	4.96826900	-1.98768300
H	-7.16410900	7.07509300	-2.30378600
H	-9.56246300	7.18257100	-1.63786100
H	-10.68814600	5.18514300	-0.65250300
H	-5.00819800	0.86987300	-7.18151300
C	-2.17580600	3.04384700	-4.75437800

H	-3.10275200	2.89623500	-5.31251400
H	-2.06470800	4.10847500	-4.51153600
H	-1.33604500	2.69391800	-5.36604100
O	-2.26281200	2.26493400	-3.53204900
C	4.21549800	5.14574100	-5.85965700
C	5.45232000	4.59133400	-6.15616000
C	4.04209500	6.51564100	-6.19434900
C	6.51537000	5.31530500	-6.76148700
C	5.03536100	7.27092700	-6.77802000
C	7.78140800	4.73785600	-7.06096700
C	6.30050600	6.70397200	-7.08107700
C	8.78154900	5.48538000	-7.64639300
C	7.35391700	7.44213200	-7.68383900
C	8.56686300	6.84672300	-7.95996500
C	0.67350200	-2.05480200	-7.46437100
C	-0.45457100	-2.52892800	-8.11765700
C	1.91816900	-2.59180700	-7.88358700
C	-0.42449200	-3.53709900	-9.11552500
C	2.01704900	-3.55233100	-8.86767600
C	-1.59481400	-4.04950900	-9.74213200
C	0.85788800	-4.06249800	-9.51026400
C	-1.50996400	-5.02635500	-10.71085400
C	0.90635600	-5.06567700	-10.51536900
C	-0.24998600	-5.53478900	-11.10329300
F	2.86724300	7.10321300	-5.95191700
F	5.66415900	3.30621600	-5.84684700
F	8.03668800	3.45957500	-6.78891900
F	9.96098300	4.94058200	-7.92567400
F	9.55022100	7.53882000	-8.52359500
F	7.19641200	8.72742500	-7.99619900
F	4.77855600	8.54813100	-7.06581600
F	3.03920200	-2.16323500	-7.29936700
F	-1.64509700	-2.00138200	-7.79828500
F	-2.80986100	-3.61451400	-9.39713000
F	-2.60519800	-5.50827400	-11.28815100
F	-0.20167600	-6.47423000	-12.04043900
F	2.06884300	-5.57828500	-10.91331000
F	3.22727100	-4.00667900	-9.19584100

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C	-0.86543300	2.17401300	-1.84066200
C	-1.22189300	1.62472500	-3.20690700
N	-0.17126200	1.57230200	-4.17169600
C	-0.24032700	0.69212000	-5.26252400
C	0.74096900	1.03633200	-6.21915600
C	1.45408400	2.18012500	-5.68186300
C	0.86467500	2.49336800	-4.42514300
C	1.34084900	3.57806400	-3.67790600
C	2.39832500	4.32637700	-4.19739900
C	3.00288900	4.02818200	-5.43930900
C	2.51558000	2.94172900	-6.17926400
C	0.84409500	0.30057100	-7.40665200
C	-0.02766500	-0.77448800	-7.64003100
C	-0.98634700	-1.10696900	-6.65200100
C	-1.10068000	-0.38643000	-5.46640000
H	-1.63659100	1.87221700	-1.12464500
H	0.10096200	1.76661900	-1.51280200
H	-0.82484900	3.26777800	-1.82542400
H	-1.61569500	0.61111300	-3.09046600
H	0.91676300	3.85135600	-2.71559500
H	2.78087800	5.16837400	-3.61631600
H	2.95043800	2.69982300	-7.15129700
H	1.58887300	0.57036300	-8.15868600
H	-1.65288900	-1.95713100	-6.81044300
H	-1.84078500	-0.67444500	-4.72611800
Sc	-4.41012400	2.28599200	-2.77485000
S	-3.31587400	4.31526700	-0.08737000
O	-2.03136000	3.90872900	0.47632500
O	-4.40642800	4.70324300	0.80156800
C	-2.92693000	5.81636400	-1.14804100
F	-2.41328100	6.77400800	-0.38704500
F	-2.03249900	5.48143100	-2.08785500
F	-4.02183300	6.27462200	-1.75017700
S	-4.34971600	-0.52069000	-1.02745500
O	-5.38947000	-1.34721900	-1.64444900
O	-4.60676800	0.07692000	0.28397100
C	-2.85069500	-1.62565100	-0.82579500
F	-3.11936300	-2.59762700	0.03424900
F	-2.52358200	-2.16102500	-2.00675200
F	-1.82028100	-0.90960500	-0.38243000
S	-5.83131600	4.46560200	-4.90199800
O	-7.25065000	4.13808300	-4.76402800
O	-5.14984900	4.12836700	-6.15953600
C	-5.67925900	6.32334000	-4.73540000
F	-6.30241400	6.90475500	-5.75383300
F	-6.22884400	6.72976500	-3.59422900
F	-4.39402100	6.66601700	-4.74980700
O	-3.79565200	3.34200900	-1.17616000
O	-3.74284800	0.48540500	-2.02214300
O	-5.00226200	4.03985300	-3.68359800
C	-9.12224400	1.61702100	-3.89363800
C	-7.83712100	0.82736700	-3.53848700
C	-6.77012300	1.03641800	-4.58137600
N	-5.49918200	1.18629900	-4.38769100
C	-4.86325200	0.84340400	-5.67999500
C	-4.63420800	-0.65590600	-5.79732200
C	-4.08527300	-1.52437000	-4.85612900
C	-3.98688100	-2.88361300	-5.17115200
C	-4.45555200	-3.36090400	-6.40352900
C	-5.07014400	-2.49445800	-7.31651500
C	-5.17421800	-1.13915800	-6.99728300
C	-5.87781800	-0.03057900	-7.74933000
C	-5.98575800	1.07770400	-6.70561500
O	-7.16189900	0.87280100	-5.83765600
C	-8.11199200	-0.70421300	-3.52328800
C	-7.40336400	1.27032800	-2.16155500
N	-6.38086900	1.98392000	-1.81875700
C	-6.63293600	2.42648700	-0.41954700
C	-7.70759700	1.43926000	0.07693600
C	-8.76170300	2.24895300	0.83020500
C	-8.56743500	3.65121100	0.29578500
C	-7.35260300	3.76071100	-0.39416100
C	-6.97098400	4.95598900	-1.00152800
C	-7.82087000	6.06085400	-0.89613200
C	-9.02937700	5.96426200	-0.19108200
C	-9.41211000	4.75791800	0.40791600
O	-8.25821400	0.95898900	-1.19953400
H	-9.46908200	1.31057900	-4.88926600
H	-9.90309800	1.39435300	-3.15514000
H	-8.91965800	2.69559000	-3.90656800
H	-3.95864300	1.44196700	-5.85425100
H	-3.77218800	-1.15587800	-3.88198500
H	-3.55280400	-3.57350700	-4.44379800
H	-4.36881700	-4.42392100	-6.64140600

H	-5.47636700	-2.87817800	-8.25519700
H	-5.28310500	0.34236000	-8.60083300
H	-6.86322400	-0.32238700	-8.14239700
H	-8.44078800	-1.02662100	-4.52008300
H	-7.20606100	-1.25438700	-3.23450400
H	-8.90472000	-0.91764200	-2.79434000
H	-5.70526700	2.40963800	0.16142200
H	-7.31416100	0.55895000	0.60151100
H	-9.77240500	1.84508700	0.66684000
H	-8.55909600	2.19605200	1.91345100
H	-6.04066800	5.02090900	-1.55988200
H	-7.54072500	7.00194200	-1.37416800
H	-9.68414200	6.83645900	-0.11754300
H	-10.36179700	4.68146800	0.94393700
H	-6.05388900	2.10042900	-7.09489600
C	-2.07700000	3.47657600	-4.62468300
H	-3.01391700	3.96742600	-4.89249400
H	-1.42383600	4.18964100	-4.10596400
H	-1.59053300	3.10902200	-5.53775600
O	-2.40473600	2.36652100	-3.75678300
C	0.10148600	-1.58901300	-8.88098800
C	-1.04057300	-1.84934900	-9.74988500
C	1.32889900	-2.10962800	-9.20783900
C	-2.31683700	-1.29404800	-9.52960200
C	-0.85458800	-2.68735200	-10.90092100
C	1.54457700	-2.93264900	-10.36267000
H	2.18036000	-1.92014000	-8.54914300
C	-3.38544500	-1.57596000	-10.38356500
H	-2.47889100	-0.63123600	-8.67988500
C	-1.96006800	-2.97420100	-11.76641900
C	0.43154900	-3.23067600	-11.20666000
C	2.80846900	-3.46722100	-10.67655800
C	-3.21847100	-2.41347300	-11.48458100
H	-4.36379500	-1.13312100	-10.18506300
C	-1.74875300	-3.82333800	-12.90998900
C	0.61527200	-4.06477100	-12.35499700
H	3.65889500	-3.23900800	-10.02871900
C	2.97876500	-4.27985800	-11.79909000
H	-4.06129400	-2.63252600	-12.14532400
C	-0.52083700	-4.34576700	-13.19187300
H	-2.60283200	-4.03913600	-13.55752100
C	1.89668300	-4.57760500	-12.63037200
H	3.96681000	-4.68635300	-12.02907200
H	-0.37849900	-4.98629600	-14.06632900
H	2.03721500	-5.21404100	-13.50801600
C	4.09490200	4.89503600	-5.96586200
C	5.38546500	4.34228400	-6.35592600
C	3.87344900	6.24390500	-6.08775700
C	5.71937000	2.98380100	-6.18770600
C	6.37517900	5.22286200	-6.90737700
C	4.85238100	7.14793000	-6.62000100
H	2.90249700	6.65363400	-5.79708900
C	6.96617000	2.49099900	-6.57958600
H	4.99754100	2.30433400	-5.73438100
C	7.64875600	4.70572000	-7.31198000
C	6.11051100	6.62057600	-7.04396100
C	4.60526600	8.52741000	-6.75317300
C	7.91977200	3.33578700	-7.14579200
H	7.19444600	1.43193900	-6.43594000
C	8.62134200	5.60928000	-7.87012800
C	7.09876200	7.49716900	-7.59443500
H	3.64154400	8.92942100	-6.42966100
C	5.57476100	9.37535700	-7.29225700
H	8.89193400	2.94282600	-7.45483200
C	8.36012200	6.94099500	-8.00718100
H	9.58642000	5.20078200	-8.18175200
C	6.80800000	8.86937900	-7.70933100
H	5.36697100	10.44398400	-7.38847700
H	9.11180400	7.61233000	-8.43092800
H	7.56276100	9.53941200	-8.12939600

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C	-1.24459600	1.54964500	-2.27438600
C	-1.31787900	2.53947400	-3.42033400
N	-0.29349400	2.31263400	-4.40747100
C	-0.20062900	1.18850500	-5.22575300
C	1.02771200	1.21879900	-5.93289200
C	1.71316200	2.42883200	-5.51143400
C	0.86100400	3.07979000	-4.57557300
C	1.22878000	4.29147200	-3.98169300
C	2.45936700	4.84360700	-4.33922900
C	3.32957400	4.21897200	-5.26432900
C	2.94154100	3.00457000	-5.85103900
C	1.33067200	0.18625100	-6.83150500
C	0.41168700	-0.85539500	-7.03950200
C	-0.82240100	-0.83221800	-6.34359900
C	-1.13679200	0.17534100	-5.43895200
H	-0.23085700	1.61218800	-1.85445600
H	-1.94812800	1.80983500	-1.47957100
H	-1.42680000	0.52212600	-2.61051600
H	-1.19414900	3.55792500	-3.03174600
H	0.58559900	4.79869400	-3.26066400
H	2.77056200	5.78505200	-3.88113500
H	3.59150700	2.51644300	-6.58036000
H	2.28390600	0.18422900	-7.36504400
H	-1.55928400	-1.61662400	-6.52518500
H	-2.08852600	0.17898100	-4.92197500
Sc	-4.60661800	2.16112500	-2.94234100
S	-3.24147200	4.52228700	-0.68816900
O	-1.86791100	4.11518500	-0.39135800
O	-4.12454400	4.97495100	0.38015400
C	-3.05269300	5.97940500	-1.86465600
F	-2.55072700	7.01002500	-1.19880900
F	-2.20974400	5.65529800	-2.85837300
F	-4.21687500	6.32796800	-2.40429100
S	-4.54116800	-0.47677600	-0.84849700
O	-5.34297900	-1.53014500	-1.47113300
O	-5.05023200	0.18836900	0.35257000
C	-2.92417300	-1.28210600	-0.35249700
F	-3.16105700	-2.25463700	0.51781600
F	-2.32188100	-1.79625500	-1.43001800
F	-2.11819700	-0.37922200	0.19855100
S	-6.37475800	3.99979000	-5.15564800
O	-7.75827400	3.90683500	-4.69497900
O	-5.99923600	3.32439600	-6.40631000
C	-6.02537200	5.81679000	-5.43724000
F	-6.77207100	6.25738800	-6.44262700
F	-6.30706000	6.51403900	-4.34055000
F	-4.73786100	5.98221000	-5.74073900
O	-3.94196000	3.50399500	-1.59839200
O	-3.99583100	0.52308800	-1.87979800
O	-5.35600100	3.72810700	-4.04454500
C	-9.25859300	1.08514500	-3.97430700
C	-7.95155300	0.43599200	-3.44874800

C	-6.87820700	0.48033100	-4.50932200
N	-5.62866700	0.78667700	-4.37742800
C	-4.95632900	0.28786200	-5.59925600
C	-4.45992400	-1.14099200	-5.44226400
C	-3.67098900	-1.68484400	-4.42867500
C	-3.30311300	-3.03123000	-4.50983700
C	-3.73605200	-3.82102000	-5.58386200
C	-4.57575600	-3.28546300	-6.56867900
C	-4.94738800	-1.94154200	-6.48497100
C	-5.87302900	-1.15439100	-7.38638200
C	-6.10650200	0.14331300	-6.61415100
O	-7.25092500	0.01977700	-5.69676400
C	-8.18153100	-1.07049100	-3.13306200
C	-7.56218200	1.15526000	-2.17642200
N	-6.56122000	1.93945800	-1.95110900
C	-6.79841500	2.57642200	-0.62603400
C	-7.89755200	1.68933400	0.00157000
C	-8.96269400	2.61542700	0.58908700
C	-8.70369400	3.93722100	-0.09879400
C	-7.46963200	3.92822700	-0.76287000
C	-7.02014600	5.04445200	-1.46590400
C	-7.82367300	6.18767800	-1.49457600
C	-9.05568600	6.20703000	-0.82556200
C	-9.50385900	5.08179700	-0.12296600
O	-8.42271500	0.99484400	-1.18191900
H	-9.58778000	0.55108300	-4.87531600
H	-10.03762800	1.00435400	-3.20511600
H	-9.09279900	2.14121100	-4.22197300
H	-4.16921800	0.98148700	-5.92493800
H	-3.36500000	-1.08121000	-3.57742000
H	-2.67942300	-3.46530300	-3.72524300
H	-3.42913200	-4.86791200	-5.64398400
H	-4.94245300	-3.91384400	-7.38430100
H	-5.40312200	-0.92152600	-8.35688600
H	-6.82036000	-1.67213900	-7.60070000
H	-8.48084300	-1.59215300	-4.05162100
H	-7.26733000	-1.52475600	-2.72881800
H	-8.98451300	-1.16063400	-2.38991200
H	-5.86387100	2.60344400	-0.05299000
H	-7.52009100	0.91129800	0.67617600
H	-9.97489100	2.21686400	0.42120400
H	-8.82125400	2.69530900	1.68016900
H	-6.07317300	5.01582200	-1.99617700
H	-7.48934900	7.06550600	-2.05161100
H	-9.67556400	7.10675200	-0.85809200
H	-10.46815600	5.09739100	0.39177200
H	-6.29419900	1.03393300	-7.22517900
C	-2.72746800	3.36044200	-5.22334600
H	-3.66948800	3.14291800	-5.73254700
H	-2.72320300	4.40882200	-4.89761100
H	-1.89091500	3.16333100	-5.90368000
O	-2.63429000	2.48720400	-4.06748800
C	0.69435200	-1.93607700	-8.02470300
C	0.53493700	-3.34426800	-7.67642900
C	1.08915200	-1.59853500	-9.29560300
C	0.21675600	-3.78359600	-6.37567800
C	0.73462200	-4.33486300	-8.69564500
C	1.32523900	-2.57150600	-10.32298000
H	1.19588200	-0.54282900	-9.55819300
C	0.04819600	-5.13994700	-6.08825800
H	0.10253400	-3.05661200	-5.57240200
C	0.55681000	-5.72400000	-8.39102500
C	1.12671300	-3.95245000	-10.01582900
C	1.71917600	-2.20673200	-11.62446300
C	0.20286800	-6.10322100	-7.08380400
H	-0.20444600	-5.44433000	-5.06945700
C	0.75661300	-6.69685200	-9.43380000
C	1.32834300	-4.94154000	-11.03026500
H	1.86932300	-1.14950800	-11.85856300
C	1.91537500	-3.17850700	-12.60767600
H	0.06531100	-7.16310800	-6.85405600
C	1.12403300	-6.32556700	-10.69376400
H	0.61077300	-7.75253300	-9.18955200
C	1.72221300	-4.53101300	-12.31762100
H	2.22217400	-2.87824800	-13.61273800
H	1.27486300	-7.07883900	-11.47166100
H	1.87777000	-5.28657300	-13.09221300
C	4.61206200	4.88003500	-5.63936000
C	5.88981100	4.19006000	-5.51439500
C	4.58506900	6.16798300	-6.11277000
C	6.01260400	2.89918500	-4.96304200
C	7.08311200	4.86322000	-5.94118200
C	5.76565200	6.86979100	-6.52821200
H	3.62434600	6.68084500	-6.20814100
C	7.25484700	2.26802500	-4.86651200
H	5.12495000	2.38478000	-4.59491000
C	8.35180200	4.20436800	-5.84312400
C	7.02359800	6.19726900	-6.45023700
C	5.72020600	8.18656600	-7.02420500
C	8.41313800	2.90438300	-5.31022100
H	7.31600400	1.26600000	-4.43460900
C	9.53303700	4.89932300	-6.28533600
C	8.21488700	6.86753600	-6.87417200
H	4.75693700	8.69992600	-7.08451800
C	6.88731200	8.83286200	-7.43621000
H	9.38171700	2.40296700	-5.23629700
C	9.46951700	6.16934200	-6.77878100
H	10.49381300	4.38266100	-6.21211200
C	8.12188900	8.18370000	-7.36386900
H	6.83438300	9.85542100	-7.81834900
H	10.37746100	6.68232300	-7.10707500
H	9.03178600	8.69624000	-7.68714400

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C	-0.97683200	2.03030400	-1.91924700
C	-1.34583000	1.58720000	-3.32212600
N	-0.28930100	1.61448200	-4.29175600
C	-0.35179100	0.85180800	-5.46668800
C	0.71747100	1.20700900	-6.32234600
C	1.46327800	2.24401400	-5.64091100
C	0.81301100	2.48490800	-4.39838400
C	1.30703400	3.47027600	-3.53074500
C	2.44182400	4.18943000	-3.90872800
C	3.08204200	3.93556000	-5.13373600
C	2.60404000	2.96666100	-6.01148000
C	0.87120600	0.57579300	-7.56421700
C	-0.05858900	-0.39885800	-7.92351000
C	-1.12168100	-0.75483500	-7.07326400
C	-1.27468500	-0.12824500	-5.83691200
H	-1.75456400	1.69967700	-1.22507800
H	-0.01936100	1.58194500	-1.62009200
H	-0.91554900	3.11892900	-1.82796400
H	-1.73883500	0.56450100	-3.28447000
H	0.83699300	3.70067600	-2.57976600

H	2.83341200	4.95883800	-3.24176700
H	3.09898900	2.77647600	-6.96489400
H	1.69221800	0.84178400	-8.23146500
H	-1.83335200	-1.52462700	-7.37620000
H	-2.09419100	-0.42277900	-5.18975700
Sc	-4.55371500	2.25925700	-2.87862100
S	-3.42330800	4.45249600	-0.35009900
O	-2.27540400	3.80683900	0.28086700
O	-4.52063500	4.94225600	0.47998900
C	-2.73722200	5.95186300	-1.24527800
F	-2.40262300	6.88474300	-0.36479900
F	-1.64806500	5.60187600	-1.94283900
F	-3.64166400	6.44441100	-2.08977300
S	-4.55592500	-0.18502800	-0.67478700
O	-5.47840100	-1.16140200	-1.25589200
O	-4.99613200	0.61226400	0.47147400
C	-3.06183400	-1.15499400	-0.09445100
F	-3.43205600	-2.01913900	0.84088700
F	-2.52319200	-1.82166300	-1.11953500
F	-2.14991200	-0.32448800	0.40280800
S	-5.78745200	3.73736100	-5.63262800
O	-7.16912700	3.26052600	-5.73713200
O	-4.80115100	3.23507600	-6.59667300
C	-5.84722300	5.59397800	-5.85860800
F	-6.26021900	5.87533700	-7.08845700
F	-6.68372900	6.13172600	-4.97639300
F	-4.63007300	6.10381600	-5.67472200
O	-3.93780400	3.66716200	-1.56936800
O	-3.86619100	0.67556400	-1.75293700
O	-5.24759500	3.69164700	-4.19628400
C	-9.16700700	1.40768700	-3.96588400
C	-7.95387800	0.65107000	-3.36065500
C	-6.84540700	0.55956000	-4.37753900
N	-5.58527100	0.79418500	-4.21415500
C	-4.90708300	0.21959600	-5.40123900
C	-4.51830300	-1.23095900	-5.17411200
C	-3.80295400	-1.77959200	-4.10981500
C	-3.57409300	-3.15898900	-4.09113400
C	-4.06626700	-3.97184900	-5.12160800
C	-4.81461400	-3.42120600	-6.17012600
C	-5.04776800	-2.04425100	-6.18591500
C	-5.86244100	-1.22612600	-7.16371400
C	-6.03856000	0.10785000	-6.44154900
O	-7.20928000	0.06845000	-5.55424200
C	-8.33719900	-0.80974900	-2.99415100
C	-7.55619800	1.39899700	-2.10977500
N	-6.52456700	2.14692600	-1.89363600
C	-6.80045600	2.90487000	-0.64191400
C	-7.96990200	2.12566600	-0.00340600
C	-9.01885100	3.14636400	0.43886800
C	-8.66717900	4.38356200	-0.35759100
C	-7.39844600	4.26590100	-0.94163100
C	-6.86268100	5.29662700	-1.71555900
C	-7.61955600	6.45709300	-1.90159400
C	-8.88743300	6.58276400	-1.31551500
C	-9.41866600	5.54736400	-0.53763100
O	-8.46577500	1.35283900	-1.14827700
H	-9.50126800	0.88588600	-4.87194400
H	-9.98593900	1.42694300	-3.23537400
H	-8.88401100	2.43314100	-4.23752500
H	-4.07626300	0.86311200	-5.72444700
H	-3.46091400	-1.15105100	-3.29048100
H	-3.02151300	-3.60062100	-3.25884300
H	-3.88271000	-5.04888200	-5.09600400
H	-5.22399200	-4.06324200	-6.95426500
H	-5.32030300	-1.05894100	-8.10986900
H	-6.83204400	-1.67986100	-7.41833300
H	-8.65054700	-1.34287200	-3.90136500
H	-7.48196100	-1.32622600	-2.53764000
H	-9.17018100	-0.79486400	-2.27929000
H	-5.90619900	2.94420900	-0.01381200
H	-7.66738200	1.39639900	0.75868200
H	-10.03936400	2.77502400	0.25938700
H	-8.92362600	3.32727900	1.52286100
H	-5.88054800	5.19609900	-2.17327500
H	-7.21961300	7.26733600	-2.51537000
H	-9.46797400	7.49575100	-1.47119300
H	-10.40875700	5.64575900	-0.08472300
H	-6.15985000	0.98752400	-7.08590100
C	-2.16079800	3.60064900	-4.48611000
H	-3.07522200	4.18531600	-4.59568600
H	-1.43764400	4.16968200	-3.88990100
H	-1.75115200	3.37755200	-5.47991400
O	-2.51170700	2.36822100	-3.81172100
Br	4.63454800	4.94804400	-5.60161100
Br	0.10790600	-1.27752900	-9.61420600

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C	-1.29013300	1.16958400	-2.11377900
C	-1.28811700	2.16104200	-3.26073000
N	-0.20189100	1.95108600	-4.17916500
C	-0.00691400	0.82203800	-4.97471300
C	1.20327500	0.97050300	-5.70211200
C	1.76012800	2.25536000	-5.32499000
C	0.85903100	2.83404300	-4.39040800
C	1.10334500	4.09378500	-3.83037400
C	2.25809500	4.77278000	-4.21996100
C	3.15001300	4.19888700	-5.14588200
C	2.91870600	2.94469200	-5.70712000
C	1.61052300	-0.02939700	-6.59660300
C	0.79100100	-1.14687500	-6.75071800
C	-0.42109700	-1.28225400	-6.04724100
C	-0.83177800	-0.29259900	-5.15587100
H	-0.29938700	1.22034400	-1.64125100
H	-2.03098400	1.44572900	-1.35984500
H	-1.47271800	0.14219600	-2.44796700
H	-1.18799300	3.17374800	-2.85455700
H	0.42048300	4.55091500	-3.11383500
H	2.47228000	5.75742600	-3.80191500
H	3.61844000	2.51227100	-6.42375200
H	2.53840400	0.06735600	-7.16220900
H	-1.05040000	-2.16069700	-6.20035300
H	-1.77904600	-0.38914600	-4.63442500
Sc	-4.59289100	2.08575000	-2.93506100
S	-3.04517000	4.34212100	-0.68022000
O	-1.70220000	3.84994600	-0.37040000
O	-3.90910700	4.84612000	0.38060000
C	-2.74555300	5.78548800	-1.85161100
F	-2.10843600	6.74579100	-1.19670200
F	-1.97819300	5.38209500	-2.87878600
F	-3.88135200	6.26620500	-2.34470600
S	-4.80880800	-0.60632000	-0.93202300
O	-5.66184300	-1.56436600	-1.63487200
O	-5.31810200	0.05174900	0.27258100

C	-3.28636100	-1.56186500	-0.40447100
F	-3.64289400	-2.55994900	0.39245300
F	-2.66743800	-2.06025300	-1.48046300
F	-2.44530400	-0.75753200	0.23870200
S	-6.09985300	4.08246900	-5.19754400
O	-7.49782900	4.11581100	-4.77426600
O	-5.75351400	3.37296300	-6.43778000
C	-5.57427700	5.85857400	-5.46554500
F	-6.22898000	6.35971100	-6.50581600
F	-5.84409800	6.58370100	-4.38374600
F	-4.26443800	5.90350400	-5.70624700
O	-3.79511900	3.36905000	-1.60010800
O	-4.13750500	0.38718400	-1.89385400
O	-5.14035800	3.72026900	-4.05817100
C	-9.32038600	1.52114100	-3.93551100
C	-8.09577000	0.71643700	-3.42265800
C	-7.03061500	0.65309400	-4.49157700
N	-5.75633300	0.84575900	-4.38134200
C	-5.14769500	0.30395200	-5.62123500
C	-4.74302500	-1.15207300	-5.46988400
C	-3.94362500	-1.73383400	-4.48669600
C	-3.70931600	-3.11164300	-4.53362200
C	-4.28233800	-3.89248400	-5.54721100
C	-5.11596300	-3.31041200	-6.51043400
C	-5.35175700	-1.93468100	-6.46104800
C	-6.23452300	-1.09156000	-7.35416700
C	-6.33175400	0.23851700	-6.60811400
O	-7.46413900	0.23077300	-5.67168700
C	-8.50185600	-0.75406100	-3.11966900
C	-7.62463000	1.37971600	-2.14892900
N	-6.55090600	2.06479800	-1.93407400
C	-6.71965000	2.72637900	-0.61129100
C	-7.88779600	1.94553200	0.03167600
C	-8.85629700	2.96771700	0.62700200
C	-8.49349700	4.25415500	-0.08070600
C	-7.27492500	4.12881600	-0.76110100
C	-6.74747500	5.18684500	-1.49865100
C	-7.45130300	6.39362900	-1.53908200
C	-8.66393200	6.53146800	-0.84875300
C	-9.19388100	5.46213200	-0.11622500
O	-8.48655000	1.30160600	-1.14654100
H	-9.71409200	1.03844700	-4.83957100
H	-10.09982800	1.52477900	-3.16250400
H	-9.03250000	2.55257300	-4.17525500
H	-4.32810200	0.94696800	-5.96652100
H	-3.54655800	-1.13627400	-3.66919600
H	-3.09226200	-3.57771300	-3.76232300
H	-4.09493200	-4.96883400	-5.57293400
H	-5.58607700	-3.92730500	-7.28059700
H	-5.77512000	-0.92444000	-8.34309800
H	-7.22966300	-1.52817600	-7.52829100
H	-8.86742900	-1.22658300	-4.04073700
H	-7.64580000	-1.31861800	-2.72768600
H	-9.30533700	-0.75509700	-2.37162600
H	-5.78176700	2.68078400	-0.04465700
H	-7.57850900	1.13607100	0.70340600
H	-9.90276700	2.65938100	0.48080100
H	-8.68827700	3.04397300	1.71461700
H	-5.82006100	5.06467300	-2.04967200
H	-7.05516500	7.22744600	-2.12263400
H	-9.20590900	7.47979300	-0.89034900
H	-10.14546800	5.56927600	0.41106500
H	-6.45256500	1.12929000	-7.23574000
C	-2.54073100	2.95006700	-5.18972500
H	-3.51615800	2.86762700	-5.67461800
H	-2.36614900	4.00039800	-4.91859600
H	-1.76418800	2.59154600	-5.87563700
O	-2.56491100	2.12781200	-3.99422400
Br	1.31399600	-2.53203900	-7.96316000
Br	4.72010100	5.17284300	-5.64326700

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C	-0.97881500	2.02700800	-1.92250700
C	-1.34712200	1.58564800	-3.32620100
N	-0.29101600	1.61521400	-4.29499500
C	-0.35104600	0.85298200	-5.47085300
C	0.72025000	1.20873800	-6.32390100
C	1.46406100	2.24584700	-5.64098600
C	0.81130900	2.48655100	-4.39969600
C	1.30313400	3.47265900	-3.53137600
C	2.43809000	4.19171300	-3.90738900
C	3.08148300	3.93825300	-5.13090700
C	2.60509300	2.96895000	-6.00899200
C	0.87749200	0.57721500	-7.56486900
C	-0.05036600	-0.39805700	-7.92722500
C	-1.11577500	-0.75349300	-7.07951100
C	-1.27291700	-0.12727700	-5.84390500
H	-1.75597400	1.69460000	-1.22856100
H	-0.02067700	1.57954400	-1.62415600
H	-0.91870400	3.11555400	-1.82979300
H	-1.74033600	0.56295500	-3.29048100
H	0.83069000	3.70319700	-2.58165900
H	2.83315800	4.96290500	-3.24463900
H	3.10650300	2.78380000	-6.95991800
H	1.69807300	0.83862100	-8.23434600
H	-1.82281300	-1.52415300	-7.39074000
H	-2.09429200	-0.42165600	-5.19902000
Sc	-4.55393000	2.25892800	-2.87912800
S	-3.42169400	4.45051300	-0.35036200
O	-2.27502700	3.80227300	0.28020000
O	-4.51807700	4.94180900	0.48010600
C	-2.73280900	5.94925800	-1.24441600
F	-2.39692600	6.88107800	-0.36327200
F	-1.64398600	5.59794400	-1.94185900
F	-3.63616300	6.44385100	-2.08888300
S	-4.55795700	-0.18593900	-0.67499700
O	-5.47901100	-1.16300200	-1.25721000
O	-5.00002800	0.61054600	0.47111400
C	-3.06371000	-1.15485400	-0.09328300
F	-3.43441800	-2.01984100	0.84113600
F	-2.52306600	-1.82056600	-1.11792300
F	-2.15321400	-0.32382600	0.40566200
S	-5.78949800	3.73684700	-5.63279500
O	-7.17108300	3.25990200	-5.73815200
O	-4.80284300	3.23499200	-6.59673200
C	-5.84949800	5.59347400	-5.85858600
F	-6.26191800	5.87493000	-7.08864000
F	-6.68655700	6.13102700	-4.97677100
F	-4.63254500	6.10360300	-5.67405300
O	-3.93774100	3.66709900	-1.57013900
O	-3.86794900	0.67557100	-1.75212800
O	-5.25034800	3.69100600	-4.19629500
C	-9.16775400	1.40856400	-3.96506400
C	-7.95498700	0.65146300	-3.35968300

C	-6.84658400	0.55897800	-4.37659900
N	-5.58641400	0.79364400	-4.21377400
C	-4.90838000	0.21854500	-5.40072200
C	-4.51857800	-1.23157900	-5.17263300
C	-3.80153900	-1.77873400	-4.10872100
C	-3.57253300	-3.15807800	-4.08853200
C	-4.06610200	-3.97236500	-5.11720500
C	-4.81576300	-3.42314400	-6.16552100
C	-5.04904300	-2.04623100	-6.18281600
C	-5.86465400	-1.22948200	-7.16097800
C	-6.04034600	0.10543600	-6.44044100
O	-7.21080200	0.06702000	-5.55286800
C	-8.33933600	-0.80897600	-2.99277600
C	-7.55686200	1.39963400	-2.10908400
N	-6.52503500	2.14731500	-1.89333800
C	-6.80029000	2.90542300	-0.64160800
C	-7.97016600	2.12699400	-0.00288900
C	-9.01861400	3.14835200	0.43909700
C	-8.66605100	4.38534700	-0.35728000
C	-7.39732800	4.26690900	-0.94118900
C	-6.86073700	5.29744900	-1.71480800
C	-7.61682100	6.45844500	-1.90076200
C	-8.88471800	6.58485000	-1.31488400
C	-9.41673900	5.54967900	-0.53724000
O	-8.46641200	1.35402400	-1.14743500
H	-9.50215300	0.88688800	-4.87114600
H	-9.98673200	1.42812200	-3.23461000
H	-8.88435200	2.43389600	-4.23668600
H	-4.07808700	0.86239200	-5.72460500
H	-3.45835300	-1.14911900	-3.29070000
H	-3.01880100	-3.59855100	-3.25639600
H	-3.88252800	-5.04937000	-5.09035000
H	-5.22607700	-4.06623800	-6.94831300
H	-5.32335800	-1.06356600	-8.10783500
H	-6.83445900	-1.68360600	-7.41414500
H	-8.65333500	-1.34201600	-3.89981600
H	-7.48441200	-1.32603600	-2.53638600
H	-9.17214800	-0.79328900	-2.27773400
H	-5.90592500	2.94417800	-0.01362500
H	-7.66795500	1.39786800	0.75944900
H	-10.03930400	2.77760900	0.25937500
H	-8.92356400	3.32926300	1.52310700
H	-5.87855300	5.19637200	-2.17230000
H	-7.21624100	7.26854400	-2.51431600
H	-9.46463000	7.49825000	-1.47049700
H	-10.40681600	5.64866700	-0.08442300
H	-6.16183500	0.98432700	-7.08583500
C	-2.16365600	3.59959100	-4.48907800
H	-3.07808700	4.18419200	-4.59909900
H	-1.44054600	4.16892800	-3.89310400
H	-1.75369200	3.37599100	-5.48263300
O	-2.51441200	2.36754100	-3.81413800
Cl	0.10782600	-1.20550400	-9.47622300
Cl	4.50587600	4.86736500	-5.55631800

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C	-1.29042700	1.16669800	-2.11522300
C	-1.28792900	2.15898700	-3.26150700
N	-0.20237500	1.95092900	-4.17995900
C	-0.00417100	0.82129300	-4.97457100
C	1.20635200	0.97187700	-5.70115600
C	1.76005200	2.25812400	-5.32512700
C	0.85716100	2.83612100	-4.39181500
C	1.09884700	4.09709400	-3.83308100
C	2.25236200	4.77730100	-4.22266000
C	3.14661800	4.20461900	-5.14722800
C	2.91734400	2.94940900	-5.70687600
C	1.61635600	-0.02790000	-6.59411300
C	0.80017500	-1.14769800	-6.74857800
C	-0.41236300	-1.28437500	-6.04589300
C	-0.82649400	-0.29539200	-5.15599000
H	-0.29966400	1.21685100	-1.64265300
H	-2.03120900	1.44252800	-1.36107000
H	-1.47324600	0.13956300	-2.45001300
H	-1.18884800	3.17140200	-2.85441200
H	0.41453500	4.55356800	-3.11756700
H	2.47059300	5.76309300	-3.80950900
H	3.62250900	2.52333200	-6.42186600
H	2.54315400	0.06425200	-7.16212200
H	-1.03469300	-2.16684600	-6.20385900
H	-1.77422900	-0.39322900	-4.63560800
Sc	-4.59208700	2.08514200	-2.93564900
S	-3.04460000	4.34036300	-0.67973500
O	-1.70172400	3.84773500	-0.37030000
O	-3.90792600	4.84482200	0.38140200
C	-2.74500000	5.78362400	-1.85124600
F	-2.10332900	6.74194800	-1.19778800
F	-1.98204900	5.37899000	-2.88112800
F	-3.88119800	6.26756000	-2.34029000
S	-4.81004200	-0.60769100	-0.93312200
O	-5.66333900	-1.56526900	-1.63632100
O	-5.31917600	0.04985600	0.27185200
C	-3.28793900	-1.56392000	-0.40587000
F	-3.64488500	-2.56218900	0.39071000
F	-2.66909300	-2.06221300	-1.48194500
F	-2.44663700	-0.76015800	0.23768800
S	-6.09967000	4.08317000	-5.19670600
O	-7.49735500	4.11796100	-4.77252900
O	-5.75498200	3.37320700	-6.43714800
C	-5.57271000	5.85874900	-5.46527700
F	-6.22800700	6.36051900	-6.50491500
F	-5.84079200	6.58419300	-4.38323100
F	-4.26308500	5.90252100	-5.70728200
O	-3.79529600	3.36766000	-1.59933100
O	-4.13854100	0.38600600	-1.89444400
O	-5.13971600	3.72033100	-4.05801000
C	-9.32045000	1.52342400	-3.93487800
C	-8.09625400	0.71780300	-3.42243800
C	-7.03136100	0.65405000	-4.49158500
N	-5.75696700	0.84603300	-4.38180000
C	-5.14897000	0.30388800	-5.62191000
C	-4.74485200	-1.15224700	-5.47026100
C	-3.94477100	-1.73383400	-4.48753200
C	-3.71200800	-3.11193500	-4.53332900
C	-4.28711700	-3.89321700	-5.54538700
C	-5.12099500	-3.31119700	-6.50842500
C	-5.35520600	-1.93515800	-6.46019900
C	-6.23759500	-1.09192300	-7.35357000
C	-6.33352600	0.23868700	-6.60829500
O	-7.46556300	0.23202500	-5.67158900
C	-8.50324100	-0.75250000	-3.11974800
C	-7.62447800	1.38049200	-2.14866600
N	-6.55048600	2.06512200	-1.93398000
C	-6.71874300	2.72645000	-0.61103300

C	-7.88694400	1.94583500	0.03211300
C	-8.85493300	2.96820700	0.62797300
C	-8.49203500	4.25463800	-0.07969400
C	-7.27373200	4.12903700	-0.76052500
C	-6.74637900	5.18693500	-1.49831800
C	-7.44994500	6.39388100	-1.53846100
C	-8.66225400	6.53200700	-0.84762800
C	-9.19216000	5.46277300	-0.11491400
O	-8.48623100	1.30239400	-1.14605400
H	-9.71467800	1.04118200	-4.83895300
H	-10.09971700	1.52742200	-3.16169500
H	-9.03191300	2.55471300	-4.17445600
H	-4.32930100	0.94659500	-5.96753400
H	-3.54600600	-1.13585500	-3.67116600
H	-3.09459800	-3.57786200	-3.76223100
H	-4.10108900	-4.96983700	-5.57008400
H	-5.59256900	-3.92833700	-7.27750400
H	-5.77829800	-0.92581000	-8.34272500
H	-7.23315000	-1.52780400	-7.52715900
H	-8.86936300	-1.22455200	-4.04083800
H	-7.64746100	-1.31771900	-2.72811400
H	-9.30652700	-0.75319800	-2.37149300
H	-5.78073100	2.68055000	-0.04466100
H	-7.57770900	1.13614800	0.70359100
H	-9.90154900	2.66019900	0.48211100
H	-8.68648400	3.04425300	1.71553900
H	-5.81928900	5.06449700	-2.04980700
H	-7.05387000	7.22758200	-2.12222500
H	-9.20404100	7.48045100	-0.88901500
H	-10.14354100	5.57010400	0.41271500
H	-6.45398100	1.12919200	-7.23638000
C	-2.54120500	2.94617100	-5.19143900
H	-3.51736600	2.86539000	-5.67516700
H	-2.36382200	3.99654800	-4.92225700
H	-1.76612800	2.58471300	-5.87747100
O	-2.56603600	2.12597700	-3.99466300
Cl	1.28367500	-2.41802200	-7.85887500
Cl	4.58531800	5.10036800	-5.60242300

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C	-0.96438100	1.97767400	-1.78320500
C	-1.29656900	1.50806300	-3.18608900
N	-0.22497700	1.50599600	-4.12415700
C	-0.29074000	0.74776000	-5.30815100
C	0.77346000	1.10724000	-6.16890200
C	1.52476200	2.14315600	-5.48540300
C	0.88184900	2.37960400	-4.23720100
C	1.39091000	3.35631500	-3.37567800
C	2.52845500	4.07739500	-3.75793200
C	3.17039700	3.83691200	-4.99003200
C	2.66154900	2.86226500	-5.85725500
C	0.91945900	0.48196300	-7.40961000
C	-0.00527100	-0.50032600	-7.79358800
C	-1.06274100	-0.85304200	-6.92725900
C	-1.20717400	-0.22953400	-5.68387100
H	-1.76768400	1.67812800	-1.10403600
H	-0.02375300	1.52053600	-1.44599900
H	-0.88351600	3.06715800	-1.71760900
H	-1.71443800	0.49535600	-3.14218200
H	0.93232100	3.58379200	-2.41790300
H	2.90835200	4.83529700	-3.07355000
H	3.16097200	2.68560600	-6.81157200
H	1.73218100	0.74002700	-8.09091100
H	-1.78787700	-1.61742900	-7.20606600
H	-2.02191100	-0.53034800	-5.03376100
Sc	-4.50368300	2.22608600	-2.84844200
S	-3.43703700	4.44745500	-0.31317800
O	-2.30405800	3.81331300	0.35534000
O	-4.54788500	4.96048700	0.48472700
C	-2.72732800	5.92325900	-1.22866000
F	-2.40018800	6.87259100	-0.36203200
F	-1.63073200	5.55311900	-1.90212400
F	-3.61576400	6.40528700	-2.09650200
S	-4.60188800	-0.19652900	-0.61808300
O	-5.52349700	-1.16843700	-1.20864600
O	-5.05854700	0.61786900	0.50977600
C	-3.13534200	-1.17912700	0.00899000
F	-3.53998700	-2.02939900	0.94346400
F	-2.57959800	-1.86353400	-0.99508500
F	-2.22561600	-0.35561100	0.52134000
S	-5.66429200	3.69429400	-5.63914400
O	-7.05126800	3.24024500	-5.77353800
O	-4.66466000	3.16444200	-6.57440300
C	-5.68730500	5.54855200	-5.88931600
F	-6.07167900	5.82144500	-7.13071200
F	-6.53174100	6.11239700	-5.03084800
F	-4.46576500	6.04094200	-5.68826300
O	-3.93230200	3.63662800	-1.52220700
O	-3.87636900	0.64174500	-1.68863500
O	-5.16201100	3.65727500	-4.19010200
C	-9.10204800	1.40732700	-4.05246100
C	-7.91213700	0.64613200	-3.40868600
C	-6.77645800	0.53617200	-4.39328400
N	-5.51883400	0.75489300	-4.19401000
C	-4.81405600	0.16035800	-5.35571200
C	-4.46006900	-1.29572800	-5.10769100
C	-3.79087700	-1.85054300	-4.01716300
C	-3.58716500	-3.23354900	-3.98378500
C	-4.05821200	-4.04371000	-5.02628800
C	-4.76069000	-3.48601900	-6.10253000
C	-4.96894500	-2.10528100	-6.13283800
C	-5.73576100	-1.27790500	-7.14114000
C	-5.91457600	0.06127600	-6.42946800
O	-7.11200600	0.04169800	-5.57770800
C	-8.31792500	-0.80842800	-3.04131400
C	-7.54164200	1.40072900	-2.15338800
N	-6.51004800	2.14111900	-1.91563000
C	-6.81412400	2.91182300	-0.67863700
C	-8.00605600	2.14708000	-0.06490400
C	-9.05740100	3.17969600	0.34276300
C	-8.67648800	4.40688200	-0.45578200
C	-7.39436900	4.27417000	-1.00643500
C	-6.83193000	5.29297900	-1.77705600
C	-7.57505500	6.45709700	-1.99330800
C	-8.85610900	6.59807100	-1.44030400
C	-9.41443700	5.57430400	-0.66594700
O	-8.47844200	1.37014500	-1.21647500
H	-9.41591900	0.88116700	-4.96332400
H	-9.94031100	1.43877100	-3.34463100
H	-8.80345400	2.42826100	-4.32415200
H	-3.95995800	0.78435800	-5.65618900
H	-3.46381000	-1.22236000	-3.19160800
H	-3.07022300	-3.67985900	-3.13130100
H	-3.89486300	-5.12369300	-4.98865900

H	-5.15530500	-4.12532700	-6.89652700
H	-5.15756300	-1.12181800	-8.06778500
H	-6.70297900	-1.71685700	-7.42872300
H	-8.60962000	-1.34680300	-3.95268500
H	-7.48073100	-1.32786300	-2.55569700
H	-9.17094500	-0.78050500	-2.35085400
H	-5.93664500	2.95138800	-0.02734600
H	-7.72929700	1.42143200	0.71038800
H	-10.07624500	2.81482000	0.14170700
H	-8.98696100	3.36953800	1.42716900
H	-5.84004200	5.17985200	-2.20976600
H	-7.15367800	7.25795500	-2.60507800
H	-9.42567400	7.51370300	-1.61941200
H	-10.41487400	5.68431300	-0.23914800
H	-6.00316300	0.94008600	-7.08024000
C	-2.06650000	3.50833800	-4.41746800
H	-2.96536600	4.10998600	-4.56085000
H	-1.34026300	4.07813300	-3.82573300
H	-1.64326700	3.24731300	-5.39626500
O	-2.45487800	2.30482800	-3.71399100
O	4.27856900	4.50052000	-5.41727800
O	0.19249100	-1.06156400	-9.01784600
C	4.84612400	5.50057600	-4.59715100
H	5.71837800	5.89161200	-5.13806600
H	4.14057500	6.33072400	-4.41070800
H	5.18138400	5.09568000	-3.62486500
C	-0.69680100	-2.06036000	-9.47059400
H	-1.73286700	-1.68352100	-9.55377900
H	-0.34842400	-2.36234700	-10.46748400
H	-0.69546600	-2.94550500	-8.80854200

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C	-1.28581700	1.11985800	-1.81236500
C	-1.18210200	2.11011900	-2.95616600
N	-0.12959000	1.82671100	-3.87793500
C	-0.06473700	0.71012800	-4.72181100
C	1.01818800	0.86724500	-5.62685800
C	1.63286200	2.14834300	-5.32153300
C	0.88432800	2.72009400	-4.25653600
C	1.20851800	3.97951500	-3.75126000
C	2.29002800	4.66759700	-4.31336700
C	3.04593800	4.10478800	-5.36527000
C	2.71463800	2.84018600	-5.87100800
C	1.26453900	-0.10785900	-6.59811100
C	0.41923500	-1.22463300	-6.67974600
C	-0.66920700	-1.35746000	-5.79018200
C	-0.91359700	-0.39060900	-4.81171200
H	-0.30257200	1.08543900	-1.32302500
H	-2.01265000	1.45766700	-1.06871600
H	-1.54933600	0.11086700	-2.14665500
H	-1.01128400	3.11040700	-2.54183500
H	0.63968400	4.43968500	-2.94190400
H	2.53878400	5.65214400	-3.91858500
H	3.30710700	2.42415500	-6.68790400
H	2.08835300	-0.01497800	-7.30818500
H	-1.34736100	-2.20859100	-5.84859800
H	-1.76598900	-0.50292700	-4.15090700
Sc	-4.50020000	2.09449300	-2.70757600
S	-3.05605700	4.29626100	-0.35182500
O	-1.74335100	3.75256200	-0.00086100
O	-3.92017200	4.86059100	0.67751400
C	-2.66839700	5.70955000	-1.53328100
F	-2.01783500	6.65658300	-0.87075700
F	-1.88627300	5.26961400	-2.53276000
F	-3.77292600	6.22406200	-2.06405200
S	-4.94543100	-0.55604200	-0.66352000
O	-5.76228700	-1.51117400	-1.41323300
O	-5.53274600	0.12489300	0.49215600
C	-3.48364000	-1.52623200	-0.00739600
F	-3.91082300	-2.46589000	0.82589400
F	-2.82980600	-2.10515500	-1.02073900
F	-2.64832800	-0.71210100	0.63060700
S	-5.94737900	4.17507900	-4.94273600
O	-7.34596900	4.28465600	-4.53246700
O	-5.63149900	3.44368200	-6.17868500
C	-5.33849400	5.92325800	-5.21624700
F	-5.94668000	6.43864800	-6.27855000
F	-5.60362500	6.67304100	-4.15080400
F	-4.02223800	5.91230200	-5.42668800
O	-3.83032100	3.34051400	-1.26979400
O	-4.18494300	0.40765600	-1.58603900
O	-5.01525000	3.76980400	-3.79755000
C	-9.05550900	1.48749400	-4.37900800
C	-7.89159600	0.72073200	-3.70045400
C	-6.68416800	0.67667800	-4.60656300
N	-5.43819500	0.83390000	-4.29615000
C	-4.66636500	0.26743500	-5.42697100
C	-4.39068500	-1.21479200	-5.23841500
C	-3.84273300	-1.86094100	-4.13168500
C	-3.66799100	-3.24740600	-4.17881000
C	-4.05467300	-3.97113300	-5.31584900
C	-4.65116300	-3.32324600	-6.40558100
C	-4.82949100	-1.93876100	-6.35540300
C	-5.49214300	-1.02660500	-7.36430400
C	-5.67070500	0.28160400	-6.59501000
O	-6.93827900	0.28344300	-5.84808400
C	-8.28860700	-0.76559400	-3.45709200
C	-7.61514200	1.37552100	-2.36505000
N	-6.57994000	2.04086700	-1.97736900
C	-6.91960500	2.65440200	-0.66328100
C	-8.18462000	1.87706500	-0.22931800
C	-9.21551200	2.89733700	0.25448400
C	-8.71585400	4.20731000	-0.31256700
C	-7.40913400	4.08173000	-0.80331800
C	-6.73954800	5.17094100	-1.35751500
C	-7.39581100	6.40308300	-1.41835500
C	-8.70194200	6.53696500	-0.92697000
C	-9.37013600	5.44004600	-0.36930300
O	-8.61531600	1.28112100	-1.50054000
H	-9.30644900	0.99460600	-5.32734600
H	-9.93432200	1.46676700	-3.72138300
H	-8.77066700	2.52883500	-4.57553700
H	-3.75221600	0.84372900	-5.61497000
H	-3.58694900	-1.30135500	-3.23496800
H	-3.24140900	-3.76404400	-3.31618700
H	-3.91385500	-5.05461900	-5.34164100
H	-4.98785800	-3.89630800	-7.27337800
H	-4.84850000	-0.84720900	-8.24223400
H	-6.45346300	-1.41003200	-7.73862200
H	-8.50044300	-1.24730600	-4.42070900
H	-7.48041100	-1.30273600	-2.94298100
H	-9.19140300	-0.79544900	-2.83319300
H	-6.07184400	2.54439300	0.02425400
H	-7.98695600	1.04193800	0.45397300

H	-10.22960800	2.62642200	-0.07702900
H	-9.22828000	2.91662700	1.35729800
H	-5.73461700	5.05566400	-1.75045600
H	-6.88682100	7.26122400	-1.86253100
H	-9.20552200	7.50549900	-0.98349900
H	-10.38976600	5.54648800	0.01032600
H	-5.66659700	1.19581300	-7.20010600
C	-2.38728000	3.00391700	-4.88325100
H	-3.36613200	2.99797600	-5.36753800
H	-2.12696900	4.03544800	-4.61142300
H	-1.64312500	2.58511000	-5.57101200
O	-2.47401800	2.18492200	-3.68916700
O	0.71147200	-2.12808200	-7.65614000
O	4.11050300	4.72004000	-5.95095100
C	4.50575400	5.99880700	-5.50166500
H	5.37204700	6.29101000	-6.11045700
H	3.70579800	6.74969500	-5.63687200
H	4.80512200	5.98874800	-4.43763500
C	-0.10899800	-3.26797300	-7.80511100
H	-1.15532700	-2.99723200	-8.03796500
H	0.30425700	-3.84460400	-8.64361000
H	-0.10477900	-3.90117500	-6.89915400

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C	-0.98185700	2.01290900	-1.93172500
C	-1.34567600	1.58115300	-3.33966300
N	-0.29246000	1.62211300	-4.30644800
C	-0.34497700	0.85944600	-5.48493700
C	0.73176500	1.21943800	-6.32988200
C	1.46919900	2.25905200	-5.64153500
C	0.80918500	2.49877700	-4.40360600
C	1.28866000	3.48663800	-3.52992800
C	2.42572700	4.20728200	-3.90433500
C	3.08844900	3.96581800	-5.12012500
C	2.61058500	2.99119900	-5.99420800
C	0.89123000	0.58247800	-7.56887100
C	-0.02606500	-0.39837800	-7.94871800
C	-1.09246500	-0.74586900	-7.09850400
C	-1.26488800	-0.12207000	-5.86109000
H	-1.75658100	1.67021900	-1.24007600
H	-0.02024600	1.57017300	-1.63757800
H	-0.92752800	3.10084500	-1.83106900
H	-1.73978000	0.55853400	-3.31373800
H	0.80425600	3.71293900	-2.58506700
H	2.80281900	4.97856100	-3.22828700
H	3.97587800	4.54743600	-5.37978800
H	3.11098800	2.79822900	-6.94618600
H	1.72128400	0.85452200	-8.22523200
H	0.08311800	-0.90145500	-8.91228800
H	-1.80434200	-1.51765200	-7.40231500
H	-2.08852700	-0.41314100	-5.21720900
Sc	-4.54895200	2.25635400	-2.88251400
S	-3.41812800	4.44323400	-0.34934300
O	-2.27643900	3.78787600	0.28278000
O	-4.51171000	4.94229100	0.48058400
C	-2.71928000	5.93782400	-1.24255700
F	-2.37834500	6.86749000	-0.36058300
F	-1.63256900	5.58100600	-1.93973100
F	-3.61960300	6.43870300	-2.08688300
S	-4.56608400	-0.18920000	-0.67516800
O	-5.48729900	-1.16563000	-1.25847700
O	-5.00945900	0.60642300	0.47122500
C	-3.07474400	-1.16054400	-0.09028800
F	-3.44990800	-2.02553000	0.84285100
F	-2.53216100	-1.82701700	-1.11318700
F	-2.16439200	-0.33162400	0.41221600
S	-5.79804400	3.73441000	-5.63108600
O	-7.18122200	3.26092500	-5.73278400
O	-4.81623900	3.23021700	-6.59868800
C	-5.85552600	5.59080800	-5.85884700
F	-6.26991600	5.87157100	-7.08871600
F	-6.69042000	6.13119500	-4.97650400
F	-4.63778600	6.10016000	-5.67740600
O	-3.93908500	3.66384200	-1.56906600
O	-3.87395500	0.67183900	-1.75031200
O	-5.25530600	3.68883300	-4.19648900
C	-9.16802700	1.41009000	-3.96392400
C	-7.95496900	0.65315900	-3.35911500
C	-6.84676600	0.55884600	-4.37629100
N	-5.58621100	0.79117700	-4.21436200
C	-4.90898700	0.21244000	-5.40036400
C	-4.52191800	-1.23769500	-5.16791500
C	-3.80250100	-1.78207300	-4.10432400
C	-3.58011400	-3.16231700	-4.07714300
C	-4.08183200	-3.98025600	-5.09896500
C	-4.83203900	-3.43331400	-6.14805600
C	-5.05857500	-2.05539300	-6.17228300
C	-5.87095800	-1.23990300	-7.15418700
C	-6.04187800	0.09858100	-6.43918900
O	-7.21245800	0.06587400	-5.55189100
C	-8.34029800	-0.80684400	-2.99141600
C	-7.55581400	1.40189900	-2.10925000
N	-6.52351500	2.14865300	-1.89459100
C	-6.79716600	2.90706700	-0.64290200
C	-7.96799500	2.13056400	-0.00349400
C	-9.01493700	3.15358600	0.43842400
C	-8.66028400	4.39025600	-0.35753700
C	-7.39187500	4.26978400	-0.94176200
C	-6.85344900	5.30002400	-1.71454500
C	-7.60744900	6.46255500	-1.89948600
C	-8.87508000	6.59088400	-1.31346600
C	-9.40888200	5.55609500	-0.53652900
O	-8.46557800	1.35756600	-1.14710100
H	-9.50199400	0.88921200	-4.87063500
H	-9.98705400	1.42820300	-3.23346600
H	-8.88534600	2.43583700	-4.23440700
H	-4.07693400	0.85355400	-5.72519400
H	-3.45193600	-1.14933700	-3.29189000
H	-3.02494900	-3.60055600	-3.24478000
H	-3.90371500	-5.05805200	-5.06625400
H	-5.24793400	-4.07872800	-6.92604000
H	-5.32821100	-1.07983500	-8.10124000
H	-6.84243000	-1.69119800	-7.40610200
H	-8.65605600	-1.33966000	-3.89798300
H	-7.48540300	-1.32467800	-2.53599600
H	-9.17216300	-0.79010400	-2.27527900
H	-5.90255800	2.94432700	-0.01527100
H	-7.66619200	1.40176400	0.75930400
H	-10.03618500	2.78455000	0.25826900
H	-8.91999500	3.33421000	1.52249700
H	-5.87139300	5.19742400	-2.17193300
H	-7.20542400	7.27238000	-2.51246000
H	-9.45332700	7.50548600	-1.46832500
H	-10.39869600	5.65657000	-0.08342700

H	-6.16095900	0.97544600	-7.08784000
C	-2.17023300	3.59734900	-4.49842800
H	-3.08358600	4.18429700	-4.60518400
H	-1.44202000	4.16545000	-3.90757000
H	-1.76509800	3.37027700	-5.49310800
O	-2.52035500	2.36788000	-3.81889300

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C	-1.29158600	1.13757900	-2.09557100
C	-1.28640100	2.12743700	-3.24385400
N	-0.20086200	1.93397900	-4.15846700
C	0.03576600	0.79618400	-4.93473900
C	1.23706500	0.98148400	-5.66951200
C	1.74174500	2.29705200	-5.32238800
C	0.82195100	2.85925000	-4.39621100
C	1.01113500	4.14065700	-3.86381800
C	2.13744000	4.85526900	-4.27841600
C	3.05831000	4.31191300	-5.19460100
C	2.86645500	3.03377200	-5.71977400
C	1.67473600	-0.02346500	-6.54450600
C	0.90814300	-1.18142300	-6.68608300
C	-0.29572200	-1.33651900	-5.97202000
C	-0.74922900	-0.35101400	-5.09366200
H	-0.30396100	1.19420000	-1.61716900
H	-2.03821900	1.41291400	-1.34662900
H	-1.46825200	0.10849000	-2.42682000
H	-1.19834900	3.13995600	-2.83639500
H	0.31028400	4.57932200	-3.15280400
H	2.30447000	5.85833400	-3.87827700
H	3.92961400	4.89860400	-5.49473000
H	3.57909100	2.60966800	-6.43133900
H	2.59912800	0.10564600	-7.11275700
H	1.23760800	-1.97090600	-7.36562800
H	-0.89759200	-2.23902300	-6.10645600
H	-1.69276400	-0.46848000	-4.56856000
Sc	-4.58277500	2.08048700	-2.92748900
S	-3.02380100	4.34612600	-0.69950100
O	-1.67177400	3.86154700	-0.41723400
O	-3.85083800	4.88820500	0.37170900
C	-2.75743600	5.74847800	-1.92869800
F	-1.93514400	6.63972700	-1.39102100
F	-2.19577800	5.26727800	-3.04932100
F	-3.89933000	6.34321500	-2.25368300
S	-4.83486900	-0.62868300	-0.94648300
O	-5.68920800	-1.57576400	-1.66280000
O	-5.34806000	0.01937800	0.26209800
C	-3.32155400	-1.59781000	-0.41763800
F	-3.68960500	-2.60120900	0.36797400
F	-2.69774800	-2.09066800	-1.49326000
F	-2.48033100	-0.80473000	0.23902000
S	-6.07804900	4.11029200	-5.16737100
O	-7.47167500	4.16409400	-4.73163000
O	-5.75460200	3.39775600	-6.41207000
C	-5.52841200	5.87903300	-5.43576700
F	-6.17060700	6.38613700	-6.48139700
F	-5.79759700	6.60924500	-4.35703600
F	-4.21713000	5.90814500	-5.66723700
O	-3.80512500	3.34259000	-1.55899300
O	-4.15256100	0.36960800	-1.89404200
O	-5.11320200	3.73203200	-4.03748300
C	-9.31330100	1.56247700	-3.95070200
C	-8.09929700	0.74225600	-3.43719800
C	-7.02980100	0.67574000	-4.50163000
N	-5.75446000	0.85814900	-4.38776200
C	-5.14725200	0.31354300	-5.62797100
C	-4.75409100	-1.14560700	-5.47666500
C	-3.95622200	-1.73272100	-4.49553800
C	-3.74077200	-3.11374300	-4.53658800
C	-4.32843000	-3.89207400	-5.54362300
C	-5.15638600	-3.30350800	-6.50776600
C	-5.37405100	-1.92463800	-6.46380700
C	-6.24520900	-1.07382400	-7.36094300
C	-6.33023900	0.25829300	-6.61703000
O	-7.46445400	0.26081400	-5.68424700
C	-8.52099700	-0.72623500	-3.14606700
C	-7.62826300	1.39176800	-2.15691000
N	-6.55072900	2.06722200	-1.93347900
C	-6.71927200	2.71742400	-0.60521100
C	-7.89422000	1.93882500	0.02774600
C	-8.85636300	2.96201700	0.63171100
C	-8.48362300	4.25257900	-0.06320200
C	-7.26520900	4.12479000	-0.74355200
C	-6.73138600	5.18497300	-1.47306900
C	-7.42680400	6.39684100	-1.50392300
C	-8.63848100	6.53729900	-0.81256800
C	-9.17593800	5.46540700	-0.08916900
O	-8.49472500	1.31110800	-1.15789600
H	-9.70841000	1.08900700	-4.85902400
H	-10.09586800	1.57019200	-3.18084500
H	-9.01342400	2.59222400	-4.18311400
H	-4.32345400	0.95095800	-5.97147800
H	-3.54537800	-1.13648700	-3.68402400
H	-3.12649100	-3.58388000	-3.76556700
H	-4.15626500	-4.97114100	-5.56400900
H	-5.63643200	-3.91747000	-7.27419600
H	-5.78047300	-0.91346800	-8.34854400
H	-7.24460100	-1.49954800	-7.53772400
H	-8.88623900	-1.18939900	-4.07197400
H	-7.67223900	-1.30137500	-2.75345500
H	-9.32819800	-0.72450600	-2.40205600
H	-5.78300200	2.65983700	-0.03715800
H	-7.59192500	1.12067900	0.69207900
H	-9.90481700	2.66264200	0.48101900
H	-8.68942900	3.02642600	1.72027700
H	-5.80603200	5.06052900	-2.02662000
H	-7.02495900	7.23224600	-2.08129800
H	-9.17416800	7.48950500	-0.84661300
H	-10.12734600	5.57435800	0.43811300
H	-6.44140700	1.14955000	-7.24590100
C	-2.51974000	2.83201800	-5.22367200
H	-3.52967400	2.86810300	-5.63775600
H	-2.17934400	3.85975400	-5.03807900
H	-1.85240600	2.32633500	-5.93199500
O	-2.57219200	2.09143100	-3.97781100

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C	-0.97250300	2.04801300	-1.87342700
C	-1.33124100	1.59619300	-3.27586700
N	-0.27298400	1.61533500	-4.23898200
C	-0.34043800	0.85174300	-5.41432200
C	0.71915200	1.21037900	-6.27872900
C	1.46850000	2.25070000	-5.60145200
C	0.82823200	2.48846400	-4.35389600
C	1.33301300	3.47168500	-3.49114900

C	2.46471800	4.18537500	-3.88502800
C	3.12268300	3.95836400	-5.11661800
C	2.60407400	2.97635900	-5.97284000
C	0.85971800	0.57471000	-7.51741400
C	-0.05637800	-0.41684600	-7.90540700
C	-1.10571900	-0.75496400	-7.01619500
C	-1.25837200	-0.13358600	-5.77872000
H	-1.75769500	1.72674100	-1.18299300
H	-0.01932200	1.59749700	-1.56387600
H	-0.90479100	3.13708400	-1.79086600
H	-1.73152500	0.57638200	-3.23554200
H	0.86705100	3.70643800	-2.53889700
H	2.83742400	4.96675400	-3.21948700
H	3.09317200	2.75913700	-6.92478400
H	1.69429300	0.83863900	-8.17036100
H	-1.83875500	-1.51000200	-7.30878200
H	-2.07469800	-0.42624800	-5.12733000
Sc	-4.54212100	2.26312900	-2.88051600
S	-3.45581600	4.46717300	-0.34179800
O	-2.31665600	3.82280800	0.30605600
O	-4.56163900	4.96301500	0.47368400
C	-2.75733300	5.96192000	-1.23494300
F	-2.43114100	6.89760200	-0.35379100
F	-1.66167300	5.60868200	-1.91955400
F	-3.65223000	6.45342500	-2.09055100
S	-4.57811200	-0.16782800	-0.66331000
O	-5.49656100	-1.14469800	-1.25030800
O	-5.03030000	0.63601800	0.47378800
C	-3.09478700	-1.13931200	-0.05864600
F	-3.47978800	-1.99581400	0.87820800
F	-2.54629300	-1.81537100	-1.07214900
F	-2.18587600	-0.30909300	0.44434200
S	-5.73754700	3.72654000	-5.65974500
O	-7.11780100	3.25023600	-5.78582500
O	-4.73595600	3.21930200	-6.60509400
C	-5.79369500	5.58196300	-5.89598200
F	-6.18676800	5.85732900	-7.13394600
F	-6.64476800	6.12418600	-5.03037600
F	-4.58005300	6.09377800	-5.69502600
O	-3.95823800	3.67773500	-1.56278700
O	-3.87242600	0.68478000	-1.73691400
O	-5.22306400	3.68820600	-4.21446800
C	-9.14185000	1.41186400	-4.02809800
C	-7.93995200	0.65494800	-3.40133500
C	-6.81675600	0.55588400	-4.40111600
N	-5.55869400	0.78744500	-4.21955100
C	-4.86505700	0.20433400	-5.39392300
C	-4.48755900	-1.24744900	-5.15618300
C	-3.79144300	-1.79629300	-4.07949600
C	-3.56651000	-3.17618200	-4.05534300
C	-4.04313000	-3.98914900	-5.09313100
C	-4.77238000	-3.43800100	-6.15476300
C	-5.00198800	-2.06051900	-6.17574400
C	-5.79694700	-1.24098000	-7.16844600
C	-5.98050400	0.09451500	-6.45108200
O	-7.16456300	0.06038900	-5.58118600
C	-8.33229600	-0.80309800	-3.03361000
C	-7.55893100	1.40782200	-2.14826600
N	-6.53016300	2.15595500	-1.92093700
C	-6.82408100	2.91973400	-0.67703500
C	-8.00264200	2.14389600	-0.05152000
C	-9.05707500	3.16702000	0.37180200
C	-8.69432400	4.40017800	-0.42597700
C	-7.41768100	4.27934600	-0.99189400
C	-6.87136400	5.30602100	-1.76382700
C	-7.62549200	6.46554300	-1.96625700
C	-8.90124300	6.59440700	-1.39824900
C	-9.44315400	5.56306300	-0.62232200
O	-8.48278300	1.36650000	-1.19960000
H	-9.46475700	0.88608600	-4.93599100
H	-9.97114600	1.43801200	-3.30957600
H	-8.85144400	2.43477800	-4.30153400
H	-4.02461200	0.84055600	-5.70681600
H	-3.45956600	-1.16669300	-3.25685600
H	-3.02845900	-3.61810500	-3.21370400
H	-3.86254900	-5.06661800	-5.06314300
H	-5.16992200	-4.07981800	-6.94519300
H	-5.23739200	-1.07645700	-8.10490700
H	-6.76348800	-1.69171300	-7.43959100
H	-8.63191500	-1.34039800	-3.94301100
H	-7.48557600	-1.31880000	-2.56056900
H	-9.17670700	-0.78290100	-2.33241000
H	-5.93913400	2.96236100	-0.03625900
H	-7.71106800	1.41805600	0.71812000
H	-10.07527600	2.79516700	0.18055800
H	-8.97613500	3.35323000	1.45607900
H	-5.88317900	5.20285000	-2.20761500
H	-7.21702100	7.27248100	-2.57879600
H	-9.47950800	7.50660100	-1.56662800
H	-10.43936900	5.66379600	-0.18354300
H	-6.08931200	0.97343000	-7.09866500
C	-2.13516600	3.60685000	-4.45755400
H	-3.04372400	4.20081100	-4.56719700
H	-1.40387200	4.17100000	-3.86680900
H	-1.73030600	3.37395700	-5.45106900
O	-2.49599800	2.38173700	-3.77564000
C	4.32661600	4.74525000	-5.49328000
C	4.54036700	5.14895400	-6.82576300
C	5.28762900	5.10866900	-4.52983400
C	5.67258000	5.88552300	-7.18190000
H	3.79793800	4.90318800	-7.58875600
C	6.41904700	5.84716800	-4.88498300
H	5.15933600	4.78892200	-3.49302800
C	6.61772900	6.23901500	-6.21304200
H	5.81218300	6.19340500	-8.22147900
H	7.15426700	6.11072600	-4.12017000
H	7.50291100	6.81654300	-6.49106100
C	0.06680500	-1.09943100	-9.22067700
C	-0.23088500	-2.46949900	-9.35779800
C	0.48294100	-0.39528300	-10.36739500
C	-0.11643700	-3.11064800	-10.59361700
H	-0.53357000	-3.04587300	-8.48036600
C	0.59974900	-1.03642400	-11.60300600
H	0.69486600	0.67411900	-10.29528100
C	0.30011200	-2.39759500	-11.72277300
H	-0.34563000	-4.17661600	-10.67260000
H	0.91795600	-0.46626600	-12.47973200
H	0.39032700	-2.89915700	-12.68956600

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C	-1.22195300	1.31685300	-1.68472500
C	-1.12530900	2.26945300	-2.86006500
N	-0.05164600	1.96957500	-3.76307800
C	0.00930600	0.84399300	-4.58983600

C	1.05771700	1.00904800	-5.53083200
C	1.65696100	2.30480200	-5.26022200
C	0.93344900	2.87352000	-4.17860000
C	1.24828700	4.14603000	-3.69064400
C	2.29857800	4.83516900	-4.29574400
C	3.04663700	4.29140800	-5.36955900
C	2.71058000	3.01434300	-5.84580800
C	1.27587800	0.03040400	-6.50857100
C	0.44925600	-1.10471000	-6.56531500
C	-0.59035800	-1.23558800	-5.61229800
C	-0.82150600	-0.27739800	-4.63039900
H	-0.24875700	1.33031900	-1.17471000
H	-1.97508600	1.65764600	-0.96924100
H	-1.44781100	0.28951800	-1.98804800
H	-0.97361500	3.28645800	-2.47941100
H	0.68907700	4.60560100	-2.87422700
H	2.53577700	5.83979000	-3.93962200
H	3.28085800	2.56287400	-6.66041800
H	2.06254200	0.17657300	-7.25180400
H	-1.23294900	-2.11739600	-5.62970000
H	-1.63602500	-0.40577900	-3.92619600
Sc	-4.45379500	2.12677100	-2.69842600
S	-3.19147500	4.40608000	-0.31190500
O	-1.87313400	3.92485600	0.10276500
O	-4.12215000	4.94856500	0.66983200
C	-2.81475100	5.81517700	-1.50122500
F	-2.23494500	6.80075300	-0.82977400
F	-1.97223000	5.39310100	-2.45852000
F	-3.91708900	6.27126500	-2.08721300
S	-4.84140200	-0.50315300	-0.63296900
O	-5.63678200	-1.48519900	-1.37107800
O	-5.44969700	0.18946800	0.50475700
C	-3.36850200	-1.43458200	0.05431500
F	-3.78689300	-2.37131200	0.89496200
F	-2.68969800	-2.01295200	-0.94259200
F	-2.55876400	-0.59413300	0.69138000
S	-5.90880100	4.14114000	-4.98941400
O	-7.32509900	4.18078600	-4.63067000
O	-5.51213400	3.42927300	-6.21349100
C	-5.37481000	5.91714700	-5.24056300
F	-5.95589800	6.39906900	-6.33316800
F	-5.72756300	6.65508900	-4.19273000
F	-4.05100200	5.97033500	-5.38793700
O	-3.88453400	3.40273100	-1.24482800
O	-4.08935000	0.45554900	-1.56897300
O	-5.00103200	3.77693600	-3.81114100
C	-8.90792000	1.31454900	-4.55427300
C	-7.73456700	0.61048900	-3.82735900
C	-6.49012500	0.62122100	-4.68266900
N	-5.26516400	0.81469700	-4.31206900
C	-4.42830100	0.26351700	-5.40368400
C	-4.14879400	-1.21804800	-5.21153900
C	-3.67261900	-1.87193600	-4.07682900
C	-3.47103700	-3.25459500	-4.13122100
C	-3.75896600	-3.96657000	-5.30433500
C	-4.28873000	-3.31228800	-6.42430400
C	-4.49777300	-1.93249700	-6.36583400
C	-5.11402200	-1.01673500	-7.40050600
C	-5.36945500	0.27244100	-6.62162500
O	-6.67268100	0.22767600	-5.93635800
C	-8.06262600	-0.89462100	-3.59311600
C	-7.54294700	1.27817800	-2.48338600
N	-6.55268800	1.98480500	-2.05253200
C	-6.97279400	2.58461600	-0.75509700
C	-8.21906700	1.75238900	-0.37297200
C	-9.31151400	2.72573200	0.07011400
C	-8.84731700	4.05708800	-0.47714400
C	-7.51782500	3.98944600	-0.91547600
C	-6.87373600	5.10861200	-1.43950400
C	-7.57967100	6.31154000	-1.52454300
C	-8.90944100	6.38704500	-1.08704800
C	-9.55161800	5.26049100	-0.55873500
O	-8.57310700	1.14229900	-1.66129600
H	-9.09572300	0.80676000	-5.50933800
H	-9.80999500	1.25105500	-3.93187100
H	-8.66846500	2.36832700	-4.74467400
H	-3.50934600	0.84682100	-5.53966100
H	-3.48746500	-1.32125200	-3.15784700
H	-3.09635000	-3.77745300	-3.24843800
H	-3.59250000	-5.04609400	-5.33721600
H	-4.55091800	-3.87733300	-7.32246700
H	-4.41954400	-0.80614900	-8.23155800
H	-6.04012300	-1.41410600	-7.84278800
H	-8.20815500	-1.38981600	-4.56220700
H	-7.24944200	-1.38658300	-3.04276600
H	-8.98778600	-0.97007400	-3.00695100
H	-6.15057700	2.51105400	-0.03271000
H	-8.01296100	0.92434400	0.31681600
H	-10.29910100	2.41129200	-0.30064900
H	-9.36791200	2.74276700	1.17157900
H	-5.84902200	5.03877300	-1.78996100
H	-7.09050500	7.19267100	-1.94532400
H	-9.45168500	7.33315400	-1.16238400
H	-10.58932300	5.32168000	-0.22034100
H	-5.36189500	1.19675200	-7.21107900
C	-2.31784600	3.11417500	-4.81245200
H	-3.28015700	3.05534700	-5.32514900
H	-2.11890800	4.15837700	-4.53786800
H	-1.53487000	2.73160100	-5.47783100
O	-2.39711700	2.29571500	-3.61624600
C	0.63387900	-2.14366100	-7.61283100
C	-0.47403400	-2.82310100	-8.15917700
C	1.91541800	-2.47986300	-8.09067300
C	-0.30554200	-3.79846200	-9.14451000
H	-1.48292900	-2.57413700	-7.82127200
C	2.08373600	-3.45335800	-9.07843900
H	2.79479900	-1.99011200	-7.66594300
C	0.97413900	-4.11828200	-9.61078700
H	-1.18158300	-4.30713800	-9.55560800
H	3.08982800	-3.70087800	-9.42700300
H	1.10592600	-4.88133300	-10.38199300
C	4.16150900	5.06296000	-5.98088300
C	4.39233900	5.02557400	-7.36999500
C	5.01890700	5.85186000	-5.18935200
C	5.44116500	5.74687700	-7.94534500
H	3.72665700	4.44251800	-8.01086400
C	6.06649200	6.57544700	-5.76440600
H	4.87793400	5.88066800	-4.10630800
C	6.28357300	6.52625900	-7.14542500
H	5.59506500	5.70723700	-9.02690600
H	6.72264600	7.17465100	-5.12769600
H	7.10328500	7.09195600	-7.59536300

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C	-0.94684500	2.03394700	-1.76713000
C	-1.29421400	1.56566700	-3.16623800
N	-0.23225400	1.56075800	-4.12126000
C	-0.33783300	0.81958300	-5.31052300
C	0.67594800	1.20972400	-6.21359800
C	1.44619000	2.24249000	-5.54420000
C	0.85830700	2.44677800	-4.26553400
C	1.39857900	3.40973200	-3.40745800
C	2.50847000	4.14509700	-3.83819000
C	3.11299700	3.95946700	-5.09890600
C	2.55716700	2.98853300	-5.94522500
C	0.75555800	0.60938900	-7.47480800
C	-0.16923600	-0.37715600	-7.85770100
C	-1.16019100	-0.75045300	-6.92366600
C	-1.25432000	-0.16719700	-5.65788700
H	-1.74889000	1.74049800	-1.08325900
H	-0.00790100	1.56837400	-1.43677000
H	-0.85570200	3.12293300	-1.70249400
H	-1.70969600	0.55246100	-3.11594500
H	0.98582900	3.60986900	-2.42280000
H	2.90555500	4.88919300	-3.14839100
H	2.98227300	2.80337700	-6.93412200
H	1.54444300	0.92545800	-8.16082100
H	-1.89289600	-1.51849800	-7.17055100
H	-2.02424400	-0.49939400	-4.97012700
Sc	-4.51121400	2.23858900	-2.85103600
S	-3.48533300	4.44601500	-0.28853100
O	-2.35434300	3.80802600	0.37967300
O	-4.60452300	4.94270700	0.50823900
C	-2.77700900	5.93872900	-1.17709700
F	-2.46307300	6.87759200	-0.29434000
F	-1.67294600	5.58522100	-1.84685800
F	-3.66159000	6.42777100	-2.04528900
S	-4.59740400	-0.17994900	-0.62441200
O	-5.52010000	-1.15081300	-1.21509000
O	-5.05332400	0.63574100	0.50276400
C	-3.13120000	-1.16323100	0.00202900
F	-3.53407200	-2.00644300	0.94365300
F	-2.58277200	-1.85536500	-1.00061900
F	-2.21646100	-0.33944000	0.50494000
S	-5.64138200	3.71367800	-5.65087100
O	-7.02246700	3.24839700	-5.80681300
O	-4.62455200	3.19995800	-6.57630500
C	-5.67854500	5.56959100	-5.88684000
F	-6.04533400	5.84876700	-7.13217700
F	-6.54222400	6.11831600	-5.03780800
F	-4.46526500	6.07237800	-5.66210000
O	-3.96763900	3.65034500	-1.51276100
O	-3.87059000	0.65765500	-1.69542200
O	-5.15879100	3.67031500	-4.19535100
C	-9.09522900	1.40253600	-4.10227800
C	-7.90698600	0.64545600	-3.45110100
C	-6.76257600	0.54616500	-4.42617300
N	-5.50762000	0.76610700	-4.21184200
C	-4.79124900	0.17813100	-5.36983800
C	-4.44547100	-1.28120900	-5.12921800
C	-3.79624600	-1.84817000	-4.03290800
C	-3.59308700	-3.23151300	-4.01175700
C	-4.04490700	-4.02965900	-5.07199300
C	-4.72873500	-3.45991100	-6.15386900
C	-4.93704200	-2.07905000	-6.17164400
C	-5.68702700	-1.23967100	-7.18253400
C	-5.87843100	0.09021100	-6.45705100
O	-7.08496000	0.05926800	-5.61741500
C	-8.30555200	-0.81344800	-3.09273200
C	-7.55142500	1.39553700	-2.18878000
N	-6.52461100	2.13791100	-1.93610000
C	-6.84488500	2.90097800	-0.69829800
C	-8.03901900	2.12744500	-0.10057200
C	-9.09827900	3.15298800	0.30416700
C	-8.71627300	4.38603400	-0.48475800
C	-7.42873600	4.26215100	-1.02479700
C	-6.86470600	5.28744400	-1.78561200
C	-7.61161700	6.44901500	-2.00263100
C	-8.89805900	6.58114100	-1.46008900
C	-9.45806500	5.55087000	-0.69562500
O	-8.49748700	1.35642400	-1.26161700
H	-9.39996100	0.87661500	-5.01636900
H	-9.93912400	1.42986200	-3.40101700
H	-8.79841100	2.42511200	-4.37028300
H	-3.93095800	0.80008400	-5.65653100
H	-3.48323500	-1.22899500	-3.19511400
H	-3.09095100	-3.68764800	-3.15557600
H	-3.88112000	-5.10987100	-5.04430400
H	-5.10843000	-4.08993900	-6.96236600
H	-5.09159200	-1.07084500	-8.09614000
H	-6.64829300	-1.67567400	-7.49349800
H	-8.58322000	-1.35132600	-4.00877300
H	-7.46908600	-1.32779400	-2.60013000
H	-9.16582900	-0.79462300	-2.41102400
H	-5.97452700	2.94132000	-0.03778200
H	-7.76669300	1.39776500	0.67262300
H	-10.11383400	2.78468000	0.09299600
H	-9.03725600	3.33726200	1.39010500
H	-5.86855600	5.18130500	-2.21019200
H	-7.18883300	7.25490100	-2.60679600
H	-9.47051000	7.49487800	-1.63966700
H	-10.46271200	5.65388800	-0.27704800
H	-5.96207400	0.97632300	-7.09845300
C	-2.07092300	3.57663700	-4.37153000
H	-2.96991300	4.18427700	-4.48597800
H	-1.33211800	4.13194700	-3.78203500
H	-1.66723500	3.33316500	-5.36307600
O	-2.45094400	2.36026700	-3.68509900
C	4.33454500	4.77308100	-5.56761400
C	-0.07712300	-1.00971000	-9.25965400
C	3.96878000	5.55103200	-6.85221400
H	4.83186600	6.13933600	-7.20498500
H	3.66923000	4.87622500	-7.66859000
H	3.13415600	6.24555000	-6.66550500
C	4.80266600	5.78699400	-4.50892200
H	5.10516200	5.29152700	-3.57308800
H	5.67489600	6.34315600	-4.88669200
H	4.01810500	6.52240100	-4.27133900
C	5.50677200	3.81102900	-5.86633600
H	6.39109400	4.37537700	-6.20537000
H	5.78740400	3.24338500	-4.96478900
H	5.25131000	3.08647600	-6.65457800
C	1.29006300	-1.71276300	-9.41688400
H	1.37604300	-2.17001200	-10.41642800
H	2.12751800	-1.00828800	-9.29876100
H	1.41018300	-2.50837100	-8.66433000
C	-0.21314700	0.09611300	-10.33089300
H	-0.15203600	-0.33796900	-11.34248900

H	-1.18086500	0.61457700	-10.23804900
H	0.58273800	0.85131900	-10.24383300
C	-1.18493300	-2.05064200	-9.50256300
H	-1.12590500	-2.88713800	-8.78880800
H	-2.18919900	-1.60443100	-9.42568900
H	-1.08481400	-2.47086600	-10.51555000

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C	-1.25207100	1.26548000	-1.76114400
C	-1.16181700	2.24354200	-2.91626100
N	-0.10023100	1.95988600	-3.83319900
C	-0.03893500	0.84553500	-4.67699300
C	1.03534000	1.00520000	-5.58843200
C	1.65206700	2.28612000	-5.28237600
C	0.91024000	2.85356000	-4.21283300
C	1.23772400	4.11276000	-3.70852500
C	2.31646300	4.79211900	-4.28443100
C	3.08260200	4.25534500	-5.34319900
C	2.72888200	2.98754300	-5.83248300
C	1.26527000	0.02982800	-6.56566300
C	0.42972100	-1.09590100	-6.66680700
C	-0.63949200	-1.21141900	-5.75154000
C	-0.88430600	-0.25826600	-4.76130500
H	-0.27233700	1.25923100	-1.26362600
H	-1.99281100	1.59492800	-1.02747500
H	-1.48930400	0.24723800	-2.08704200
H	-1.00508600	3.25230900	-2.51626300
H	0.67489900	4.57270700	-2.89455300
H	2.55887600	5.77527200	-3.88237000
H	3.28829200	2.53411000	-6.65367800
H	2.09552000	0.16722500	-7.26203000
H	-1.32106700	-2.05990700	-5.79921200
H	-1.72686800	-0.37782800	-4.08932600
Sc	-4.48262800	2.12627000	-2.70303700
S	-3.15665200	4.37220900	-0.31931100
O	-1.83839300	3.86824100	0.06751400
O	-4.06429400	4.91261300	0.68515400
C	-2.78190000	5.79342200	-1.49499400
F	-2.18556700	6.76540500	-0.81795400
F	-1.95519300	5.37721900	-2.46818100
F	-3.88753100	6.26650400	-2.06143800
S	-4.87442500	-0.51384400	-0.64237000
O	-5.67808700	-1.48943000	-1.38002400
O	-5.47138300	0.17176300	0.50566900
C	-3.39807300	-1.45338800	0.02588700
F	-3.81151200	-2.39084200	0.86856700
F	-2.73264800	-2.03213400	-0.97965500
F	-2.57775500	-0.61852800	0.65674700
S	-5.95918200	4.16091800	-4.96261900
O	-7.36832200	4.22030600	-4.57887600
O	-5.59497900	3.44463000	-6.19418800
C	-5.40696100	5.93003700	-5.22186700
F	-6.01312100	6.42616700	-6.29445000
F	-5.71735500	6.66791800	-4.16049200
F	-4.08735600	5.96557300	-5.40841800
O	-3.87786000	3.39208500	-1.25498300
O	-4.12884400	0.44980600	-1.57739400
O	-5.03558500	3.78503000	-3.80097300
C	-8.98235800	1.37009700	-4.46893800
C	-7.80458200	0.64844600	-3.76630300
C	-6.57752400	0.64529000	-4.64665200
N	-5.34341000	0.83102300	-4.30460600
C	-4.53320000	0.27629400	-5.41451700
C	-4.24801400	-1.20428300	-5.22312900
C	-3.73264500	-1.85128200	-4.10140300
C	-3.53536900	-3.23456200	-4.15302700
C	-3.86748100	-3.95445800	-5.30941200
C	-4.43353900	-3.30679800	-6.41524300
C	-4.63563000	-1.92591000	-6.36042500
C	-5.27713300	-1.01540000	-7.38428300
C	-5.50421000	0.28166200	-6.60950500
O	-6.79119200	0.25045200	-5.89510500
C	-8.14927700	-0.85216400	-3.52851400
C	-7.57829400	1.31207300	-2.42580700
N	-6.57244200	2.00822300	-2.01537200
C	-6.95917500	2.61067200	-0.70903600
C	-8.20705800	1.79245000	-0.30214000
C	-9.27955200	2.77808500	0.16227500
C	-8.81087100	4.10443400	-0.39316900
C	-7.49116100	4.02180500	-0.85766400
C	-6.84495500	5.13371600	-1.39438000
C	-7.53869400	6.34464300	-1.46521600
C	-8.85846900	6.43526400	-1.00114000
C	-9.50282000	5.31588100	-0.46037200
O	-8.59320400	1.18623400	-1.58291000
H	-9.19557100	0.86722000	-5.42126300
H	-9.87288600	1.31713100	-3.82913100
H	-8.73265700	2.42109600	-4.66160800
H	-3.61862300	0.86068200	-5.57449200
H	-3.51553700	-1.29519100	-3.19258300
H	-3.13148200	-3.75182700	-3.27988400
H	-3.70626300	-5.03490100	-5.33962200
H	-4.72727000	-3.87741800	-7.29999600
H	-4.60544300	-0.81590700	-8.23654000
H	-6.21764400	-1.41112900	-7.79667800
H	-8.32277800	-1.34261600	-4.49539400
H	-7.33166300	-1.35725500	-2.99702700
H	-9.06263500	-0.91586500	-2.92276800
H	-6.12315600	2.52734900	-0.00373700
H	-7.99653600	0.96237800	0.38370800
H	-10.27762600	2.47530200	-0.18966700
H	-9.31474700	2.79506300	1.26463000
H	-5.82845000	5.05209700	-1.76558200
H	-7.04800700	7.22021700	-1.89574000
H	-9.39126100	7.38754600	-1.06546600
H	-10.53283700	5.38874000	-0.10139900
H	-5.50391400	1.20140500	-7.20621300
C	-2.37951500	3.11974800	-4.84242700
H	-3.34030200	3.04969400	-5.35708800
H	-2.19947700	4.16397300	-4.55533800
H	-1.58856800	2.75824600	-5.50986600
O	-2.44603500	2.28641800	-3.65636000
C	4.27360400	5.00653400	-5.97084500
C	0.68565900	-2.14557600	-7.76558800
C	4.00040900	5.23608000	-7.47483600
H	4.84310600	5.77183400	-7.94215200
H	3.86722700	4.28733500	-8.01678200
H	3.08914500	5.83807300	-7.62005600
C	5.55708900	4.16130400	-5.80553700
H	6.42131800	4.68205900	-6.24993300
H	5.77464400	3.98389700	-4.74019900
H	5.46862100	3.18125900	-6.29874500
C	4.51409200	6.37693700	-5.31319300
H	3.64299800	7.04195300	-5.42187300

H	4.74315100	6.28179400	-4.24023300
H	5.37211500	6.87376400	-5.79257400
C	2.09896100	-2.74399300	-7.58606900
H	2.30119600	-3.49704900	-8.36556400
H	2.88137300	-1.97290700	-7.65594800
H	2.19489500	-3.23329800	-6.60366800
C	-0.33514200	-3.29731700	-7.71834200
H	-0.29782700	-3.83900900	-6.76038200
H	-1.36635000	-2.93970600	-7.86550200
H	-0.11591800	-4.02119800	-8.51887400
C	0.58560800	-1.47071300	-9.15246100
H	0.76519700	-2.20659200	-9.95360700
H	-0.41552400	-1.03623900	-9.30475000
H	1.32436700	-0.66323200	-9.26959400

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C	-0.60929900	1.50952100	-2.04760700
C	-1.36810300	1.58788300	-3.40696400
N	-0.49608600	1.77163800	-4.53078300
C	-0.61252200	1.05389500	-5.73553400
C	0.28416700	1.59107900	-6.69134700
C	1.00481900	2.66092200	-6.03311100
C	0.51640900	2.74155400	-4.70124400
C	1.04142100	3.69320300	-3.81275800
C	2.05063500	4.54303600	-4.27064300
C	2.53810300	4.46648700	-5.58744500
C	2.01585200	3.52617100	-6.47341000
C	0.35726300	1.03560400	-7.97669100
C	-0.44848000	-0.05962600	-8.28824400
C	-1.29998900	-0.61434100	-7.31503200
C	-1.38459000	-0.07358400	-6.03013400
H	0.42815600	1.81781000	-2.23664600
H	-1.88902000	0.63840300	-3.56131400
H	0.68368800	3.79332100	-2.78965300
H	2.46488100	5.28455300	-3.58329900
H	3.32695100	5.14780200	-5.91407700
H	2.38504400	3.45830900	-7.49949700
H	1.04419100	1.45208600	-8.71725100
H	-0.40452200	-0.50297200	-9.28564000
H	-1.89959600	-1.49618600	-7.55478900
H	-2.01237200	-0.55312000	-5.28412800
Sc	-4.60571100	2.39063900	-2.59879200
S	-3.88433000	4.87415700	-0.17817200
O	-2.82379700	4.38122200	0.69366300
O	-5.11283200	5.39968100	0.41268500
C	-3.13497000	6.29891600	-1.14707200
F	-3.06978300	7.37394700	-0.37406900
F	-1.90337200	5.97856400	-1.55480500
F	-3.87847100	6.57436800	-2.22158600
S	-4.98857200	0.12189300	-0.26849400
O	-5.86194500	-0.84605600	-0.93485200
O	-5.55392600	0.99960800	0.75824800
C	-3.67128200	-0.88537300	0.60449900
F	-4.22950300	-1.55734900	1.60252200
F	-3.11249900	-1.75238500	-0.24543600
F	-2.72487800	-0.08330200	1.08487100
S	-5.40984900	3.64571400	-5.61849700
O	-6.73150100	3.13055100	-5.99003800
O	-4.23760000	3.11704100	-6.32747300
C	-5.44169200	5.48554800	-5.95654900
F	-5.58047300	5.69367700	-7.26048900
F	-6.45655800	6.04926100	-5.30782400
F	-4.29996500	6.03385300	-5.54199200
O	-4.17984100	3.91508500	-1.34721700
O	-4.10158300	0.89033800	-1.26955000
O	-5.19629100	3.68690200	-4.10244400
C	-9.00641500	1.53709400	-4.22466000
C	-7.94348400	0.75497600	-3.40196700
C	-6.70962200	0.56591700	-4.24234400
N	-5.48383700	0.83669500	-3.94267800
C	-4.65707400	0.20988800	-4.99709800
C	-4.24275300	-1.20134800	-4.62378000
C	-3.62054800	-1.64191400	-3.45613700
C	-3.32999100	-3.00319600	-3.32003100
C	-3.66957100	-3.90438600	-4.33851700
C	-4.32658500	-3.46196600	-5.49409400
C	-4.62149500	-2.10362200	-5.62789600
C	-5.35138400	-1.39174200	-6.74560600
C	-5.65117200	-0.01682600	-6.15238600
O	-6.91917300	-0.02365800	-5.41280400
C	-8.46234300	-0.65681800	-3.02179200
C	-7.69332300	1.57070400	-2.15599100
N	-6.69754200	2.34371400	-1.86944400
C	-7.14188200	3.19877800	-0.73447000
C	-8.37162100	2.44984100	-0.18077700
C	-9.47653600	3.48130200	0.04727700
C	-9.05186800	4.64806200	-0.81693300
C	-7.72086900	4.50920700	-1.23324800
C	-7.11418300	5.47286300	-2.03999600
C	-7.86132900	6.58831100	-2.42907100
C	-9.19137000	6.73656400	-2.00932000
C	-9.79480200	5.76791500	-1.19879400
O	-8.71658500	1.58493800	-1.31504700
H	-9.24873000	0.96809900	-5.13166700
H	-9.91448500	1.66377200	-3.62105600
H	-8.61564000	2.51897400	-4.52391200
H	-3.82408000	0.86927600	-5.27674500
H	-3.40165100	-0.94652600	-2.64921400
H	-2.85169300	-3.36190100	-2.40604700
H	-3.43869400	-4.96607700	-4.22087500
H	-4.61756400	-4.17304500	-6.27152000
H	-4.71083600	-1.26818900	-7.63533000
H	-6.26981800	-1.90328400	-7.07053300
H	-8.67051400	-1.22749400	-3.93626800
H	-7.71487300	-1.18697200	-2.41653100
H	-9.38846200	-0.55739800	-2.44107600
H	-6.33718600	3.31926200	-0.00478400
H	-8.15716400	1.78655200	0.66646100
H	-10.46595200	3.07253800	-0.20865500
H	-9.50475000	3.76118300	1.11400600
H	-6.08423700	5.35299000	-2.36887900
H	-7.40409000	7.34426100	-3.07147600
H	-9.76368100	7.61363100	-2.32251100
H	-10.83340600	5.88236700	-0.87735000
H	-5.71261100	0.80811300	-6.87296600
C	-2.21281700	3.88027200	-3.91044400
H	-3.09411100	4.49690900	-3.72755400
H	-1.36602100	4.31085800	-3.37047400
H	-2.02103800	3.84614900	-4.98946700
O	-2.50216700	2.54868100	-3.42150100
C	-1.17365800	2.40868100	-0.94915100
H	-2.16018800	2.07585100	-0.60746200
H	-0.50491900	2.40435500	-0.07725600
H	-1.27223200	3.45350600	-1.26601500

C	-0.54744200	0.02293200	-1.63970100
H	-0.15113400	-0.55602100	-2.49299000
H	-1.57233100	-0.34043100	-1.47133100
C	0.30001300	-0.26393600	-0.40191900
H	-0.13801900	0.18384100	0.50235400
H	0.37408900	-1.34878900	-0.22688700
H	1.32405500	0.12972100	-0.51557200

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C	-1.18234000	0.97415800	-1.69999600
C	-1.12153900	1.97212200	-2.88544800
N	0.02370600	1.82289000	-3.73337200
C	0.35183100	0.70807900	-4.50979300
C	1.46660600	1.02948800	-5.33013500
C	1.82503900	2.40355300	-5.03241900
C	0.90607200	2.86343500	-4.05291700
C	0.95848600	4.17183000	-3.55455000
C	1.95649200	5.01251600	-4.05369300
C	2.88103200	4.56917100	-5.01910600
C	2.82061100	3.26600800	-5.51311000
C	1.97966200	0.06918800	-6.21333700
C	1.37563600	-1.18731600	-6.27355700
C	0.27022700	-1.49043500	-5.45642100
C	-0.25395700	-0.55245100	-4.56437100
H	-1.73428600	0.08783200	-2.03311200
H	-1.09336200	2.99088100	-2.48629000
H	0.24992900	4.53397900	-2.80777200
H	2.01825600	6.03815400	-3.68143100
H	3.64990600	5.25433300	-5.38371700
H	3.53390500	2.91958700	-6.26496400
H	2.83764900	0.30673500	-6.84691000
H	1.76171100	-1.94424700	-6.96017700
H	-0.19201800	-2.47814700	-5.51994800
H	-1.09857800	-0.80145300	-3.92591800
Sc	-4.57573100	2.09489600	-3.17905600
S	-3.18154800	4.90771200	-1.46684200
O	-1.73771200	4.68981700	-1.31258600
O	-3.93491600	5.45704400	-0.34507500
C	-3.27117200	6.16481800	-2.86242200
F	-2.51043800	7.20465300	-2.54114800
F	-2.80922600	5.61831700	-3.98848600
F	-4.51664000	6.58568200	-3.06505600
S	-4.99464200	-0.77169600	-1.51542000
O	-6.13910200	-1.24983100	-2.29707700
O	-5.22295000	-0.38153000	-0.12167600
C	-3.80288300	-2.26228900	-1.45104200
F	-4.38276300	-3.30502900	-2.02614600
F	-2.65538200	-2.00333700	-2.08242300
F	-3.53357000	-2.55154000	-0.18314400
S	-5.83335600	3.77505300	-5.89654700
O	-7.18851800	3.22193100	-5.98794000
O	-4.89401400	3.48500700	-6.98670000
C	-6.06135600	5.63277400	-5.86540300
F	-6.73023600	5.99956500	-6.95314600
F	-6.75879900	5.98037200	-4.78488300
F	-4.88253300	6.24257300	-5.84718400
O	-3.89086000	3.69761300	-2.08560400
O	-4.15647200	0.27152000	-2.26802600
O	-5.17865200	3.56054800	-4.52530500
C	-9.07683200	2.18206000	-3.64375200
C	-8.18499600	0.97342600	-3.21191600
C	-7.24608500	0.66777900	-4.35498600
N	-5.97811100	0.86924900	-4.45477700
C	-5.55608200	0.33723000	-5.77904600
C	-4.90799400	-1.02737800	-5.69273400
C	-3.74080100	-1.38380700	-5.01878700
C	-3.33131700	-2.72041100	-5.04468300
C	-4.08145600	-3.67929100	-5.73938600
C	-5.24652700	-3.31395900	-6.42339600
C	-5.65741800	-1.97914500	-6.39654400
C	-6.84601600	-1.34639900	-7.08389600
C	-6.89776900	0.07284100	-6.50943900
O	-7.85640000	0.15197800	-5.41468100
C	-9.06775200	-0.25822200	-2.91376500
C	-7.47308900	1.45622500	-1.97474700
N	-6.37421900	2.14131800	-1.91727400
C	-6.37972900	2.80666700	-0.58935200
C	-7.36973500	1.96093700	0.23460000
C	-8.24390600	2.92893500	1.03029600
C	-8.14616400	4.21129500	0.23322800
C	-7.08720400	4.14667400	-0.68171300
C	-6.86093100	5.17019200	-1.59856000
C	-7.68159900	6.30099200	-1.55921100
C	-8.71721700	6.39221800	-0.61790000
C	-8.96223600	5.34400700	0.27864000
O	-8.15635300	1.34404600	-0.84871600
H	-9.65966400	1.89708300	-4.52963300
H	-9.76156700	2.43644000	-2.82289700
H	-8.46101500	3.05365300	-3.89767500
H	-4.92765700	1.07710900	-6.29589400
H	-3.16805900	-0.63504300	-4.47264300
H	-2.43184500	-3.02267400	-4.50507800
H	-3.75345300	-4.72174200	-5.74579800
H	-5.82712900	-4.06321300	-6.96773600
H	-6.69880600	-1.30611100	-8.17601900
H	-7.79326300	-1.87764300	-6.90436800
H	-9.61840200	-0.53980500	-3.81976600
H	-8.45138500	-1.10240100	-2.58255000
H	-9.78759200	-0.00683100	-2.12465800
H	-5.36773200	2.87046100	-0.17160400
H	-6.92128700	1.13623000	0.80068700
H	-9.27170300	2.55042200	1.13746700
H	-7.82898400	3.04224100	2.04648600
H	-6.08335600	5.07131700	-2.34987900
H	-7.51729600	7.10912800	-2.27576200
H	-9.35316000	7.28099800	-0.59697900
H	-9.79174300	5.40452300	0.98805000
H	-7.17943900	0.85531700	-7.22455300
C	-2.15692000	2.65235600	-4.97660000
H	-3.13049000	2.82994200	-5.44082600
H	-1.69489900	3.62797700	-4.77855000
H	-1.53743200	2.06922600	-5.66962000
O	-2.34901500	1.92247900	-3.73650500
C	0.23540000	0.55543600	-1.27750200
H	0.77179200	0.01467000	-2.06690200
H	0.83724400	1.43472700	-0.99523800
H	0.18476300	-0.11058700	-0.40560600
C	-1.93120400	1.58733900	-0.49748000
H	-2.91297400	1.94227200	-0.82417700
H	-1.39189000	2.49009200	-0.16923400
C	-2.13841200	0.64473100	0.68770200
H	-1.19242900	0.38119300	1.18455800
H	-2.78381000	1.12102800	1.44210300
H	-2.63605400	-0.28705700	0.38744400

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C	-0.25718600	1.61447200	-1.94998200
C	-1.14486500	1.76657400	-3.23492900
N	-0.49136000	1.96746400	-4.51385600
C	-0.68840100	1.04678700	-5.56260900
C	-0.12597500	1.55444300	-6.75828800
C	0.50369500	2.80947100	-6.41627100
C	0.29650700	3.02386000	-5.02429400
C	0.87503800	4.14112800	-4.40690700
C	1.61697500	5.03380800	-5.18271400
C	1.80030700	4.83623600	-6.56204200
C	1.24667200	3.71830300	-7.18145500
C	-0.20845100	0.81813200	-7.94799900
C	-0.82702600	-0.43225500	-7.92977100
C	-1.32974400	-0.95525800	-6.72475500
C	-1.25428300	-0.23132800	-5.53234000
H	-1.62735800	0.79281100	-3.34194100
H	0.76379000	4.33179200	-3.34550100
H	2.06561500	5.90321800	-4.69603100
H	2.38435000	5.55391700	-7.14252500
H	1.39247900	3.53924400	-8.24939200
H	0.21790300	1.21721700	-8.87141400
H	-0.89976100	-1.01965200	-8.84795200
H	-1.78185100	-1.94967200	-6.70556800
H	-1.62125500	-0.68272100	-4.61330500
Sc	-4.51615800	2.18768800	-2.56386800
S	-3.78469000	4.03049100	0.27686500
O	-2.66022500	3.23703700	0.76964800
O	-4.93706400	4.26358900	1.14586400
C	-3.09822500	5.74188800	-0.08414100
F	-2.92172400	6.39000900	1.05959400
F	-1.92519700	5.64946900	-0.71741300
F	-3.94252400	6.42690500	-0.85404900
S	-5.20393200	-0.23555300	-0.43635200
O	-5.98159100	-1.14693200	-1.27751600
O	-5.89518800	0.53727500	0.59723700
C	-3.95274500	-1.29000700	0.47817200
F	-4.59810300	-2.15856900	1.24731500
F	-3.18604200	-1.96114400	-0.38658500
F	-3.17665200	-0.51983300	1.23144100
S	-4.97460800	3.59199500	-5.57123900
O	-6.24080200	3.10090600	-6.12521300
O	-3.72371300	3.08918800	-6.15228000
C	-4.98029500	5.44598100	-5.82586000
F	-5.02271600	5.71534300	-7.12515800
F	-6.04166000	5.97927400	-5.22774900
F	-3.87423300	5.97558000	-5.30273400
O	-4.21262100	3.62067300	-1.14388400
O	-4.23360700	0.63438100	-1.26135300
O	-4.95059300	3.56597800	-4.03928000
C	-8.78631600	1.69744900	-4.57490000
C	-7.86904000	0.79367400	-3.70320000
C	-6.58311300	0.53914400	-4.44224800
N	-5.36821500	0.71853800	-4.04607100
C	-4.50842700	0.06105800	-5.06105900
C	-4.19374700	-1.37374700	-4.68857000
C	-3.63437300	-1.85603600	-3.50620800
C	-3.44043200	-3.23385300	-3.36652600
C	-3.80927600	-4.10866000	-4.39850300
C	-4.38991500	-3.62032900	-5.57597300
C	-4.58694500	-2.24443000	-5.71340700
C	-5.19392500	-1.47933700	-6.86811200
C	-5.43375500	-0.08820800	-6.28448700
O	-6.74662200	-0.00949700	-5.64011200
C	-8.52810100	-0.58722500	-3.44265400
C	-7.67658300	1.52298600	-2.39665400
N	-6.66381300	2.20728200	-1.97916100
C	-7.13959500	2.99108100	-0.80514800
C	-8.46361700	2.30024700	-0.42014500
C	-9.50918600	3.39286000	-0.19330200
C	-8.91915900	4.59887600	-0.88976100
C	-7.57001800	4.38867800	-1.20955400
C	-6.82452200	5.37417700	-1.85882800
C	-7.44728100	6.58312800	-2.18505000
C	-8.79359300	6.80099700	-1.86016800
C	-9.53769500	5.80987400	-1.20875900
O	-8.76638200	1.54974400	-1.64189400
H	-8.99438900	1.18967700	-5.52566600
H	-9.73047800	1.87870700	-4.04479200
H	-8.28955400	2.65267800	-4.79235200
H	-3.62002000	0.67035900	-5.27578200
H	-3.37872800	-1.17467100	-2.69640400
H	-3.01454000	-3.62616200	-2.44064900
H	-3.65588600	-5.18388000	-4.27672100
H	-4.69362700	-4.30762200	-6.36979800
H	-4.48633100	-1.39948600	-7.71096200
H	-6.12301400	-1.92197800	-7.25764600
H	-8.68772500	-1.10243700	-4.39860300
H	-7.88296200	-1.19927300	-2.79722000
H	-9.49608700	-0.43985000	-2.94708600
H	-6.39800500	2.97217800	-0.00398500
H	-8.36979000	1.56171800	0.38562100
H	-10.49419400	3.09217700	-0.58198000
H	-9.62670100	3.57254200	0.88868600
H	-5.78273200	5.19933900	-2.11697100
H	-6.87918900	7.35809300	-2.70515200
H	-9.26826400	7.74992500	-2.12298800
H	-10.58923700	5.97875800	-0.96196200
H	-5.38530400	0.74234000	-6.99998400
C	-2.12503100	4.04461400	-3.38801900
H	-3.00188400	4.58354800	-3.02641400
H	-1.24279900	4.45384900	-2.89295900
H	-2.05829700	4.14799500	-4.47652700
O	-2.29792800	2.65255800	-3.03930500
C	1.03906200	0.89781600	-2.36623100
H	1.66706600	1.53214400	-3.00934600
H	1.62116100	0.63788300	-1.46882600
H	0.82772700	-0.03599200	-2.91234400
C	-1.05085300	0.71367800	-0.97919900
H	-1.31715700	-0.25155400	-1.43864300
H	-0.44535600	0.49949900	-0.08570300
H	-1.97075400	1.20389900	-0.63865100
C	0.06453600	2.90983200	-1.18817900
H	-0.84769500	3.44827500	-0.90942300
H	0.57385000	2.64563900	-0.24867100
H	0.74237400	3.57831500	-1.73165300

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C	-0.87719500	0.68876300	-2.00162500
C	-1.17700200	1.74023400	-3.13237800
N	-0.11958500	1.89460300	-4.10078700
C	0.32686400	0.98007800	-5.06377700
C	1.52588100	1.47483200	-5.64555200

C	1.81532300	2.74215600	-5.00524100
C	0.78101600	2.96987900	-4.06100600
C	0.77341200	4.11306700	-3.25006900
C	1.80581000	5.03719700	-3.42418600
C	2.83096700	4.83159500	-4.36745300
C	2.84349300	3.68334100	-5.15850600
C	2.15871300	0.75338700	-6.66787600
C	1.58624900	-0.43766500	-7.11372600
C	0.37688800	-0.89735600	-6.55943200
C	-0.27034300	-0.19586600	-5.54030200
H	-1.27958200	2.71429600	-2.64360800
H	0.00589700	4.28752600	-2.49610600
H	1.81505800	5.93827900	-2.80599600
H	3.62380600	5.57562900	-4.47388200
H	3.64080100	3.51407300	-5.88630100
H	3.08302400	1.12950800	-7.11306200
H	2.06860800	-1.01034200	-7.90921000
H	-0.07590200	-1.81784600	-6.93611200
H	-1.22105600	-0.54997600	-5.14818100
Sc	-4.61954100	1.92921300	-3.00484800
S	-3.08025200	4.53839100	-1.14929400
O	-1.69131600	4.30911000	-0.74267900
O	-4.02683500	5.11169800	-0.19959400
C	-2.89753000	5.76516600	-2.56779500
F	-2.09257700	6.74324700	-2.17217600
F	-2.34798700	5.15238700	-3.62086700
F	-4.06584700	6.28205300	-2.92670800
S	-5.11365800	-0.41185400	-0.68575300
O	-6.47183700	-0.88985500	-0.96176200
O	-4.89856900	0.43138400	0.49339800
C	-4.11571800	-1.97898200	-0.41021300
F	-4.79753900	-2.76729700	0.41236900
F	-3.92392600	-2.61190900	-1.56557000
F	-2.93748300	-1.69499900	0.13656000
S	-5.95911200	3.84172400	-5.45141400
O	-7.38609200	3.81305200	-5.13166900
O	-5.49566800	3.12517500	-6.64906500
C	-5.53005000	5.63801000	-5.76397100
F	-6.04326200	6.00023600	-6.93466500
F	-6.04297600	6.40676100	-4.80677200
F	-4.20978800	5.79264700	-5.79595500
O	-3.66968500	3.30933400	-1.86263200
O	-4.42889200	0.16536300	-1.93719300
O	-5.06798500	3.55295000	-4.23583700
C	-9.40698000	1.79608300	-3.70565000
C	-8.24542700	0.85976000	-3.26011700
C	-7.26807200	0.67298400	-4.39763500
N	-5.98130700	0.80081000	-4.41984500
C	-5.51575300	0.21740300	-5.71107500
C	-5.00888400	-1.20160100	-5.56806000
C	-3.94160900	-1.66344300	-4.79805100
C	-3.65603600	-3.03207400	-4.79039000
C	-4.42904900	-3.91963000	-5.55247900
C	-5.49253700	-3.45042400	-6.33323500
C	-5.78065200	-2.08330700	-6.33700200
C	-6.84197900	-1.34404200	-7.12119500
C	-6.81645400	0.07098000	-6.53505600
O	-7.83917500	0.21698400	-5.50446900
C	-8.80788800	-0.54671200	-2.91856500
C	-7.63835100	1.51375100	-2.04394300
N	-6.52440600	2.16778100	-1.94607800
C	-6.60217900	2.92928900	-0.66955800
C	-7.70338300	2.19032500	0.11582300
C	-8.58881800	3.25051500	0.76783600
C	-8.33945300	4.47682900	-0.08280700
C	-7.20940100	4.30006300	-0.89197400
C	-6.81720400	5.27151500	-1.80925500
C	-7.55527700	6.45585300	-1.88870200
C	-8.66963800	6.65369900	-1.06052000
C	-9.07304900	5.66303200	-0.15619600
O	-8.42677600	1.53306700	-0.98315900
H	-9.88004300	1.37942700	-4.60426000
H	-10.14969100	1.85165200	-2.89929800
H	-9.03038100	2.79991600	-3.93537200
H	-4.79655800	0.89039900	-6.18959500
H	-3.34500900	-0.97453400	-4.20251100
H	-2.83194400	-3.40818000	-4.17982600
H	-4.19979100	-4.98808300	-5.53668700
H	-6.08993700	-4.14546400	-6.92892000
H	-6.59237800	-1.31050400	-8.19481100
H	-7.84542700	-1.78835400	-7.03611100
H	-9.36608800	-0.92946500	-3.78245900
H	-7.99836700	-1.23862700	-2.65897300
H	-9.48431700	-0.46353100	-2.05837000
H	-5.62659800	2.95166400	-0.16965400
H	-7.34279500	1.39216300	0.77667400
H	-9.64266900	2.93446300	0.79524100
H	-8.26538600	3.40393000	1.81147400
H	-5.97290600	5.09449200	-2.46844300
H	-7.26444200	7.22317200	-2.60948700
H	-9.23934700	7.58376200	-1.13302900
H	-9.95688300	5.81095200	0.46991800
H	-6.98017200	0.88059300	-7.25731800
C	-2.52515200	2.22178800	-5.11728300
H	-3.55927200	2.18960400	-5.46729800
H	-2.24039700	3.27462400	-5.00551000
H	-1.89948200	1.72648200	-5.86606600
O	-2.46280900	1.52717600	-3.84164500
C	0.64051800	0.74083200	-1.71462500
H	1.23874600	0.36664100	-2.55773200
H	0.97633100	1.76198400	-1.47913300
H	0.85666400	0.10879700	-0.84008900
C	-1.58802100	1.10550100	-0.69804600
H	-2.67305100	1.16469000	-0.79953200
H	-1.37760600	0.36243500	0.08457300
H	-1.23414800	2.08441300	-0.35315900
C	-1.26076400	-0.75133000	-2.36703000
H	-2.32905200	-0.83696800	-2.58684600
H	-0.68404600	-1.13153700	-3.21821400
H	-1.05197400	-1.40639800	-1.50949700

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C	-1.11003200	1.05195600	-2.40173600
C	-1.53660500	1.56367500	-3.79307300
N	-0.51499800	1.90592700	-4.73893700
C	-0.39320200	1.21981500	-5.96393800
C	0.77034300	1.66826300	-6.63653200
C	1.38650700	2.66559100	-5.78719200
C	0.57618100	2.79054300	-4.62667000
C	0.89174100	3.73720300	-3.64269900
C	2.03901400	4.51507500	-3.81351300
C	2.86184700	4.37555000	-4.94543500
C	2.53384500	3.45629200	-5.94022000
C	1.11487900	1.13124300	-7.88484100

C	0.30156900	0.14742500	-8.44632900
C	-0.84161400	-0.30436400	-7.76191900
C	-1.20127200	0.21828900	-6.51767900
H	-2.06316700	0.72395100	-4.25414000
H	0.26428300	3.89064400	-2.76998000
H	2.29175500	5.25327200	-3.04861600
H	3.75228200	4.99976800	-5.04889600
H	3.15373700	3.35342700	-6.83406900
H	2.01081300	1.47968000	-8.40415200
H	0.55495800	-0.28127100	-9.41858700
H	-1.46460800	-1.08555600	-8.20435100
H	-2.07841500	-0.17364300	-6.00585600
Sc	-4.62211200	2.43090500	-2.69471400
S	-3.66317000	4.79188600	-0.32925500
O	-2.70563400	4.01375600	0.45050100
O	-4.76536100	5.47068700	0.34722500
C	-2.67031800	6.12565800	-1.19434000
F	-2.25214000	7.02219000	-0.31153200
F	-1.60756100	5.57868600	-1.79772300
F	-3.41892200	6.72785400	-2.11724900
S	-4.79351900	0.11274100	-0.30914100
O	-5.49586800	-0.94118700	-1.04383400
O	-5.49006100	0.80791500	0.77397000
C	-3.30246600	-0.71222100	0.47229300
F	-3.71088300	-1.62363400	1.34502000
F	-2.56688000	-1.31174100	-0.47215300
F	-2.54938200	0.19074100	1.09041700
S	-5.77335500	3.58174400	-5.66786500
O	-7.11387400	3.02130800	-5.86428800
O	-4.68783100	3.07525500	-6.51882500
C	-5.90200000	5.41352700	-6.02381300
F	-6.20008600	5.59553600	-7.30498700
F	-6.84978900	5.95814000	-5.26722700
F	-4.73638300	6.00109500	-5.75520400
O	-4.15312300	4.04087600	-1.58254700
O	-4.06247500	1.08683100	-1.24966600
O	-5.36826300	3.65256500	-4.19442000
C	-9.09033900	1.29756000	-3.95630100
C	-7.91750400	0.61316100	-3.19842700
C	-6.74240900	0.46110400	-4.13105800
N	-5.51054900	0.79900700	-3.94113800
C	-4.74379200	0.22273400	-5.06874700
C	-4.17351000	-1.14516200	-4.74430600
C	-3.40504300	-1.53031100	-3.64589700
C	-2.98653000	-2.86100700	-3.54763600
C	-3.34701100	-3.79040700	-4.53282100
C	-4.15519800	-3.40939500	-5.61157100
C	-4.57717800	-2.08167600	-5.70704200
C	-5.48766600	-1.44592300	-6.73469700
C	-5.82476300	-0.08706900	-6.12315500
O	-7.01742100	-0.15969500	-5.27214900
C	-8.32367700	-0.80984200	-2.73109800
C	-7.62281700	1.49143600	-2.00394800
N	-6.65077400	2.32128900	-1.82084700
C	-7.01904900	3.17153600	-0.65604100
C	-8.19230800	2.40089600	-0.00687000
C	-9.31668000	3.40367600	0.25623000
C	-8.96062900	4.58062700	-0.62422800
C	-7.64801300	4.47714700	-1.10544200
C	-7.09951400	5.46924000	-1.92098500
C	-7.89141200	6.57015900	-2.26053500
C	-9.20526900	6.67849500	-1.78245600
C	-9.74688000	5.68627700	-0.95721800
O	-8.57591200	1.48190000	-1.08372500
H	-9.36414500	0.68568500	-4.82554600
H	-9.95478600	1.38191200	-3.28500600
H	-8.79227200	2.29305500	-4.31022900
H	-4.00281200	0.94822700	-5.43231100
H	-3.17495400	-0.82715800	-2.84899900
H	-2.39181100	-3.17448900	-2.68678600
H	-3.01495100	-4.82789600	-4.44565700
H	-4.46461800	-4.14556000	-6.35787100
H	-4.97318300	-1.29339100	-7.69848000
H	-6.39550200	-2.03332300	-6.93938600
H	-8.56572600	-1.42469600	-3.60802500
H	-7.50536400	-1.27549000	-2.16674400
H	-9.21009400	-0.73875800	-2.08752700
H	-6.15956800	3.30109000	0.00983800
H	-7.90455900	1.77616700	0.84702900
H	-10.30194800	2.96465000	0.03690300
H	-9.31736800	3.68845500	1.32192800
H	-6.07780300	5.38470000	-2.28677300
H	-7.48260400	7.34744900	-2.91009400
H	-9.81239800	7.54464400	-2.05818600
H	-10.77102800	5.77243100	-0.58466600
H	-6.00349100	0.72218000	-6.84200700
C	-2.39331900	3.85162800	-4.37398500
H	-3.21716900	4.50909400	-4.08812400
H	-1.45414700	4.32476000	-4.07860200
H	-2.43079000	3.67576600	-5.45589000
O	-2.58387700	2.60561400	-3.65565000
C	-0.07453200	-0.06392400	-2.56936000
H	0.88645500	0.33693100	-2.92872400
H	0.09920300	-0.55668600	-1.60102600
H	-0.41169300	-0.83336800	-3.28238100
C	-0.70950600	2.07017800	-1.33188900
H	-1.33430900	2.97104500	-1.36006500
H	-0.86339900	1.61950600	-0.34064600
H	0.34779600	2.35836000	-1.40373100
H	-2.03084100	0.58945900	-2.02883500

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C	-1.24748100	1.30011900	-1.88842600
C	-1.29561500	2.18003000	-3.14941800
N	-0.12751200	2.09787600	-3.99175300
C	0.24648900	1.06744000	-4.86250400
C	1.52201800	1.37163300	-5.41158700
C	1.93060000	2.64409700	-4.85091400
C	0.88434200	3.06674000	-3.98866600
C	0.96421600	4.27546800	-3.28376200
C	2.10430800	5.06003900	-3.46823500
C	3.14828500	4.65544600	-4.32258300
C	3.06803700	3.44770200	-5.01520900
C	2.10756800	0.50068200	-6.34216600
C	1.41373300	-0.64530900	-6.73002000
C	0.13409900	-0.91520900	-6.20738200
C	-0.46689200	-0.06527200	-5.27830500
H	-1.35995300	3.21941900	-2.81106300
H	0.17590300	4.60315000	-2.60632100
H	2.18585800	6.00773900	-2.93022100
H	4.02756300	5.29325500	-4.43921400
H	3.87654200	3.12837800	-5.67739700
H	3.09060100	0.72701800	-6.76235800
H	1.85775600	-1.33220600	-7.45430100

H	-0.40900100	-1.80530300	-6.53520900
H	-1.46320200	-0.27549700	-4.89990100
Sc	-4.61011100	2.05181800	-2.97848800
S	-3.23143600	4.65229200	-0.98902500
O	-1.87090100	4.39165100	-0.51986400
O	-4.22561900	5.20353700	-0.07434200
C	-2.98909900	5.92639500	-2.35577300
F	-2.38963000	6.98882300	-1.83538400
F	-2.20504400	5.41410300	-3.31433600
F	-4.13999800	6.29729300	-2.90375900
S	-4.53140000	-0.35387300	-0.57546700
O	-5.92566600	-0.19381400	-0.14725800
O	-3.45713800	-0.10621000	0.38230700
C	-4.40497300	-2.16619800	-1.04829400
F	-4.62853700	-2.90093900	0.03462200
F	-5.31825900	-2.46419500	-1.97434600
F	-3.19779800	-2.45555200	-1.53053700
S	-6.12478200	3.82627000	-5.39115500
O	-7.51904700	3.70145000	-4.96566400
O	-5.69904100	3.13249300	-6.61594100
C	-5.81109200	5.63869800	-5.74496800
F	-6.45536300	5.97650000	-6.85619300
F	-6.24521000	6.39548500	-4.74119600
F	-4.50659700	5.83876200	-5.91279900
O	-3.78935600	3.45334000	-1.77237500
O	-4.26323800	0.32196500	-1.92914400
O	-5.12913500	3.60863800	-4.24390300
C	-9.42965300	1.24910900	-3.65117600
C	-8.08293300	0.63746000	-3.18339900
C	-7.12119900	0.57038900	-4.34617100
N	-5.84786300	0.79151900	-4.36386700
C	-5.34762900	0.25182200	-5.65519700
C	-4.84348500	-1.17190100	-5.53286900
C	-3.87573100	-1.67305800	-4.66531800
C	-3.56493800	-3.03560600	-4.71140600
C	-4.22603000	-3.87964200	-5.61436700
C	-5.21744500	-3.37719900	-6.46680400
C	-5.52891300	-2.01664900	-6.41702100
C	-6.55875700	-1.24834000	-7.21490800
C	-6.62603700	0.10543000	-6.50759600
O	-7.65610500	0.09805700	-5.46439300
C	-8.27263600	-0.82641500	-2.69417700
C	-7.59097300	1.47134800	-2.02504400
N	-6.54103800	2.21702000	-1.93684800
C	-6.69726700	3.00723900	-0.68450800
C	-7.78177000	2.23572500	0.09832100
C	-8.76514300	3.26171500	0.66012400
C	-8.53179500	4.48066500	-0.20284300
C	-7.35713000	4.34507800	-0.95409400
C	-6.95610900	5.33129600	-1.85129700
C	-7.73595100	6.48483900	-1.97331100
C	-8.90084000	6.63827400	-1.20791400
C	-9.30950800	5.63475800	-0.32102300
O	-8.40871700	1.46760200	-0.98361100
H	-9.85085100	0.63241400	-4.45514200
H	-10.13258300	1.27162400	-2.80901100
H	-9.27253600	2.26924900	-4.02740300
H	-4.61623200	0.93666700	-6.09997500
H	-3.40569700	-1.02020400	-3.93243100
H	-2.81918900	-3.44229300	-4.02531200
H	-3.97794200	-4.94365300	-5.64131300
H	-5.74648700	-4.04358300	-7.15299100
H	-6.23667700	-1.10298000	-8.25976600
H	-7.54611400	-1.73379000	-7.24471800
H	-8.62374000	-1.45101500	-3.52649300
H	-7.32747700	-1.22680900	-2.30713600
H	-9.01803500	-0.84284200	-1.88857800
H	-5.73683500	3.10115500	-0.16419200
H	-7.39988600	1.50206700	0.81706100
H	-9.79906000	2.88537500	0.62845100
H	-8.52306100	3.46067400	1.71798300
H	-6.06768500	5.18938600	-2.45852200
H	-7.43806300	7.26412000	-2.67763500
H	-9.50265700	7.54459400	-1.31402300
H	-10.22796600	5.74905900	0.26075600
H	-6.83872100	0.96656100	-7.15207600
C	-2.49443300	2.66476000	-5.21167500
H	-3.47907200	2.55719600	-5.67251500
H	-2.30802800	3.73335900	-5.03972700
H	-1.73635200	2.24035800	-5.87867700
O	-2.51238800	1.95010300	-3.94638300
C	-1.18142500	-0.20710700	-2.11937600
H	-1.98202400	-0.55904300	-2.77504300
H	-0.21675900	-0.50863400	-2.55249500
H	-1.30769700	-0.71918700	-1.15618700
C	-0.06668600	1.74974800	-1.01485600
H	-0.11927600	2.81925700	-0.77572300
H	-0.08748100	1.19089600	-0.06720500
H	0.89488700	1.54106000	-1.51002800
H	-2.16616500	1.52600900	-1.33035600

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C	-0.06968200	0.08733900	0.08059700
C	0.04786900	-0.02686000	1.60226200
N	1.39890400	-0.10167200	2.09519100
C	2.40422700	-0.98913900	1.70158300
C	3.52219900	-0.82181900	2.54563800
C	3.16529400	0.17634400	3.52684600
C	1.85581800	0.60005900	3.21736100
C	1.21764900	1.54706700	4.00644600
C	1.88930800	2.02995200	5.12540900
C	3.18293000	1.61173300	5.47451800
C	3.81684400	0.68729700	4.64271300
C	4.67409500	-1.58250100	2.35524200
C	4.73291200	-2.53386500	1.34147000
C	3.58633600	-2.70814500	0.54225000
C	2.42980200	-1.95962000	0.70122700
C	-0.83685700	-1.24358800	2.12091300
C	-1.16433300	-1.01206600	3.53451900
N	-0.45334600	-1.25453400	4.59454600
C	-0.69569600	-0.58572000	5.85564700
C	0.35617800	-0.86441700	6.72089300
C	1.25327800	-1.79228700	6.04586200
C	0.73695100	-2.04765900	4.76748300
C	1.33045700	-2.97324400	3.93283900
C	2.48997900	-3.60326900	4.38086800
C	3.05938900	-3.33458300	5.62879600
C	2.40771000	-2.41743200	6.46678900
C	0.40377000	-0.26729800	7.97226500
C	-0.60704000	0.61317100	8.36397700
C	-1.65661900	0.86079900	7.46126300
C	-1.71614500	0.27932000	6.20160600
H	0.63790100	0.83120600	-0.28421700

H	-1.07786400	0.40888600	-0.17986800
H	0.12232900	-0.85326000	-0.42905400
H	-0.37562300	0.88638000	2.01621000
H	0.21907100	1.90260500	3.79022100
H	1.37008000	2.74695800	5.74307500
H	4.81596400	0.33979900	4.87028500
H	5.51701000	-1.41700800	3.01003900
H	3.59845000	-3.44699800	-0.24748000
H	1.58914800	-2.14301700	0.05068600
H	-0.30203700	-2.16497200	1.91818800
H	-1.76478700	-1.24920100	1.55182300
H	-2.03119600	-0.39072900	3.71924300
H	0.94606800	-3.22370700	2.95951900
H	2.95706200	-4.30694300	3.71046600
H	2.80028900	-2.19451100	7.44852300
H	1.23203100	-0.48894800	8.62714100
H	-2.45648300	1.52970500	7.74474100
H	-2.54175400	0.51049800	5.54302300
C	-0.61607100	1.29512300	9.73624900
C	3.90467100	2.12744700	6.72770000
C	4.36014200	-3.98879600	6.10161300
C	5.99396900	-3.35493200	1.04079700
C	-1.84127500	0.79482900	10.53029500
H	-1.86618400	1.26896100	11.51330700
H	-2.77678300	1.03058400	10.02154600
H	-1.79654000	-0.28635300	10.67415500
C	-0.71172300	2.82462700	9.55667300
H	-1.62658900	3.12149900	9.04359600
H	-0.70918300	3.31115700	10.53363300
H	0.13610200	3.20679600	8.98603500
C	0.64946700	0.98537200	10.54880100
H	0.74790900	-0.08115100	10.75907000
H	1.55308400	1.32333800	10.03812600
H	0.59946200	1.50364500	11.50705800
C	4.32020300	0.93278900	7.61024200
H	5.00727200	0.26463300	7.09163600
H	4.81937000	1.28562700	8.51513700
H	3.44627100	0.35098500	7.90851300
C	3.01652700	3.05059200	7.57301400
H	3.55918600	3.36641000	8.46539600
H	2.72709100	3.95068800	7.02798300
H	2.10899700	2.53988700	7.89887900
C	5.16388100	2.91106500	6.30733300
H	4.89634800	3.76845300	5.68676500
H	5.69442000	3.27932000	7.18839800
H	5.85305900	2.28584400	5.73800300
C	4.12302100	-4.70351000	7.44763400
H	5.04799000	-5.17614400	7.78294100
H	3.80342100	-4.01352300	8.22902700
H	3.36144900	-5.47902200	7.34697200
C	4.89432000	-5.01678600	5.09710800
H	5.82096700	-5.44983900	5.47552800
H	4.18749900	-5.83286800	4.93598000
H	5.11582900	-4.55727100	4.13451000
C	5.42412000	-2.88568400	6.28381500
H	5.12026800	-2.15136800	7.02989200
H	6.36735000	-3.32691300	6.61113500
H	5.60087500	-2.35948800	5.34429500
C	5.66378200	-4.86131200	1.04020100
H	4.92574600	-5.11700200	0.27956300
H	6.56488900	-5.44186700	0.83226400
H	5.27306000	-5.18043000	2.00746900
C	7.10959300	-3.10570200	2.06612000
H	7.97686500	-3.71947300	1.81821000
H	7.43444900	-2.06371900	2.06565900
H	6.79967900	-3.36694600	3.07930700
C	6.52451300	-2.95593600	-0.35265800
H	7.42589100	-3.52489600	-0.59134700
H	5.78812300	-3.15161000	-1.13328900
H	6.77347400	-1.89338900	-0.38248000

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Sc	-4.50682100	2.07685900	3.37837500
S	-2.84556700	4.31520800	1.16884600
O	-1.39681400	4.04350800	1.20753500
O	-3.43503400	4.78604300	-0.07934500
C	-3.03779000	5.72172400	2.40478300
F	-2.18997000	6.69707300	2.08818200
F	-2.73293000	5.28135700	3.63643000
F	-4.27253000	6.20523100	2.41701400
S	-4.29148400	-1.08609300	2.20688500
O	-5.00193400	-1.79372200	3.27544300
O	-4.90226800	-1.04545400	0.87399700
C	-2.69380400	-2.03711500	1.98733800
F	-2.94560400	-3.32231000	1.77929600
F	-1.92339800	-1.92023700	3.07849600
F	-2.01226300	-1.55408700	0.94086000
S	-6.69900300	4.17398800	4.88787500
O	-7.98995900	4.01484300	4.21443400
O	-6.56992900	3.66506500	6.26271600
C	-6.42638300	6.01998600	5.01801600
F	-7.27655900	6.53510000	5.90348000
F	-6.62877200	6.60161400	3.83602700
F	-5.17916500	6.27314000	5.41720000
O	-3.64479200	3.19524300	1.81251200
O	-3.71897700	0.25723700	2.64151400
O	-5.50893700	3.81076500	4.01243500
C	-9.26525500	1.05399600	3.45772600
C	-7.93042200	0.26976200	3.29664700
C	-7.10836400	0.45616400	4.55388000
N	-5.91542200	0.91475600	4.71312000
C	-5.55988400	0.72717900	6.14292300
C	-4.67878900	-0.48343200	6.38193000
C	-3.40186400	-0.73932600	5.87938700
C	-2.78879700	-1.95548300	6.19508600
C	-3.44005800	-2.89392300	7.00706500
C	-4.71436500	-2.62688300	7.52014000
C	-5.33157100	-1.41497400	7.20123300
C	-6.67931400	-0.90297100	7.65716300
C	-6.90726500	0.35134000	6.80747900
O	-7.74203100	0.04644100	5.65248500
C	-8.21790500	-1.24504500	3.12537900
C	-7.26367900	0.81169100	2.05563300
N	-6.27077300	1.62114400	1.96595900
C	-6.19358400	2.04108300	0.54667600
C	-7.09357100	1.02182900	-0.19134200
C	-8.00261900	1.80862300	-1.13922900
C	-7.94153300	3.22190500	-0.60325100
C	-6.90453600	3.36317200	0.32865100
C	-6.67815800	4.57633800	0.97716300
C	-7.49620500	5.66664300	0.66797500
C	-8.52357700	5.53801400	-0.27756800
C	-8.75426900	4.31387700	-0.91774600

O	-7.86610700	0.46280500	0.91759600
H	-9.82106600	0.65070800	4.31460300
H	-9.86779900	0.92937400	2.54786000
H	-9.06764800	2.12120900	3.62448800
H	-5.14358800	1.66031500	6.53496700
H	-2.91341200	-0.00570600	5.23788000
H	-1.80007300	-2.18460500	5.79581700
H	-2.94923900	-3.84281900	7.23889100
H	-5.22101500	-3.35828500	8.15547600
H	-6.66367200	-0.63759200	8.72763500
H	-7.49580900	-1.62787100	7.51594200
H	-8.73443600	-1.62104900	4.01811500
H	-7.28333900	-1.80259000	2.98664600
H	-8.86309800	-1.39174500	2.24978600
H	-5.14820300	2.05128500	0.21336100
H	-6.55291100	0.18366900	-0.64750200
H	-9.01929400	1.38683700	-1.15886500
H	-7.60647800	1.74961600	-2.16743000
H	-5.90222000	4.66091300	1.73181000
H	-7.33818900	6.61811000	1.18093900
H	-9.15865500	6.39742700	-0.50825600
H	-9.56644200	4.21233600	-1.64270100
H	-7.39107300	1.18475200	7.33281100
C	-3.03006700	3.04000400	5.87774400
H	-4.00476100	3.41954700	6.23143400
H	-2.37661300	3.91885500	5.75765200
H	-2.59428800	2.39338900	6.66262300
O	-3.17025200	2.34089900	4.67176600
C	0.11582700	1.11474800	0.34810800
C	0.41235400	1.58873300	1.77424100
N	1.58156700	0.98474400	2.39203400
C	1.81042700	-0.37813500	2.60068900
C	2.92001700	-0.54202000	3.46966900
C	3.36483000	0.78768600	3.83258200
C	2.51672000	1.69918500	3.14926000
C	2.67438000	3.07597500	3.32701500
C	3.65585900	3.52086000	4.21723200
C	4.50137700	2.63923100	4.92716500
C	4.34788900	1.26255300	4.70501900
C	3.34354400	-1.82238300	3.85135800
C	2.66566800	-2.95910000	3.39611000
C	1.54973500	-2.76223100	2.54576200
C	1.11569600	-1.50269500	2.13772400
C	-0.86563600	1.41590400	2.68261500
C	-0.77954600	2.42678700	3.74925300
N	-0.11553800	2.36134900	4.87516600
C	0.32007500	3.53750800	5.59016900
C	1.10129100	3.14458500	6.68205700
C	1.14561600	1.68454100	6.68862300
C	0.39255000	1.22140200	5.58931900
C	0.21104600	-0.13714500	5.37117900
C	0.83186700	-1.03113500	6.25206200
C	1.61442000	-0.60520400	7.33940200
C	1.75583500	0.78054800	7.54917100
C	1.68703600	4.10820200	7.50659200
C	1.49958400	5.47250200	7.23527600
C	0.71818800	5.82503300	6.11080100
C	0.12762100	4.87706900	5.27302100
H	1.04442000	1.09326400	-0.24077200
H	-0.58080700	1.83019200	-0.11104600
H	-0.34980300	0.12263400	0.31829100
H	0.62192500	2.66199200	1.69706200
H	2.03918000	3.80163000	2.81634200
H	3.74138200	4.59653700	4.36568400
H	4.97674000	0.54138700	5.23124100
H	4.20222400	-1.90707400	4.51691100
H	0.99339800	-3.62775600	2.18021200
H	0.25146200	-1.41907000	1.48711400
H	-0.95168200	0.38190700	3.01968000
H	-1.73984700	1.65060400	2.07184100
H	-1.09223200	3.42782900	3.45740200
H	-0.37885200	-0.53132300	4.55079000
H	0.70035300	-2.09259000	6.05257900
H	2.34666500	1.15960600	8.38364400
H	2.28804100	3.78011900	8.35265400
H	0.55627500	6.87788800	5.87606600
H	-0.46369500	5.20064200	4.41746000
C	3.09455300	-4.39275100	3.75939000
C	3.52609200	-5.13208200	2.47183000
H	3.83652100	-6.16413100	2.70475800
H	2.70614900	-5.18535900	1.73942500
H	4.37428700	-4.61858100	1.99170100
C	4.27729200	-4.41296000	4.74377300
H	4.54280600	-5.45347000	4.98753900
H	5.17236100	-3.93437800	4.31714000
H	4.03529800	-3.90230900	5.68829200
C	1.91043100	-5.14728800	4.40561200
H	1.05013700	-5.22533200	3.72421800
H	2.21083300	-6.17190300	4.67919100
H	1.56767100	-4.63827000	5.31967800
C	2.33415600	-1.58968400	8.27549600
C	3.85750100	-1.44384900	8.05314600
H	4.20425600	-0.42520300	8.28360700
H	4.40935600	-2.14497900	8.69985800
H	4.12125100	-1.66040000	7.00618200
C	1.93404500	-3.04875800	8.00058900
H	2.45575800	-3.71691000	8.70275800
H	0.85130000	-3.20526100	8.12773100
H	2.20962300	-3.36251000	6.98412300
C	1.99105200	-1.26589300	9.74664300
H	0.90606200	-1.33885900	9.92213800
H	2.49544600	-1.97970700	10.41729300
H	2.31561400	-0.25598300	10.03856800
C	2.08390400	6.58090500	8.12917300
C	3.01154500	6.01673600	9.22013900
H	3.42146100	6.84309600	9.82074900
H	2.47571600	5.34543400	9.90884800
H	3.86115000	5.46456500	8.78967200
C	2.89415200	7.58081100	7.27302600
H	2.27250100	8.07532300	6.51200700
H	3.31738300	8.36952700	7.91525900
H	3.72670700	7.07905800	6.75676500
C	0.91416300	7.32411600	8.81580500
H	1.30079500	8.12558000	9.46604800
H	0.23698600	7.78448500	8.08012400
H	0.32092300	6.63428400	9.43673500
C	5.56426900	3.13485400	5.92665400
C	5.33831000	2.46107100	7.29915300
H	5.43296900	1.36684000	7.24159000
H	6.07826600	2.82096400	8.03251700
H	4.33337900	2.69112100	7.68454900
C	6.97043800	2.76803500	5.40271000
H	7.16012400	3.24284000	4.42692900
H	7.74804500	3.10768300	6.10700900

H	7.08326900	1.68025700	5.27531500
C	5.49895900	4.65770300	6.13229800
H	6.24515600	4.96918300	6.87992800
H	5.71080800	5.20958800	5.20349300
H	4.50828800	4.96736600	6.49636000

tBu-Dimer pro-*racemo*

0 1

C	0.21995300	-1.07295000	0.78215800
C	0.29456700	0.40913500	1.16236400
N	1.58050600	0.81439400	1.70415800
C	2.35080400	0.18722800	2.69133900
C	3.45233700	1.02745700	3.02059400
C	3.34600300	2.20672200	2.18703800
C	2.17376400	2.04744800	1.41103500
C	1.74890800	3.06771800	0.55255700
C	2.52821400	4.21936000	0.47187100
C	3.72007300	4.40319300	1.21778700
C	4.11329600	3.37556400	2.08265500
C	4.33926100	0.66643000	4.03824700
C	4.15641100	-0.52116500	4.76192000
C	3.07308900	-1.34843800	4.39719200
C	2.17987200	-1.02272900	3.37294900
C	-0.92623700	0.90080400	2.03802100
C	-0.94935900	0.29218200	3.37861300
N	-0.26218300	0.64954500	4.43001100
C	-0.10469300	-0.20486900	5.58055300
C	0.82164400	0.37325400	6.45597600
C	1.21595000	1.66147400	5.89158100
C	0.52884800	1.83083500	4.67138900
C	0.62783900	3.01278200	3.95260100
C	1.46514600	4.01485800	4.45674600
C	2.20174200	3.86408600	5.64357400
C	2.05268200	2.66272900	6.36631100
C	1.19137200	-0.29704200	7.62303600
C	0.63379500	-1.55167400	7.91951300
C	-0.30620000	-2.09370700	7.01344600
C	-0.68416200	-1.44012900	5.83865300
H	1.14804600	-1.37730200	0.27748000
H	-0.61979700	-1.22790100	0.09487300
H	0.06212700	-1.73781000	1.64107300
H	0.17762400	0.97849100	0.23081600
H	0.81706000	3.00485300	-0.00819500
H	2.18681500	5.01243400	-0.19604800
H	5.01215100	3.46404800	2.69229200
H	5.16133100	1.34339700	4.28001900
H	2.89166800	-2.27906400	4.93352100
H	1.35651800	-1.69979200	3.15779400
H	-1.84696400	0.60126700	1.52320200
H	-0.91676800	1.99212800	2.05830600
H	-1.47624500	-0.65672900	3.48492800
H	0.08690800	3.20659000	3.03369300
H	1.53163000	4.93146900	3.87449900
H	2.58668700	2.50721000	7.30430000
H	1.91513600	0.16916100	8.28895100
H	-0.76965000	-3.05793500	7.22699400
H	-1.42154400	-1.89566600	5.17932500
Sc	-4.47459900	2.00535300	3.26311200
S	-2.46273900	4.47864500	1.69454300
O	-1.11422400	4.00395900	1.33294300
O	-3.09422400	5.46656700	0.82511600
C	-2.21571800	5.33256700	3.35966200
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F	-2.06594900	4.42828100	4.32890700
F	-3.25390600	6.10976500	3.64827100
S	-4.98715100	-0.57772100	1.13501700
O	-5.85996400	-1.41495700	1.96255500
O	-5.54831500	0.03128900	-0.07454300
C	-3.63998100	-1.73370700	0.53664400
F	-4.16743100	-2.83152900	0.01372400
F	-2.83617800	-2.08317900	1.55492300
F	-2.89488600	-1.12140800	-0.38936000
S	-6.08936900	3.92600100	5.53002600
O	-7.40706700	4.19731600	4.95027800
O	-6.02120600	3.02844700	6.69426200
C	-5.46330600	5.57474700	6.15317300
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O	-3.38555400	3.32734600	2.05358800
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C	-6.10909400	5.56567600	1.99392300
C	-6.68407700	6.83374500	2.11670000
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H	-3.06655900	-3.38126900	3.93788900
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H	-6.51351600	-4.28787700	6.38276700
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H	-5.15337200	3.18967300	0.33502900
H	-6.93828400	2.01548300	-0.95492200

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H	-7.62418100	4.18045500	-1.81219700
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H	-6.32447400	7.51213300	2.89345200
H	-8.16650500	8.22269400	1.37238900
H	-9.03232700	6.66174900	-0.37265700
H	-7.45303000	0.70353200	6.98063000
C	-2.77277000	1.76931300	5.79085700
H	-3.48312400	2.47705500	6.25335100
H	-1.78124000	2.25400800	5.80891400
H	-2.71912800	0.86320100	6.42319200
O	-3.15990400	1.45133400	4.48525300
C	3.16693000	4.94271900	6.15977900
C	4.53721000	5.69520200	1.02935800
C	5.11589000	-0.87238500	5.91489100
C	0.99480600	-2.33470700	9.19394100
C	5.08602300	5.73282000	-0.41576100
H	4.27304000	5.71390300	-1.15776100
H	5.67387200	6.65071800	-0.58274200
H	5.73916100	4.86682100	-0.60888700
C	3.63953100	6.93159200	1.26276800
H	4.22430700	7.85768200	1.13898000
H	2.80064100	6.97370900	0.55246800
H	3.21689400	6.92950300	2.27913500
C	5.72899100	5.77482900	2.00007100
H	5.40404000	5.74755500	3.05157300
H	6.44258300	4.95152400	1.84135000
H	6.27459200	6.71870500	1.84489900
C	3.11882000	6.21853200	5.30317200
H	2.11501200	6.67123400	5.29946700
H	3.82244500	6.96406700	5.70427500
H	3.40777400	6.01718700	4.26209300
C	2.80504100	5.31911100	7.61377400
H	1.77680400	5.70950200	7.67382900
H	2.88297100	4.46045600	8.29759900
H	3.48968200	6.09901200	7.98392400
C	4.60388900	4.37307200	6.11262900
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H	5.32684100	5.12712800	6.46340700
H	4.70931600	3.48179900	6.74920900
C	5.15012200	0.29081600	6.93190200
H	5.81965700	0.04841600	7.77325100
H	5.51181400	1.22476700	6.47761400
H	4.14511800	0.48272100	7.33773800
C	4.67847500	-2.14225100	6.66558700
H	4.68614600	-3.03011400	6.01453500
H	5.36664200	-2.33985800	7.50236700
H	3.66590000	-2.03139100	7.08210400
C	6.53535200	-1.09847900	5.34899900
H	7.24220100	-1.34370800	6.15910100
H	6.54012400	-1.92965200	4.62597400
H	6.91213100	-0.20170300	4.83324800
C	2.09447800	-1.63496800	10.01234200
H	3.02361300	-1.51801500	9.43329900
H	1.77676000	-0.64050900	10.36201900
H	2.33163200	-2.23634400	10.90324900
C	-0.26848300	-2.46054300	10.07651800
H	-1.07872700	-2.99445700	9.55699100
H	-0.03512300	-3.01836500	10.99785600
H	-0.64739500	-1.46694500	10.36376900
C	1.49950100	-3.74500700	8.81109000
H	1.76643000	-4.30980700	9.71859700
H	0.73604900	-4.32605000	8.27262100
H	2.39372800	-3.68502900	8.17157500

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