# Allylcopper Intermediates with N-Heterocyclic Carbene Ligands: Synthesis, Structure, and Catalysis

Vincenzo Russo, Jessica R. Herron and Zachary T. Ball

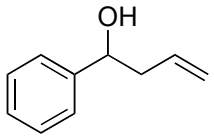
Department of Chemistry, Rice University, Houston, Texas 77005
zb1@rice.edu

## General information

All synthetic manipulations were carried out using standard Schlenk techniques under a nitrogen atmosphere or in a nitrogen-atmosphere glove box. All reactions were carried out in flame-or oven-dried glassware unless otherwise indicated. THF, ether, and benzene were distilled from sodium benzophenone ketyl under nitrogen. DMF and $Et_3N$ were distilled from calcium hydride. Anhydrous NMP was purchased from Aldrich and sparged vigorously with nitrogen for 30 min prior to first use. Pentane was sparged with nitrogen and stored in a glove box. All other solvents were reagent grade. NMR solvents were purchased from Cambridge Isotope Laboratories and were dried and degassed as follows: $C_6D_6$ over sodium/benzophenone, $CD_2Cl_2$ over $P_2O_5$, and THF-d8 over sodium/benzophenone, $CDCl_3$ (used as received). Dry NMR solvents were degassed with three freeze-pump-thaw cycles and transferred under vacuum to a storage flask. Flash chromatography was performed with 40-63 μm silica gel. NMR data was acquired with Bruker Avance 400 MHz or Bruker Avance 500 MHz instruments. Shifts for $^1H$ and $^{13}C$ NMR spectra were recorded relative to residual solvent. GC-MS was conducted on an Agilent 5973N MSD interfaced to an Agilent 6890N GC System equipped with an Rtx-35 MS column (30 m × 0.25 mm i.d., 0.10 μm film thickness; Restek, Bellefonte, PA). The analytical method entailed injection at 50 ˚C and a 5-min hold time followed by a ramp of 15 ˚C/min until a final temperature of 220 ˚C was reached. IR spectra were recorded using a Nicolet Avatar 320 FT-IR spectrometer and KBr plates. The following chemicals were purchased and used as received: 2,6-diisopropylaniline (Acros), glyoxal (40 wt. % solution in water Aldrich), formic acid (88% Fisher Scientific), paraformaldehyde (Acros), triethylamine tris(hydrofluoride) (Acros), benzaldehyde (Acros), phenylacetaldehyde (Acros), isobutyraldehyde (Acros), octanal (Acros) and allyltrimethoxysilane (Aldrich). Copper(I) chloride (Strem), sodium *tert*-butoxide (Acros), Lithium hexafluorophosphate (Acros), Lithium triflate (Aldrich), Scandium triflate (Strem), Indium triflate (Strem), Ytterbium triflate (Strem), Lanthanum triflate (Strem) and Europium triflate (Strem) were used as received, stored, and weighed in a glove box.

(IPr)CuF,[1] octyltrifluorosilane,[2] (S)-2-benzyloxypropanal,[3] (2-methyl-2-propenyl)triethoxysilane[4] and *(Z)*-crotyltrimethoxysilane[4] were synthesized according to literature protocols. We have not obtained satisfactory elemental analysis for our organocopper products; previous reports indicate that satisfactory elemental analysis cannot be obtained for this class of compounds.[5] The purity of all the compounds was assessed by $^1$H NMR and GC/MS and was found to be > 95%, unless otherwise noted.

**General procedure for catalyzed allylation: Synthesis of 1-phenyl-but-3-en-1-ol (Table 2, entry 1).**




In a glove box, a 20-mL scintillation vial equipped with a Teflon-coated stir bar and a rubber septum was charged with (IPr)CuF (22.4 mg, 0.047 mmol) and anhydrous THF (4.0 mL). The vial was then taken out of the glove box and sealed with electrical tape. Octyltrifluorosilane (19.0 mg, 0.096 mmol) and allyltrimethoxysilane (229.1 mg, 1.41 mmol) were added to the solution by syringe and the mixture was stirred for 5 min. Benzaldehyde (100 mg, 0.942 mmol), previously redistilled to remove traces of benzoic acid, was added to the solution and the mixture was stirred for 48 h. The reaction was then quenched with aq HCl (0.1 mL, 2 N soln) and stirred for 1 h. Ether (15 mL) was added, and the mixture was washed with water (2 × 50 mL) and brine (50 mL). The organic layer was dried over $MgSO_4$ and concentrated under vacuum. Kügelrohr distillation (chamber at 100 ˚C, 15 torr) of the residue afforded the final product (113 mg, 81%) as a colorless oil. Spectral data is consistent with that previously reported.[6] GC/MS, *m/z*: $t_R$ = 7.89 min; $[M]^+$ calcd, 148.2; found, 148.1; (> 95%).

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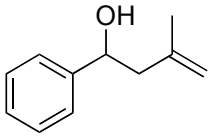
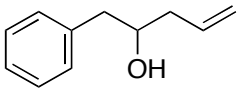
[1] Herron, J. R.; Ball, Z. T. *J. Am. Chem. Soc.* **2008**, *130*, 16486-18487.
[2] Tamao, K.; Kakui, T.; Akita, M.; Iwahara, T.; Kanatani, R.; Yoshida, J.; Kumada, M. *Tetrahedron*, **1983**, *39*, 983 – 990.
[3] Ito, Y.; Kawabata, T.; Terashima, S. *Tetrahedron Letters*, **1986**, *27*, 5751 – 5754.
[4] Furuya, N.; Sukawa, T. *J. Organometallic Chem.* **1975**, *96*, C1-C3.
[5] (a) Mankad, N. P.; Laitar, D. S.; Sadighi, J. P. *Organometallics* **2004**, *23*, 3369-3371; (b) Goj, L. A.; Blue, E. D.; Delp, S. A.; Gunnoe, T. B.; Cundari, T. R.; Pierpont, A. W.; Petersen, J. L.; Boyle, P. D. *Inorg. Chem.* **2006**, *45*, 9032-9045.
[6] Lipshutz, B. H.; Wilhelm, R. S.; Kozlowski, J. A.; Parker, D. *J. Org. Chem.* **1984**, *49*, 3928-3938.

**1-phenyl-3-methyl-3-buten-1-ol (Table 2, entry 2).**



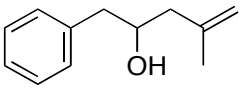

The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (22.4 mg, 0.047 mmol), octyltrifluorosilane (19.0 mg, 0.096 mmol), (2-methyl-2-propenyl)triethoxysilane (310.6 mg, 1.42 mmol) and benzaldehyde (100.0 mg, 0.942 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 115.5 mg (75%) of a colorless oil. Data was comparable to that available in the literature.[7] GC/MS, *m/z*: $t_R$ = 8.61 min; $[M]^+$ calcd, 162.2; found, 162.1; (> 95%).

**1-phenyl-4-penten-2-ol (Table 2, entry 3).**




The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (19.6 mg, 0.042 mmol), octyltrifluorosilane (16.4 mg, 0.083 mmol), allyltrimethoxysilane (202.2 mg, 1.25 mmol) and phenylacetaldehyde (100.0 mg, 0.832 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 98.6 mg (73%) of a colorless oil. Data was comparable to that available in the literature.[8] GC/MS, *m/z*: $t_R$ = 8.66 min; $[M]^+$ calcd, 162.2; found, 162.1; (> 95%).

**4-methyl-1-phenyl-4-penten-2-ol (Table 2, entry 4).**




The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (19.6 mg, 0.042 mmol), octyltrifluorosilane (16.4 mg, 0.083 mmol), (2-methyl-2-propenyl)triethoxysilane (271.6 mg, 1.25 mmol) and phenylacetaldehyde (100.0 mg, 0.832 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 105.0 mg (71.6%) of a colorless oil. Data was comparable to that available in the literature.[9] GC/MS, *m/z*: $t_R$ = 9.31 min; $[M]^+$ calcd, 176.3; found, 176.1; (> 95%).

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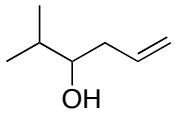
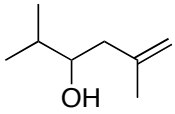
[7] Rieke, R. D.; Klein, W. R.; Wu, T. C. *J. Org. Chem.* **1993**, *58*, 2492-2500.
[8] Barentsen, H. M.; Sieval, A. B.; Cornelisse, J. *Tetrahedron* **1995**, *51*, 7495-7520.
[9] McCluskey, A.; Muderawan, I. W.; Muntari; Young, D. J. *J. Org. Chem.* **2001**, *66*, 7811-7817.

**2-methyl-5-hexen-3-ol (Table 2, entry 5).**



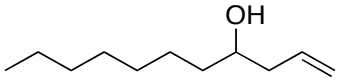

The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (32.0 mg, 0.068 mmol), octyltrifluorosilane (28.0 mg, 0.14 mmol), allyltrimethoxysilane (337.0 mg, 2.08 mmol) and isobutyraldehyde (100.0 mg, 1.34 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 89.2 mg (56%) of a colorless oil. Data was comparable to that available in the literature.[10] GC/MS, *m/z*: $t_R$ = 3.79 min; $[M - C_3H_7]^+$ calcd, 71.1; found, 71.1; (> 95%).

**2,5-dimethyl-5-hexen-3-ol (Table 2, entry 6).**




The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (32.0 mg, 0.068 mmol), octyltrifluorosilane (28.0 mg, 0.14 mmol), (2-methyl-2-propenyl)triethoxysilane (453.8 mg, 2.08 mmol) and isobutyraldehyde (100.0 mg, 1.34 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 115.6 mg (65%) of a colorless oil. Data was comparable to that available in the literature.[11] GC/MS, *m/z*: $t_R$ = 3.66 min; $[M - C_3H_7]^+$ calcd, 85.1; found, 85.2; (> 95%).

**1-undecen-4-ol (Table 2, entry 7).**




The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (18.4 mg, 0.039 mmol), octyltrifluorosilane (15.4 mg, 0.078 mmol), allyltrimethoxysilane (190.7 mg, 1.17 mmol) and octanal (100.0 mg, 0.779 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 116.7 mg (88%) of a colorless oil. Data was comparable to that available in the literature.[12] GC/MS, *m/z*: $t_R$ = 7.60 min; $[M - C_3H_5]^+$ calcd, 127.1; found, 127.2; (> 95%).

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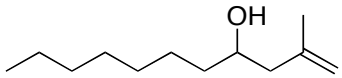
[10] Wada, M.; Ohki, H.; Akiba, K. *Bull. Chem. Soc. Jpn.* **1990**, *63*, 1738-1747.
[11] Miura, K.; Wang, D.; Hosomi, A. *J. Am. Chem. Soc.* **2005**, *127*, 9366-9367.
[12] Fürstner, A.; Shi, N. *J. Am. Chem. Soc.* **1996**, *118*, 12349-12357.

**2-methyl-1-undecen-4-ol (Table 2, entry 8).**

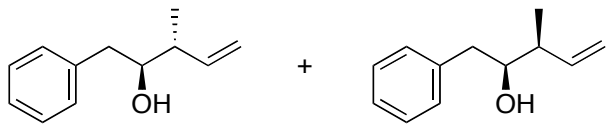



The procedure described for **(Table 2, entry 1)** was followed using (IPr)CuF (18.4 mg, 0.039 mmol), octyltrifluorosilane (15.4 mg, 0.078 mmol), (2-methyl-2-propenyl)triethoxysilane (254.8 mg, 1.17 mmol) and octanal (100.0 mg, 0.779 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr) and column chromatography ($SiO_2$, 20:1, hexane/EtOAc), affording 100.0 mg (72%) of a colorless oil. $^1$H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, $J$ = 6.9 Hz, 3 H), 1.2-1.5 (m, 12 H), 1.75 (s, 3 H), 2.09 (dd, $J$ = 13.5, 9.5 Hz, 1 H), 2.22 (dd, $J$ = 13.5, 3.5 Hz, 1 H), 3.70 (m, 1 H), 4.80 (m, 1 H), 4.89 (m, 1 H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 14.3, 22.6, 22.9, 25.9, 29.5, 29.9, 32.0, 37.3, 46.4, 68.9, 113.6, 143.1. IR (neat): 723, 889, 1081, 1126, 1275, 1457, 1647, 2856, 2956, 2928, 3075, 3370 cm$^{-1}$. GC/MS, *m/z* (rel. int. %) calculated for $[M - C_4H_9]^+$, 127.1; found, 127.2 (48), 111.2 (12), 83.2 (10), 69.2 (80), 56.2 (100); $t_R$ = 8.32 min; (>95%).

**2-methyl-1-phenyl-3-buten-1-ol (Table 3, entry 1).**


The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (22.4 mg, 0.047 mmol), octyltrifluorosilane (19.0 mg, 0.096 mmol), crotyltrimethoxysilane (250.0 mg, 1.42 mmol) and benzaldehyde (100.0 mg, 0.942 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 120.9 mg (78%) of a colorless oil. The product was identified as a 1:2 mixture of syn and anti diastereomers by NMR[13]: $^1$H NMR (400 MHz, $CDCl_3$): δ 0.89 (d, $J$ = 6.8 Hz, 2.0 H), 1.03 (d, $J$ = 6.8 Hz, 1 H), 2.20 (s, 1 H), 2.50 (m, 0.67 H), 2.60 (m, 0.33 H), 4.38 (d, $J$ = 7.2 Hz, 0.67 H), 4.65 (d, $J$ = 7.2 Hz, 0.33 H), 5.08 (m, 0.67 H), 5.22 (m, 1.33 H), 5.72-5.90 (m, 1 H), 7.21-7.40 (m, 5 H). GC/MS, *m/z*: $t_R$ = 8.38 min; $[M]^+$ calcd, 162.2; found, 162.2; (> 95%).

**3-methyl-1-phenyl-4-penten-2-ol (Table 3, entry 2).**




The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (19.6 mg,

[13] Tokuda, M.; Satoh, S.; Suginome, H. *J. Org. Chem.*, **1989**, *54*, 5608-5613.

0.042 mmol), octyltrifluorosilane (16.4 mg, 0.083 mmol), crotyltrimethoxysilane (220.0 mg, 1.25 mmol) and phenylacetaldehyde (100.0 mg, 0.832 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 96.7 mg (66%) of a 2.5:1 mixture of the syn and anti diastereomers. Data was comparable to that available in the literature.[14] The diastereomers are indistinguishable by $^{1}$H NMR and their ratio was obtained from $^{13}$C NMR (100 MHz, $CDCl_3$): δ 14.77, 16.6, 40.99, 41.06, 43.25, 43.52, 75.89, 76.0, 115.55, 116.4, 126.56, 126.6, 128.69, 128.75, 129.54, 129.58, 139.12, 139.17, 140.13, 141.13. From the $^{13}$C NMR the ratio between the syn and the anti isomers was calculated to be 2.5:1. GC/MS, *m/z*: $t_R$ = 9.34 min; $[M]^+$ calcd, 176.3; found, 176.1; (> 95%).

**2,4-dimethyl-5-hexen-3-ol (Table 3, entry 3).**


The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (32.0 mg, 0.068 mmol), octyltrifluorosilane (28.0 mg, 0.14 mmol), crotyltrimethoxysilane (366.5 mg, 2.08 mmol) and isobutyraldehyde (100.0 mg, 1.34 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 108.4 mg (61%) of a 4:1 mixture of syn and anti diastereomers. Data was comparable to that available in the literature[15]: $^{1}$H NMR (400 MHz, $CDCl_3$): δ 0.93 (d, *J* = 7.2 Hz, 3 H), 0.97 (d, *J* = 6.8 Hz, 3 H), 1.03 (d, *J* = 6.8 Hz, 3 H), 1.75 (m, 1 H), 2.25-2.45 (m, 1 H), 3.10 (dd, *J* = 5.6, 5.6 Hz, 0.80 H), 3.17 (dd, *J* = 6,6 Hz, 0.20 H), 5.0-5.15 (m, 2 H), 5.7-5.9 (m, 1 H). GC/MS, *m/z*: $t_R$ = 3.40 min (anti isomer); $[M - C_3H_7]^+$ calcd, 85.1; found, 85.1; $t_R$ = 3.58 min (syn isomer); $[M - C_3H_7]^+$ calcd, 85.1; found, 85.1; (> 95% for sum of two isomers).

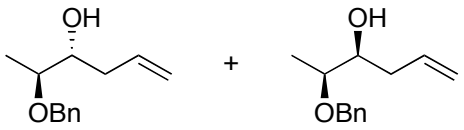
**3-methyl-1-undecen-4-ol (Table 3, entry 4).**


The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (18.4 mg, 0.039 mmol), octyltrifluorosilane (15.4 mg, 0.078 mmol), crotyltrimethoxysilane (207.5 mg, 1.17 mmol) and octanal (100.0 mg, 0.779 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 114.4 mg (79.3%) of a colorless oil as a 1:3 mixture of syn:anti diastereomers. Data was comparable to that

[14] McCluskey, A.; Muderawan, I. W.; Muntari; Young, D. J. *J. Org. Chem.* **2001**, *66*, 7811-7817.
[15] Helm, M. D.; Mayer, P.; Knochel, P. *Chem. Commun.* **2008**, *16*, 1916-1917.

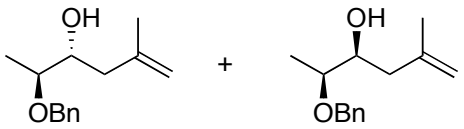
available in the literature[16]: $^1$H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, *J* = 7.2 Hz, 3 H), 1.03 (d, *J* = 7.2 Hz, 2.25 H), 1.04 (d, *J* = 6.8 Hz, 0.75 H), 1.2-1.5 (m, 12 H), 2.10-2.35 (m, 1 H), 3.35 (m, 0.75 H), 3.5 (m, 0.25 H), 5.0-5.2 (m, 2 H), 5.7-5.9 (m, 1 H). GC/MS, *m/z*: $t_R$ = 8.08 min (anti isomer); $[M - C_4H_9]^+$ calcd, 127.1; found, 127.2; $t_R$ = 8.16 min (syn isomer); $[M - C_4H_9]^+$ calcd, 127.1; found, 127.2; (> 95% for sum of two isomers).

**(S,S)-2-(benzyloxy)hex-5-en-3-ol and (S,R)-2-(benzyloxy)hex-5-en-3-ol.**




The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (14.4 mg, 0.031 mmol), octyltrifluorosilane (12.0 mg, 0.060 mmol), allyltrimethoxysilane (148.3 mg, 0.914 mmol) and (S)-2-benzyloxypropanal (100.0 mg, 0.609 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 107.5 mg (86%) of a colorless oil. The ratio between the syn and the anti diastereomers, determined by $^1$H NMR, was 1:1.5. Data was comparable to that available in the literature[17]: $^1$H NMR (400 MHz, $CDCl_3$): δ 1.20 (d, *J* = 6.4 Hz, 2 H), 1.21 (d, *J* = 6 Hz, 1.2 H), 2.15-2.40 (m, 1.8 H), 3.45 (qd, *J* = 6 Hz, 0.40 H), 3.51 (m, 1 H), 3.78 (m, 0.60 H), 4.47 (dd, *J* = 25.2, 11.2 Hz, 1 H), 4.64 (dd, *J* = 18, 11.6 Hz, 1 H), 5.0-5.20 (m, 2 H), 5.75-6.0 (m, 1 H), 7.20-7.40 (m, 5 H). GC/MS, *m/z*: $t_R$ = 10.56 min (syn isomer); $[M - C_3H_5]^+$ calcd, 165.2; found, 165.1; $t_R$ = 10.60 min (anti isomer); $[M - C_3H_5]^+$ calcd, 165.2; found, 165.1; (> 95% for sum of two isomers).

**(S,S)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol and (S,R)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol.**

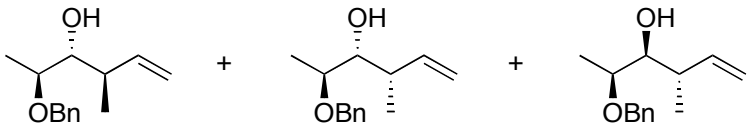



The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (14.4 mg, 0.031 mmol), octyltrifluorosilane (12.0 mg, 0.060 mmol), (2-methyl-2-propenyl)triethoxysilane (199.0 mg, 0.914 mmol) and (S)-2-benzyloxypropanal (100.0 mg, 0.609 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr) and column chromatography ($SiO_2$, 4:1, hexane/EtOAc), affording 100.7 mg (75%) of a colorless oil as a 1:1.9 syn/anti mixture. Data was comparable to that available

[16] Dinh, T. Q.; Du, X.; Smith, C. D.; Armstrong, R. W. *J. Org. Chem.* **1997**, *62*, 6773-6783.
[17] Stojanovic, A.; Renaud, P.; Schenk, K. *Helvetica Chimica Acta* **1998**, *81*, 268-284.

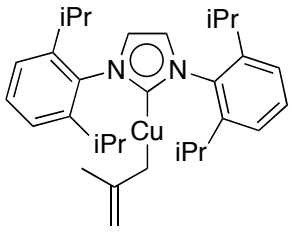
in the literature[18]: $^1$H NMR (400 MHz, $CDCl_3$): δ 1.21 (d, *J* = 6.4 Hz, 1.97 H), 1.22 (d, *J* = 6 Hz, 1.03 H), 1.75 (s, 3 H), 2.1-2.3 (m, 1 H), 3.46 (qd, *J* = 6.4 Hz, 0.34 H), 3.51 (m, 0.66 H), 3.65 (m, 0.34 H), 3.87 (m, 0.66 H), 4.49 (dd, *J* = 25.2, 11.2 Hz, 1 H), 4.65 (dd, *J* = 18, 11.6 Hz, 1 H), 4.78-4.9 (m, 2 H), 7.22-7.40 (m, 5 H). GC/MS, *m/z*: $t_R$ = 11.15 min (anti isomer); $[M - C_4H_7]^+$ calcd, 165.2; found, 165.1; $t_R$ = 11.18 min (syn isomer); $[M - C_4H_7]^+$ calcd, 165.2; found, 165.1; (> 95% for sum of two isomers).

**(2S,3R,4R)-2-(benzyloxy)-4-methyl-5-hexen-3-ol, (2S,3R,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol and (2S,3S,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol.**




The procedure described for **(Table 1, entry 1)** was followed using (IPr)CuF (14.4 mg, 0.031 mmol), octyltrifluorosilane (12.0 mg, 0.060 mmol), crotyltrimethoxysilane (160.0 mg, 0.914 mmol) and (S)-2-benzyloxypropanal (100.0 mg, 0.609 mmol). The product was purified via Kügelrohr distillation (chamber at 100 ˚C, 15 torr), affording 115.2 mg (85%) of a colorless oil. The ratio and the identity of the diastereomers was determined by $^{13}$C NMR and GC-MS, and was calculated to be 1:3.4:1.14, (2S,3S,4S):(2S,3R,4R):(2S,3R,4S). The amount of diastereomer (2S,3R,4R) was less than 5% of the material. Data was comparable to that available in the literature[19]: $^1$H NMR (400 MHz, $CDCl_3$): δ 0.99 (d, *J* = 7.2 Hz, 1.84 H), 1.08 (d, *J* = 5.6 Hz, 0.63 H), 1.10 (d, *J* = 5.6 Hz, 0.53 H), 1.90 (d, *J* = 6.4 Hz, 0.53 H), 1.92 (d, *J* = 7.2 Hz, 0.63 H), 1.22 (d, *J* = 6 Hz, 1.84 H), 2.25-2.40 (m, 0.37 H), 2.40-2.50 (m, 0.63 H), 3.55 (m, 2 H), 4.48 (dd, *J* = 25.2, 11.2 Hz, 1 H), 4.60 (dd, *J* = 18, 11.6 Hz, 1 H), 4.95-5.08 (m, 0.73 H), 5.08-5.19 (m, 1.92 H), 5.66 (ddd, *J* = 18.8, 10.8, 8 Hz, 0.26 H), 5.86 (ddd, *J* = 18, 10, 8 Hz, 1 H), 7.21-7.41 (m, 7.22 H). GC/MS, *m/z*: $t_R$ = 10.92 min (2S,3R,4S isomer); $[M - C_4H_7]^+$ calcd, 165.2; found, 165.1; $t_R$ = 10.97 min (2S,3S,4S isomer); $[M - C_4H_7]^+$ calcd, 165.2; found, 165.1; $t_R$ = 11.18 min (2S,3R,4R isomer); $[M - C_4H_7]^+$ calcd, 165.2; found, 165.1; (> 95% for sum of three isomers).

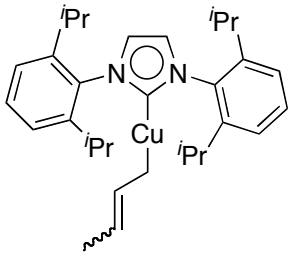
**Synthesis of [1,3-bis(2′,6′-diisopropylphenyl)imidazol-2-ylidene]copper(I) 2-methallyl (3).**




[18] Heathcock, C. H.; Kiyooka, S.; Blumenkopf, T. A. *J. Org. Chem.* **1984**, *49*, 4214-4223.
[19] Martin, S. F.; Li, W. *J. Org. Chem.* **1989**, *54*, 6129-6133.

In the glove box, (IPr)CuF (20.0 mg, 0.042 mmol) was dissolved in THF-$d_8$ (0.50 mL) in an NMR tube. The tube was then sealed with a rubber septum and taken out of the box. (2-methyl-2-propenyl)triethoxysilane (9.3 mg, 0.042 mmol) was added via syringe to the solution in the NMR tube and a spectrum (400 MHz) was recorded after 10 min. Two singlet resonances, at 2.14 (4 H) and 1.09 (3 H) ppm, were observed, corresponding to the allylcopper species in fast equilibrium between the $\eta^1$ and $\eta^3$ coordination modes.

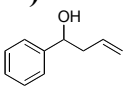
**Synthesis of [1,3-bis(2′,6′-diisopropylphenyl)imidazol-2-ylidene]copper(I) 1-methallyl (4).**



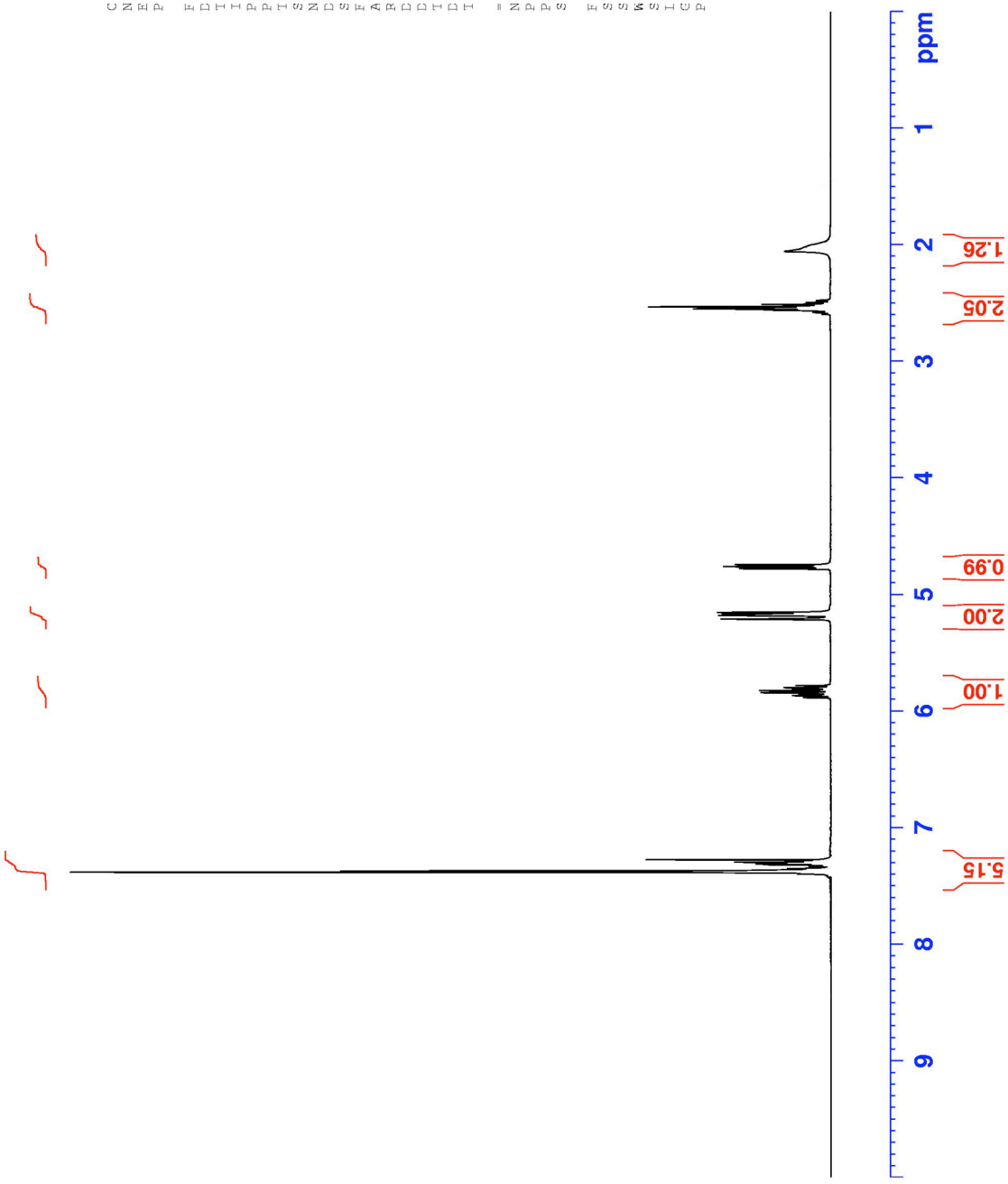

In the glove box, (IPr)CuF (20.0 mg, 0.042 mmol) was dissolved in THF-$d_8$ (0.50 mL) in an NMR tube. The tube was then sealed with a rubber septum and taken out of the box. Crotyltrimethoxysilane (7.5 mg, 0.042 mmol) was added via syringe to the solution in the NMR tube and a spectrum (400 MHz) was recorded after 10 min. The spectrum showed for resonances at 5.39, 3.93, 0.99 and 0.59 ppm, corresponding to the allylcopper species.

**NMR spectra**

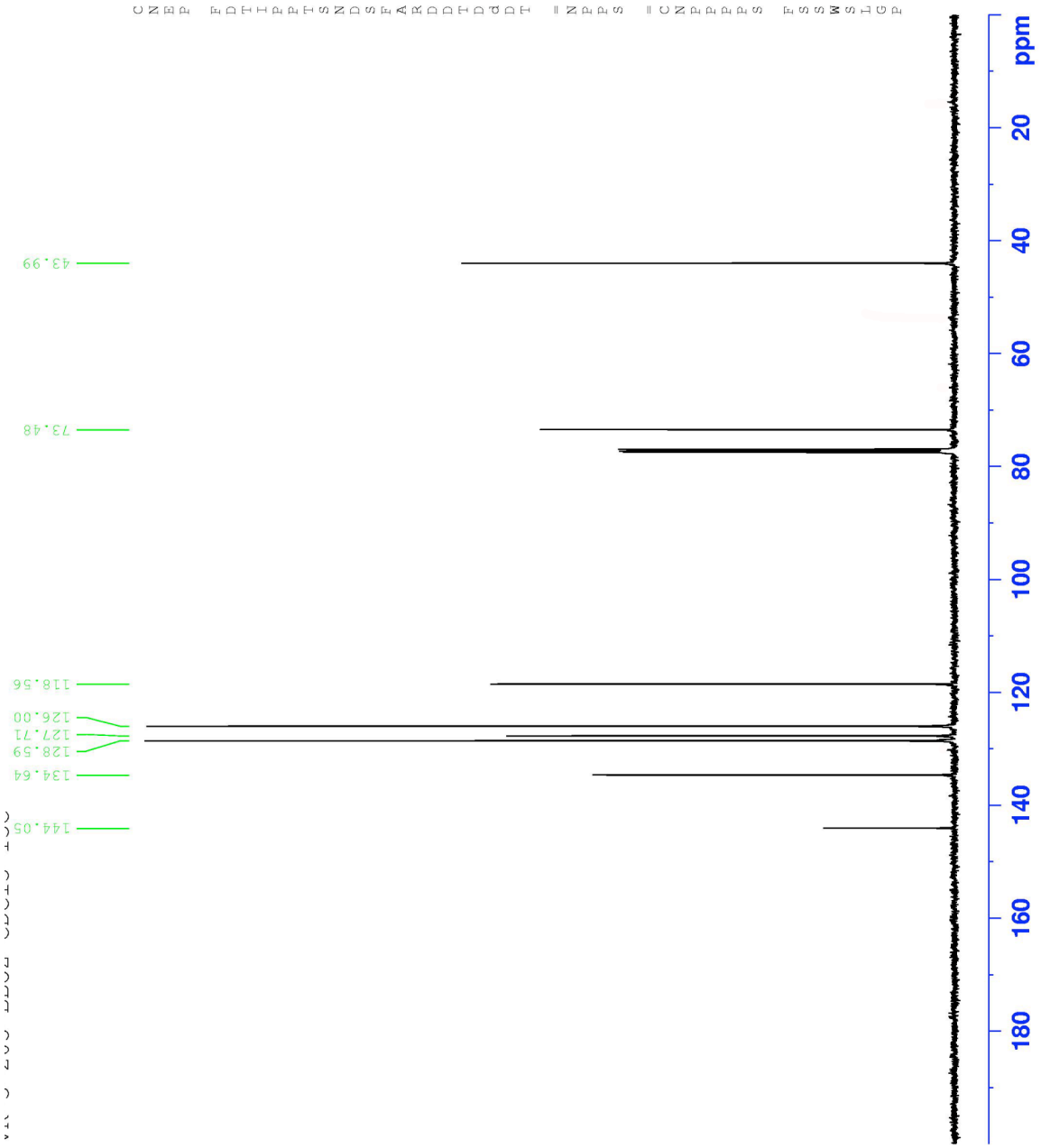
**1-phenyl-but-3-en-1-ol (Table 2, entry 1)**



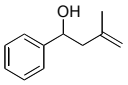

**$^1$H NMR (400 MHz, $CDCl_3$)**



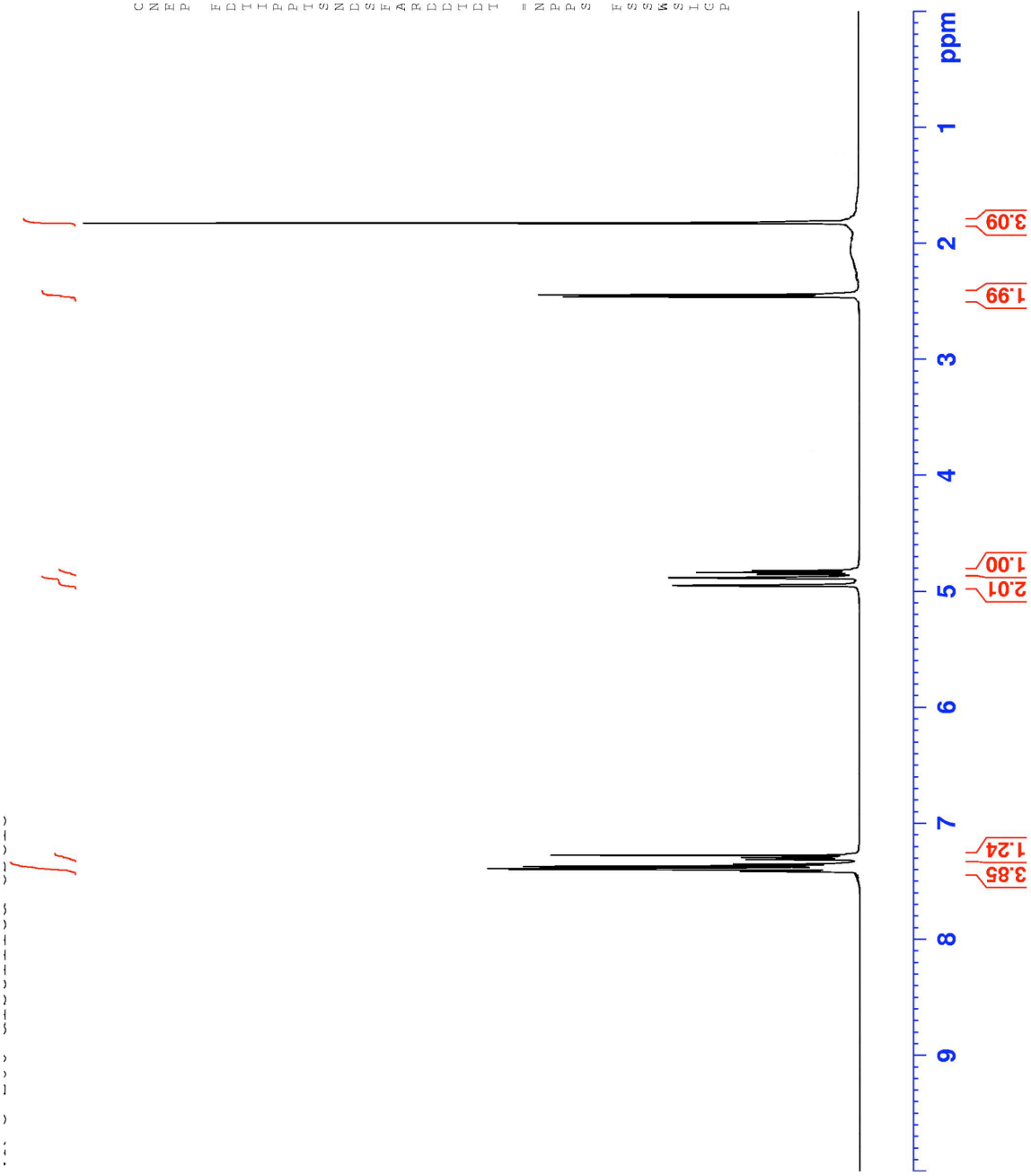
**$^{13}C$ NMR (125 MHz, $CDCl_3$)**



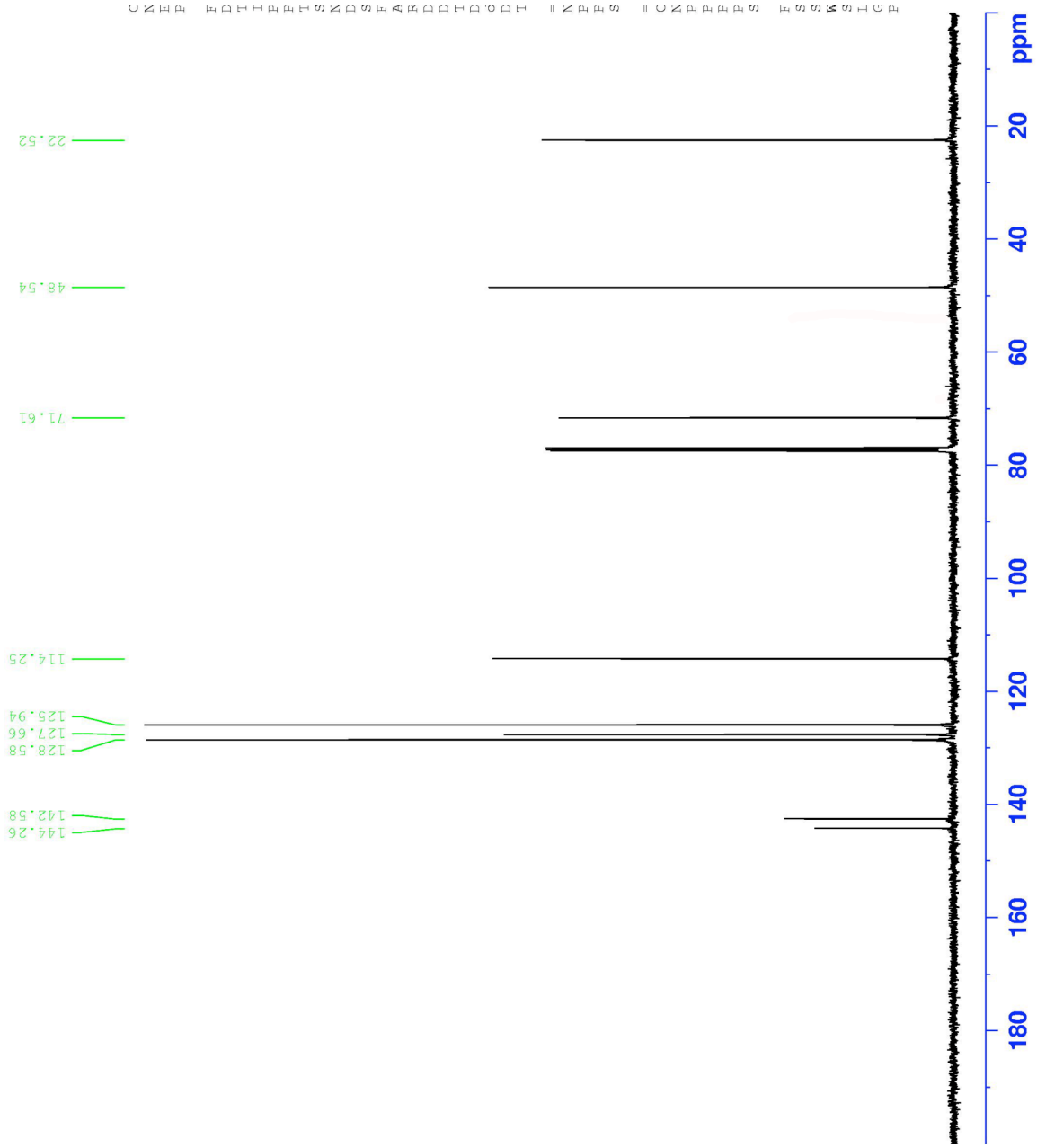
**1-phenyl-3-methyl-3-buten-1-ol (Table 2, entry 2)**



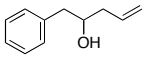

**$^1$H NMR (400 MHz, $CDCl_3$)**



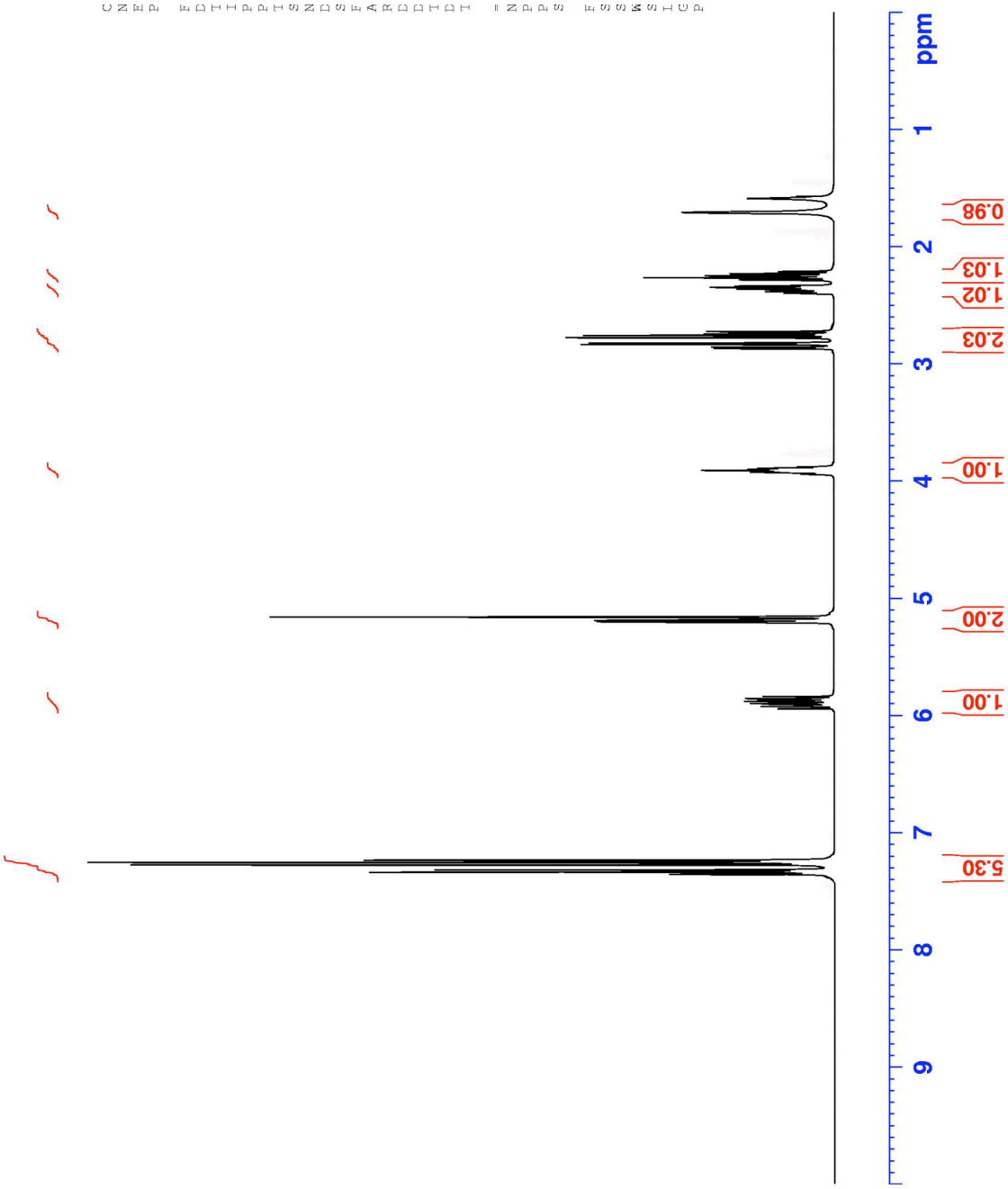
**$^{13}C$ NMR (125 MHz, $CDCl_3$)**



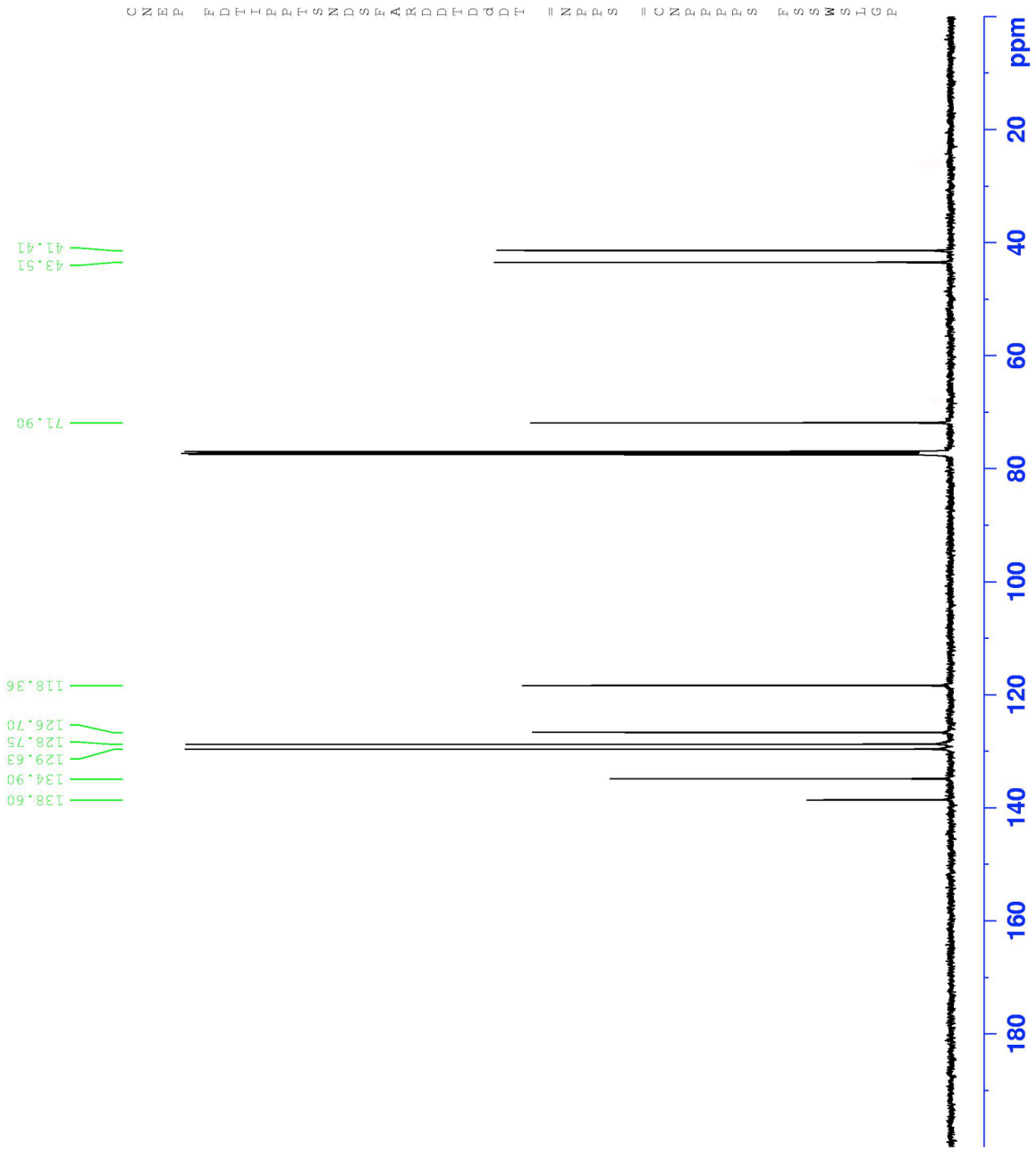
**1-phenyl-4-penten-2-ol (Table 2, entry 3)**



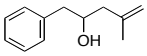

**$^1$H NMR (400 MHz, $CDCl_3$)**



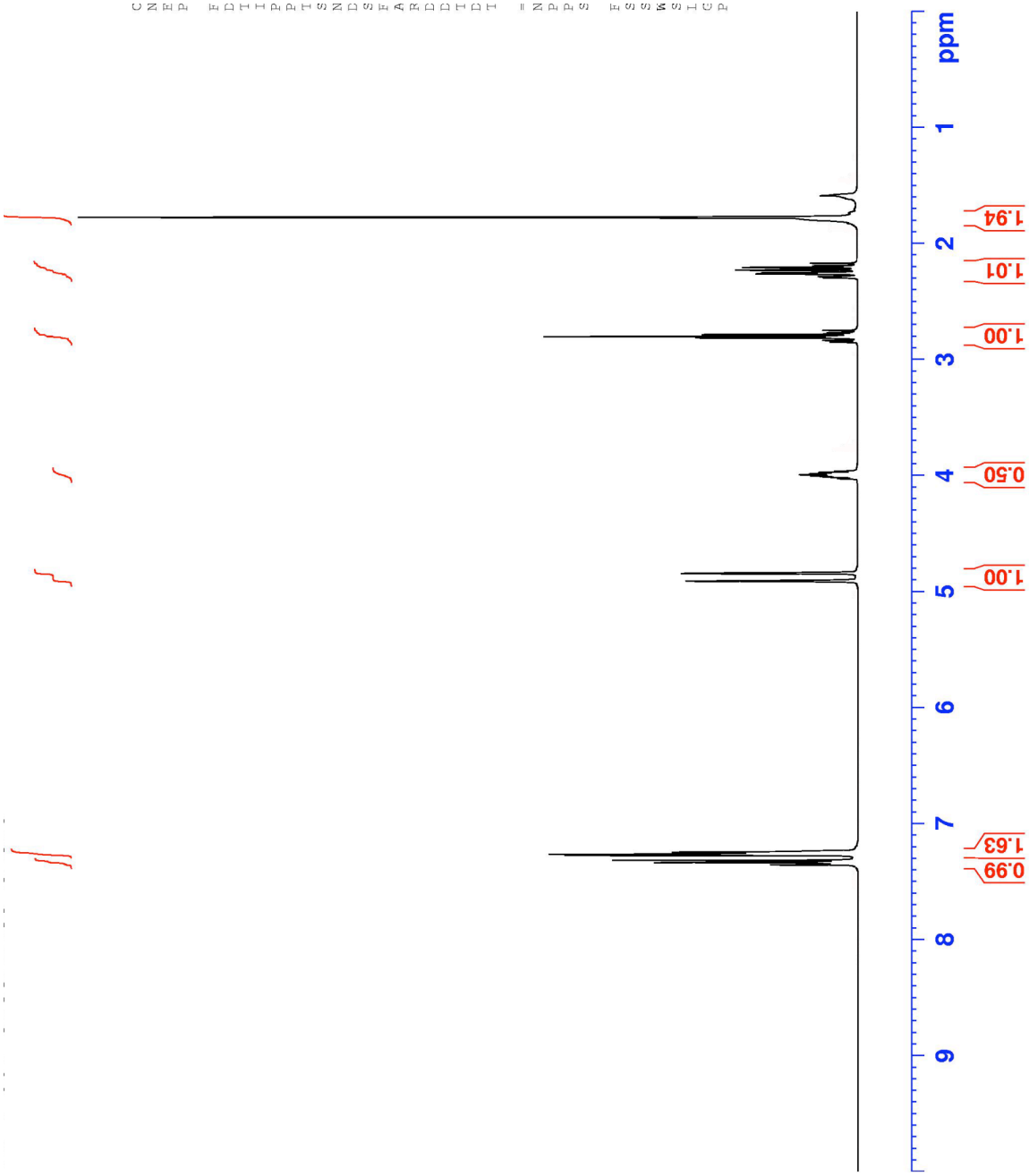
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



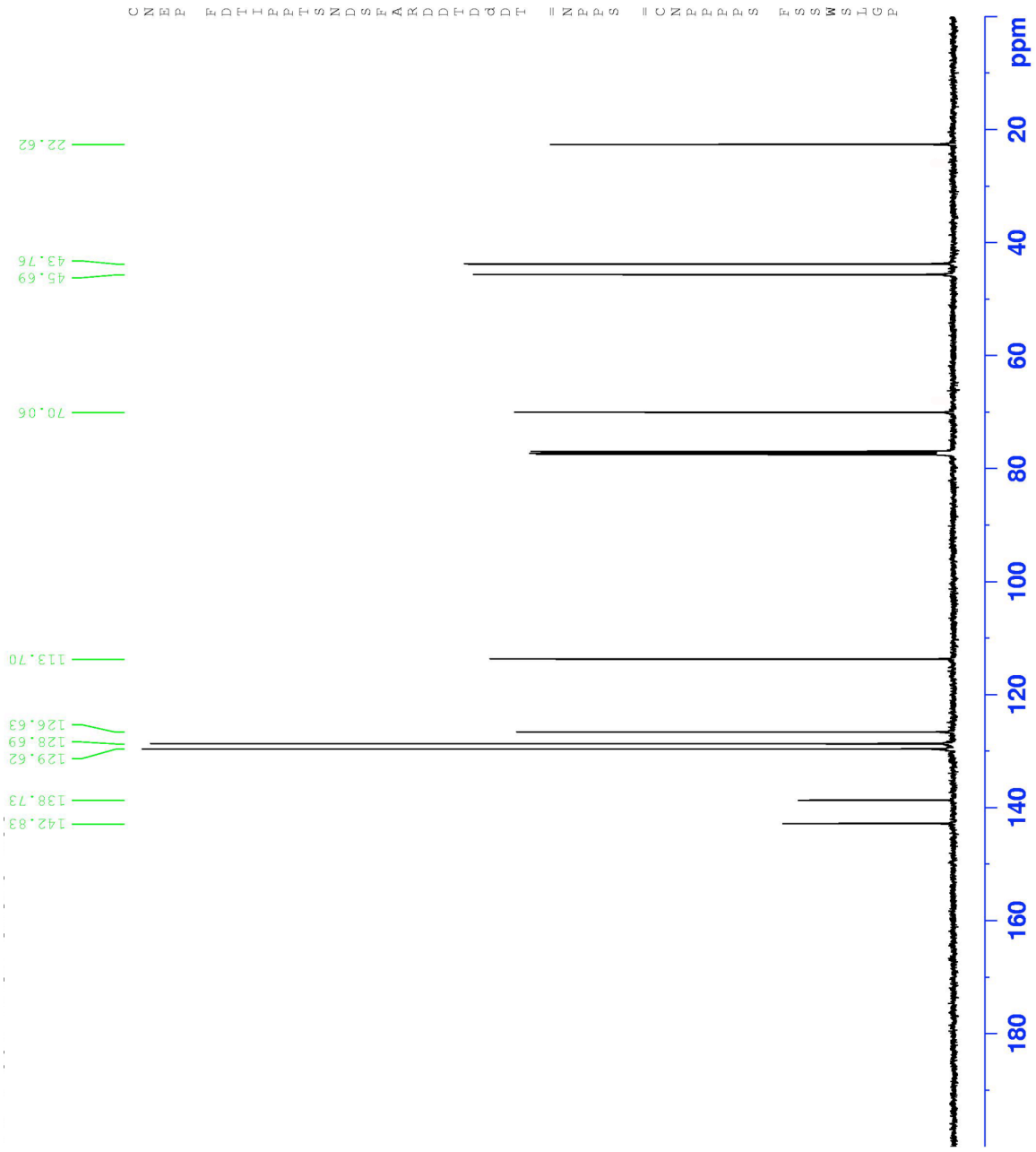
**4-methyl-1-phenyl-4-penten-2-ol (Table 2, entry 4)**



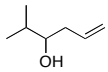

**$^1$H NMR (400 MHz, $CDCl_3$)**



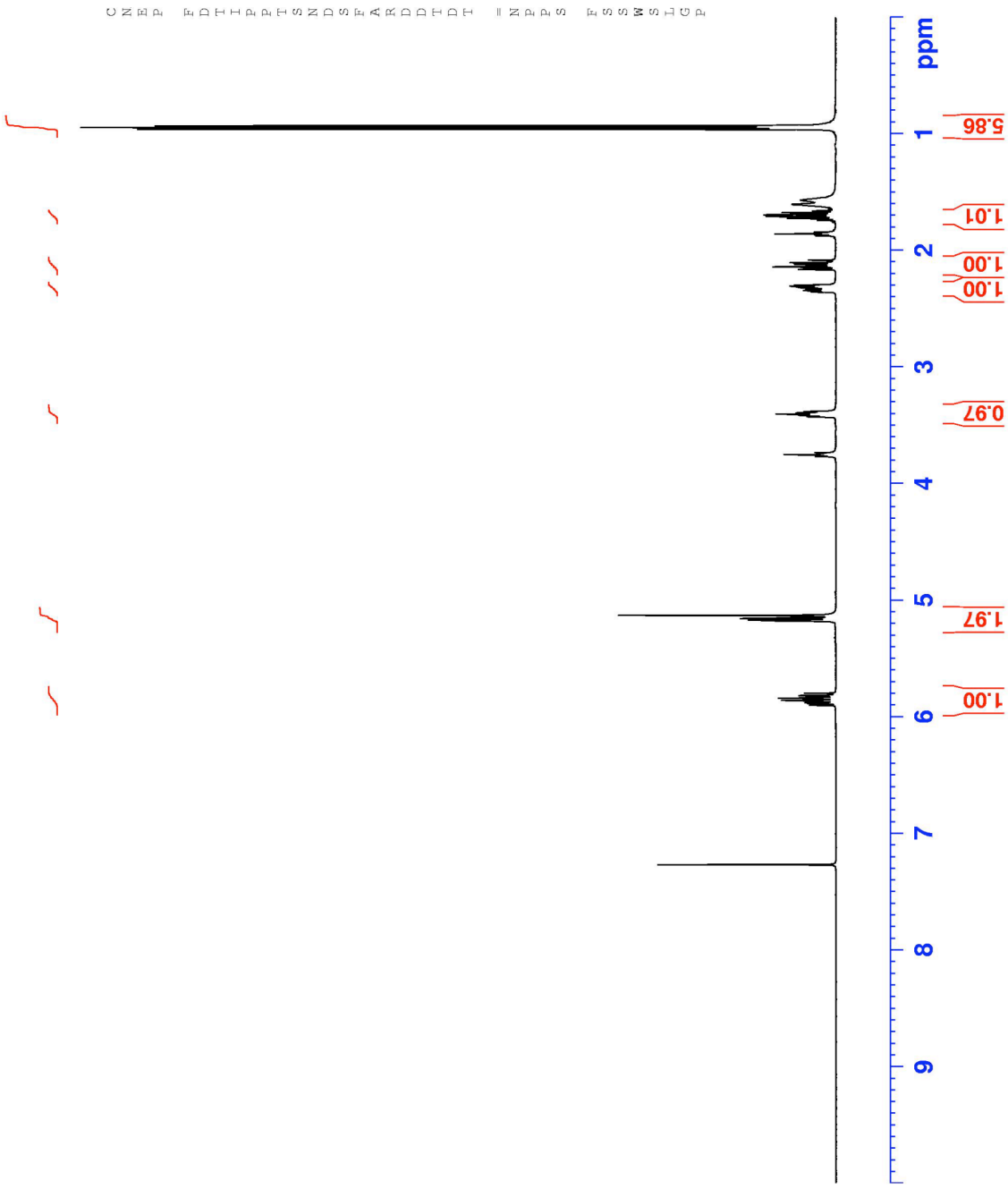
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



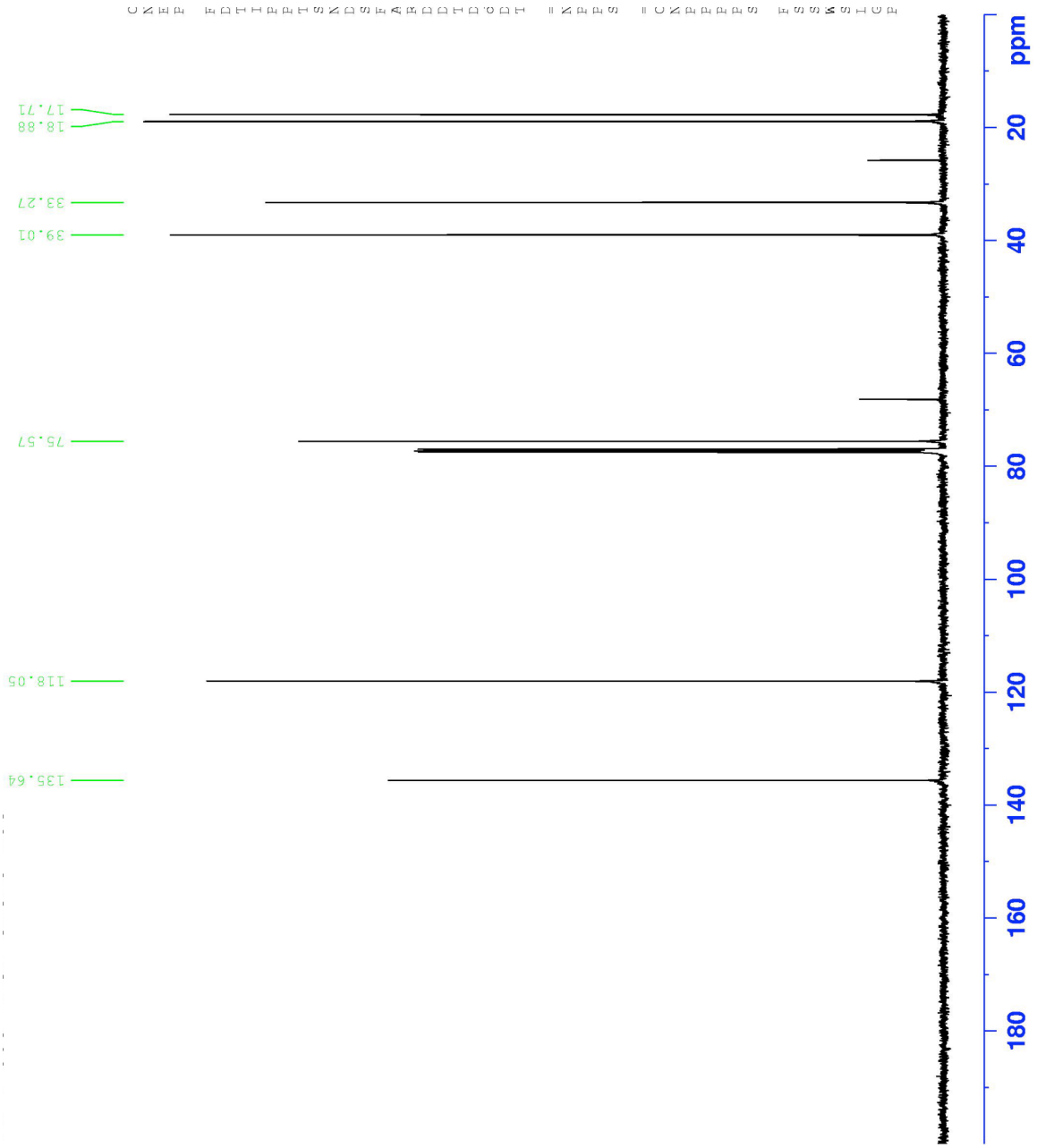
**2-methyl-5-hexen-3-ol (Table 2, entry 5)**



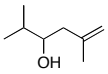

**$^1$H NMR (400 MHz, $CDCl_3$)**



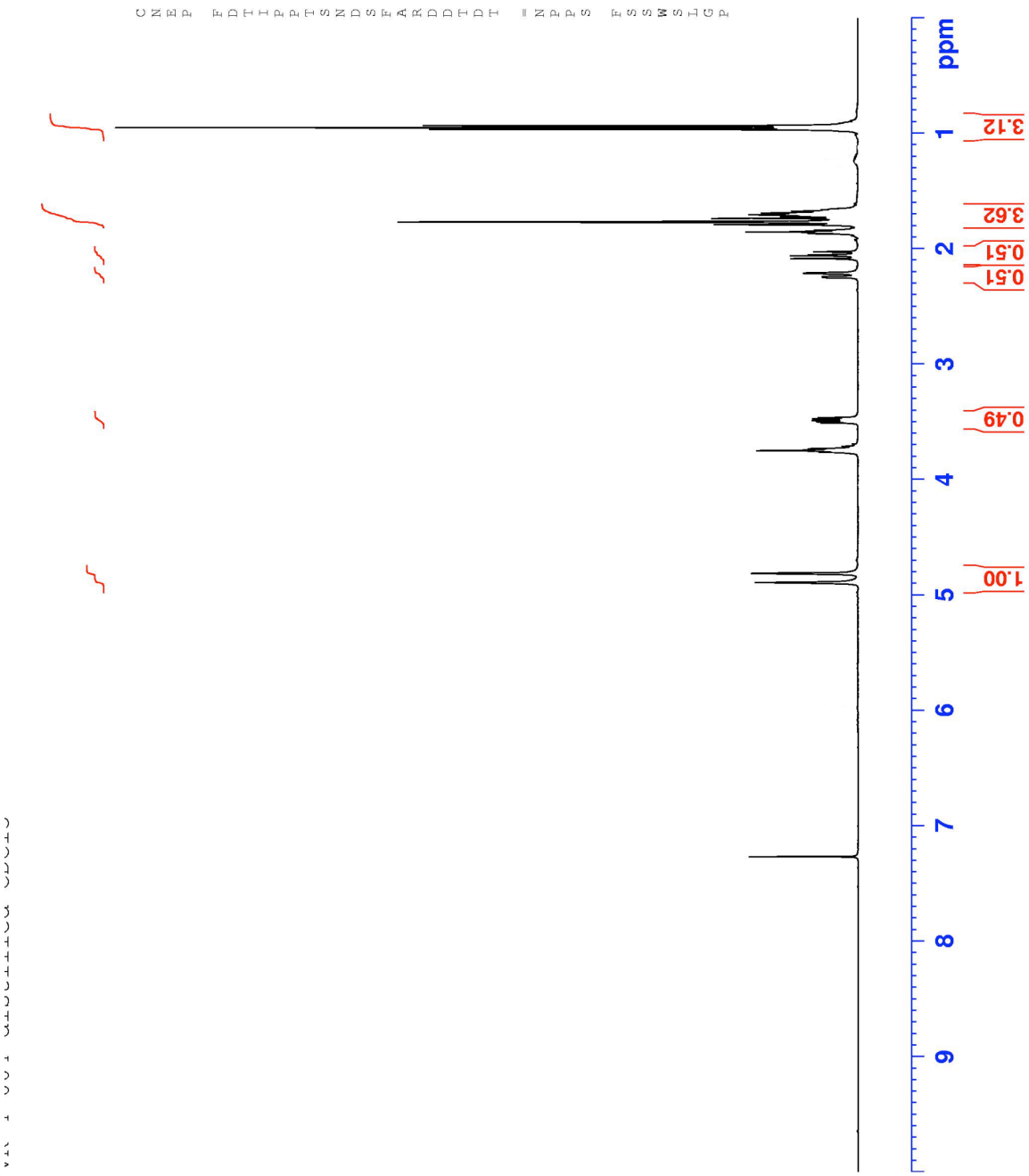
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



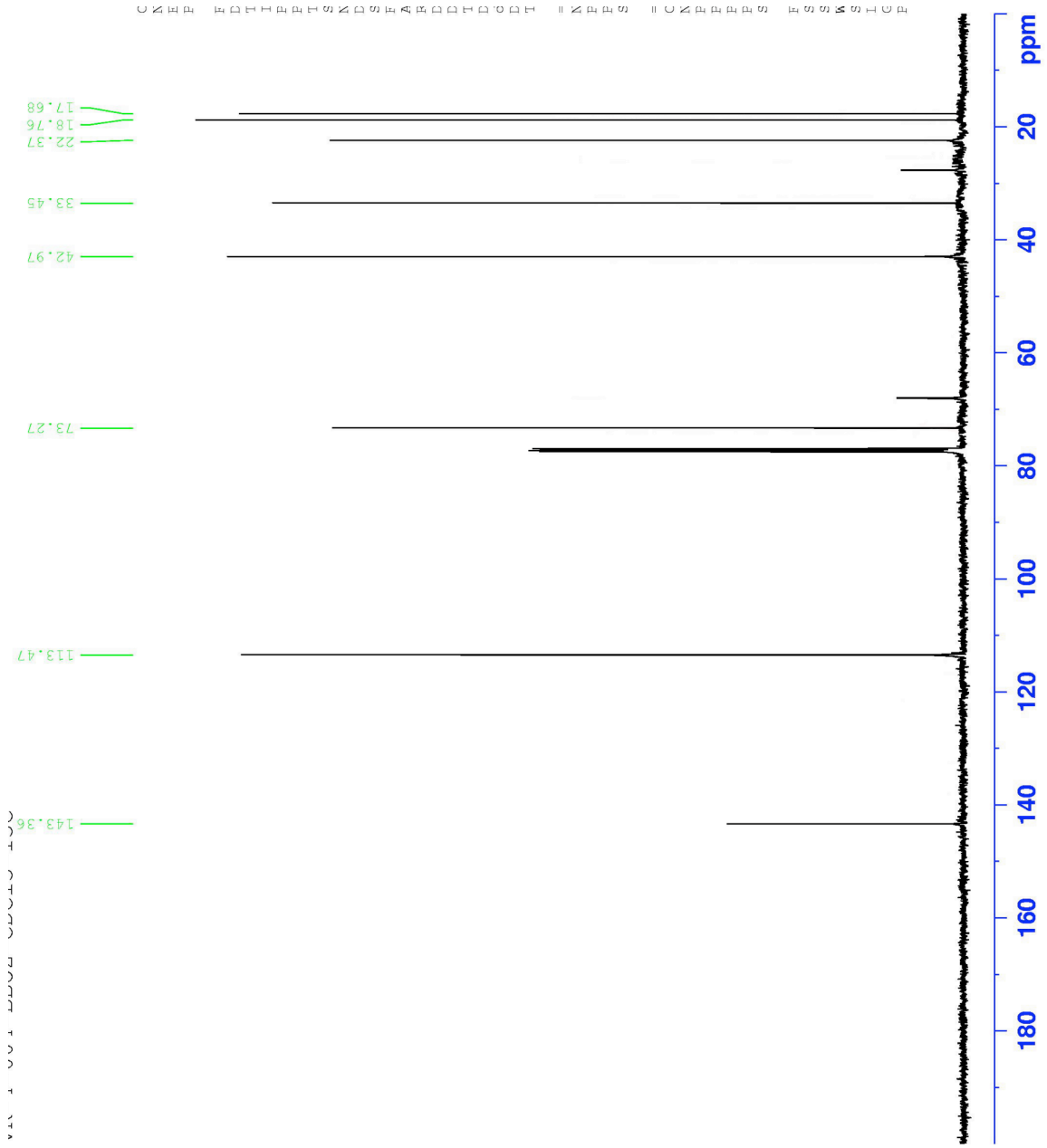
**2,5-dimethyl-5-hexen-3-ol (Table 2, entry 6)**



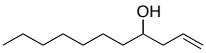

**$^1$H NMR (400 MHz, $CDCl_3$)**



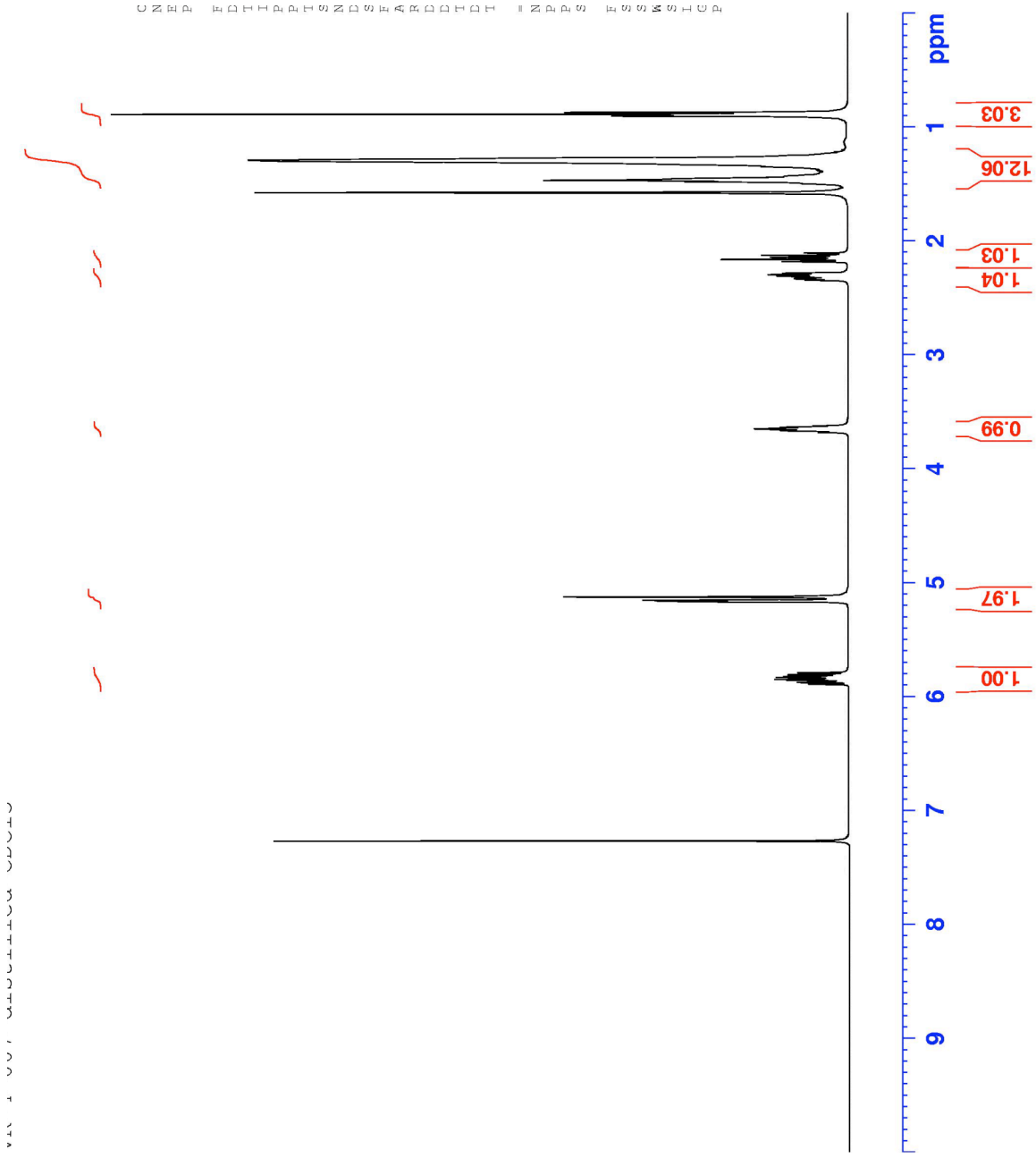
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



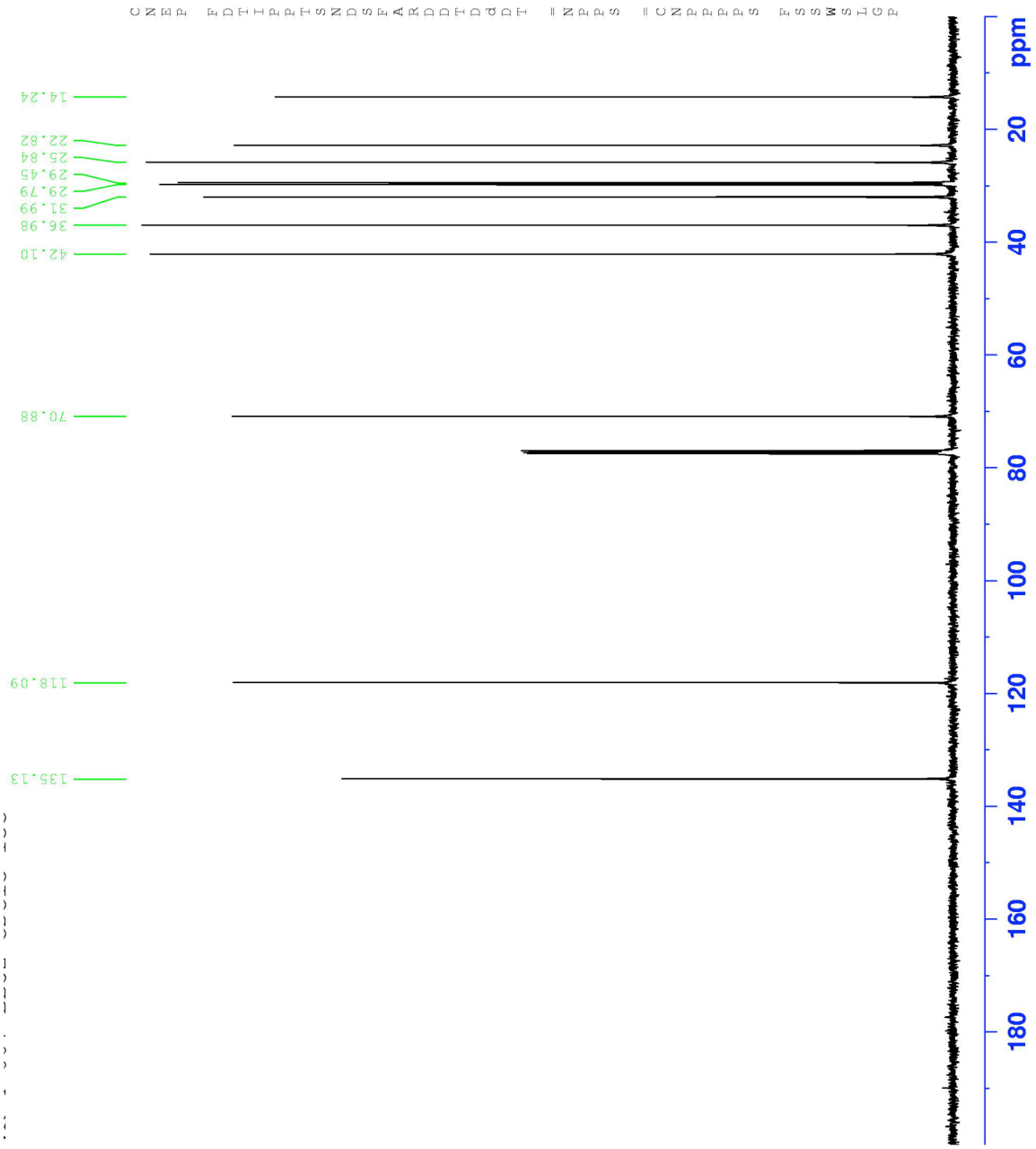
**1-undecen-4-ol (Table 2, entry 7)**



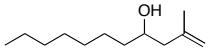

**$^1$H NMR (400 MHz, $CDCl_3$)**



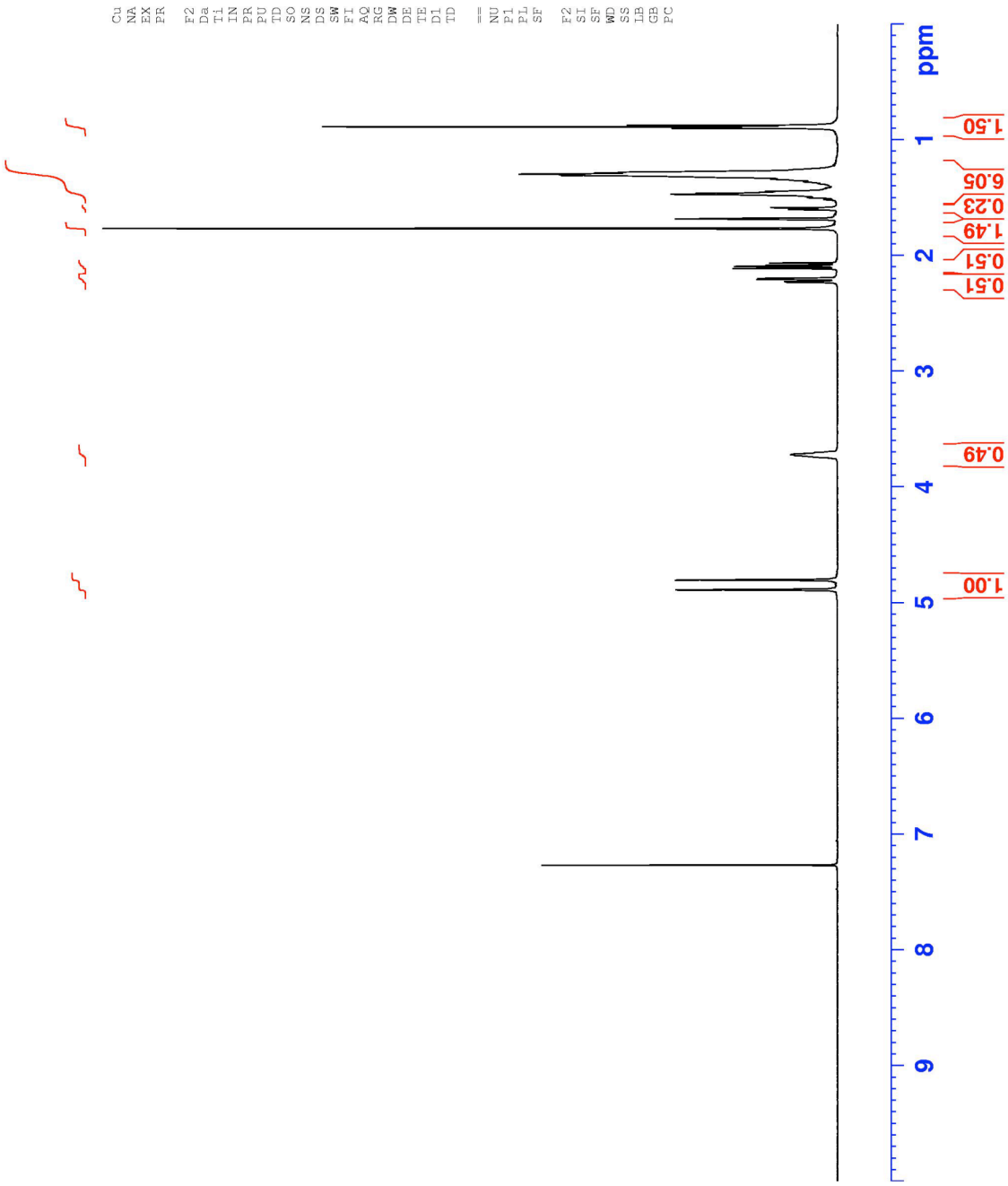
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



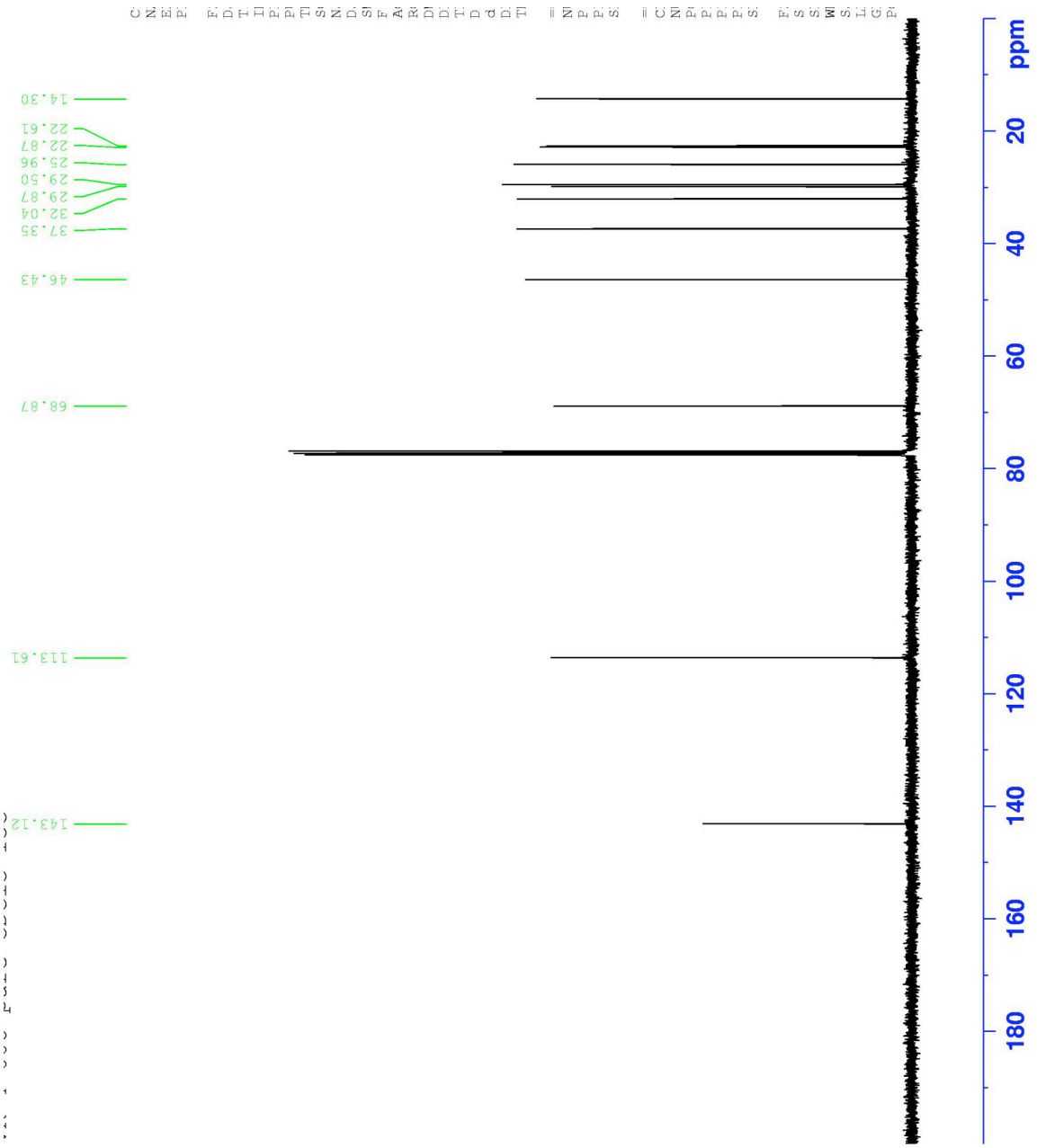
**2-methyl-1-undecen-4-ol (Table 2, entry 8)**




**$^1$H NMR (400 MHz, $CDCl_3$)**

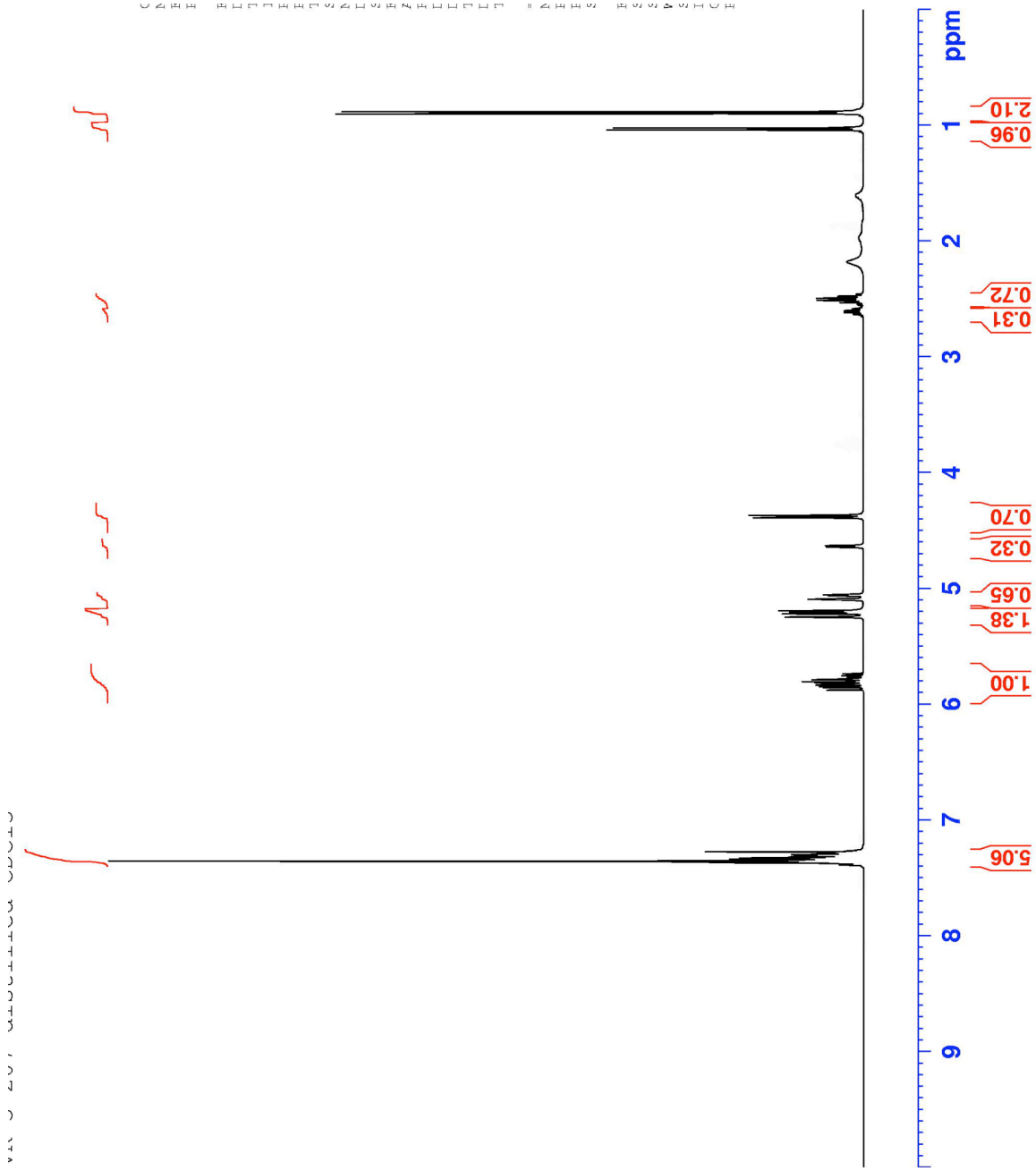


**$^{13}$C NMR (125 MHz, $CDCl_3$)**

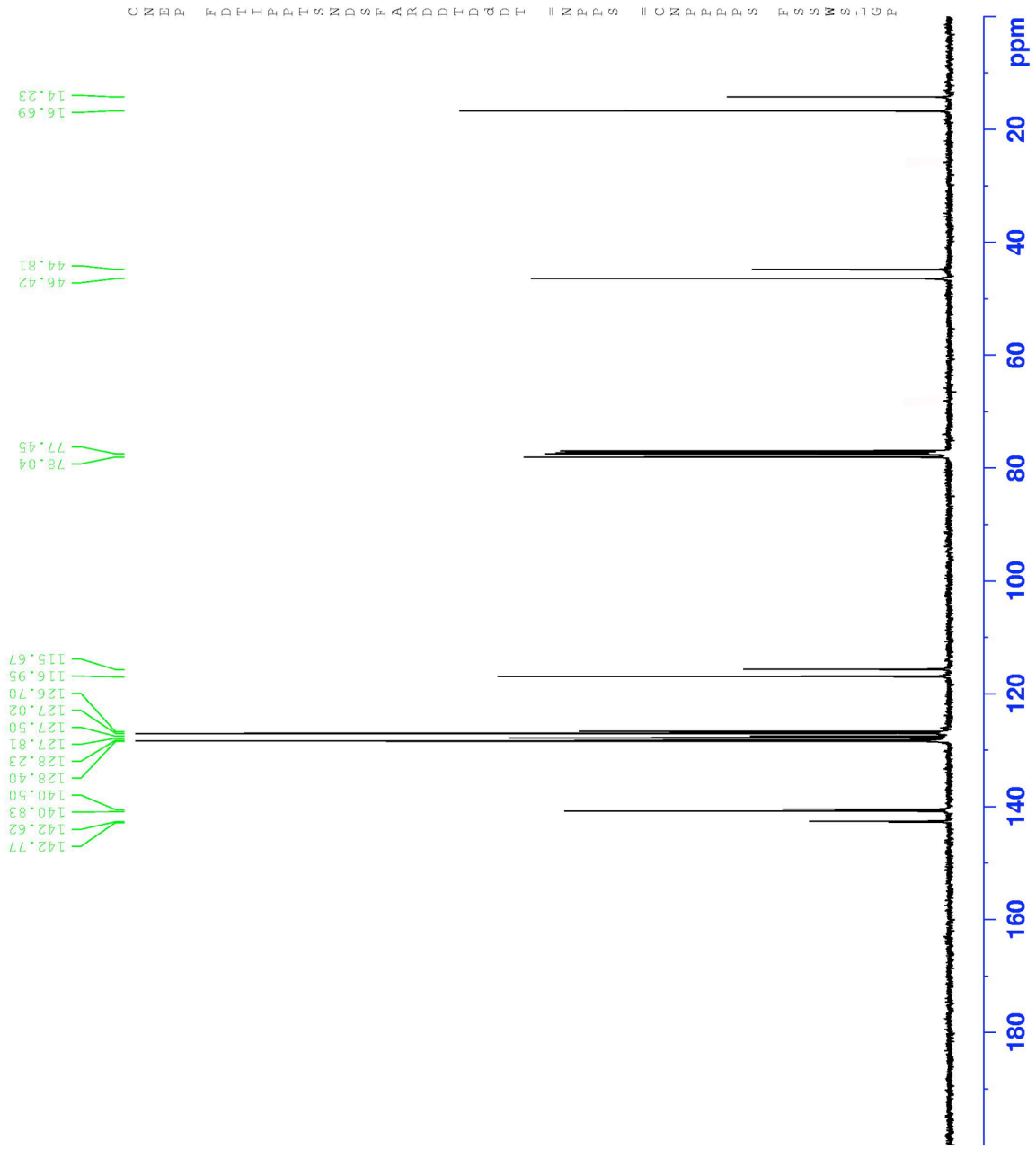


**2-methyl-1-phenyl-3-buten-1-ol (Table 3, entry 1)**


**$^1$H NMR (400 MHz, $CDCl_3$)**

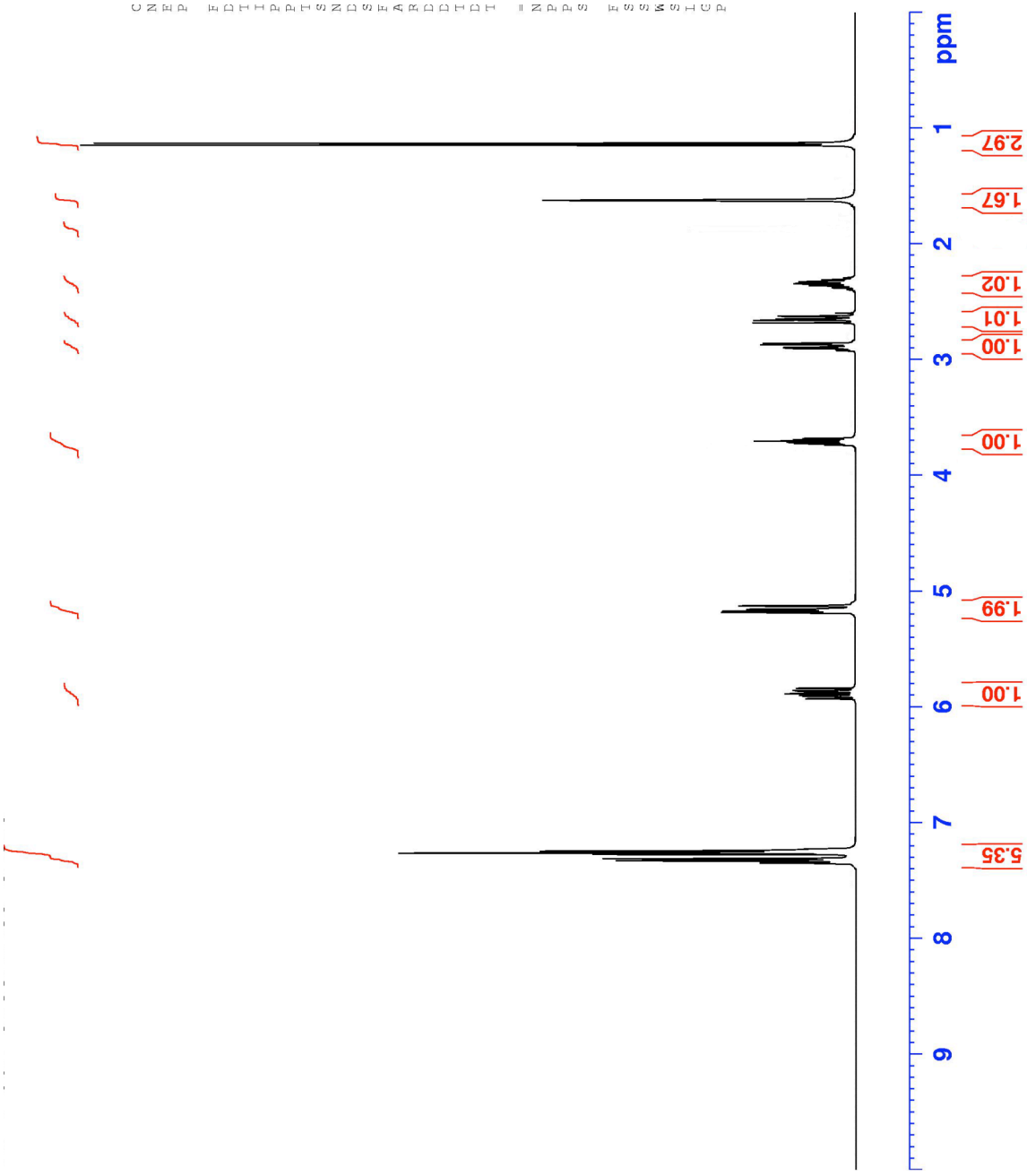


**$^{13}C$ NMR (125 MHz, $CDCl_3$)**

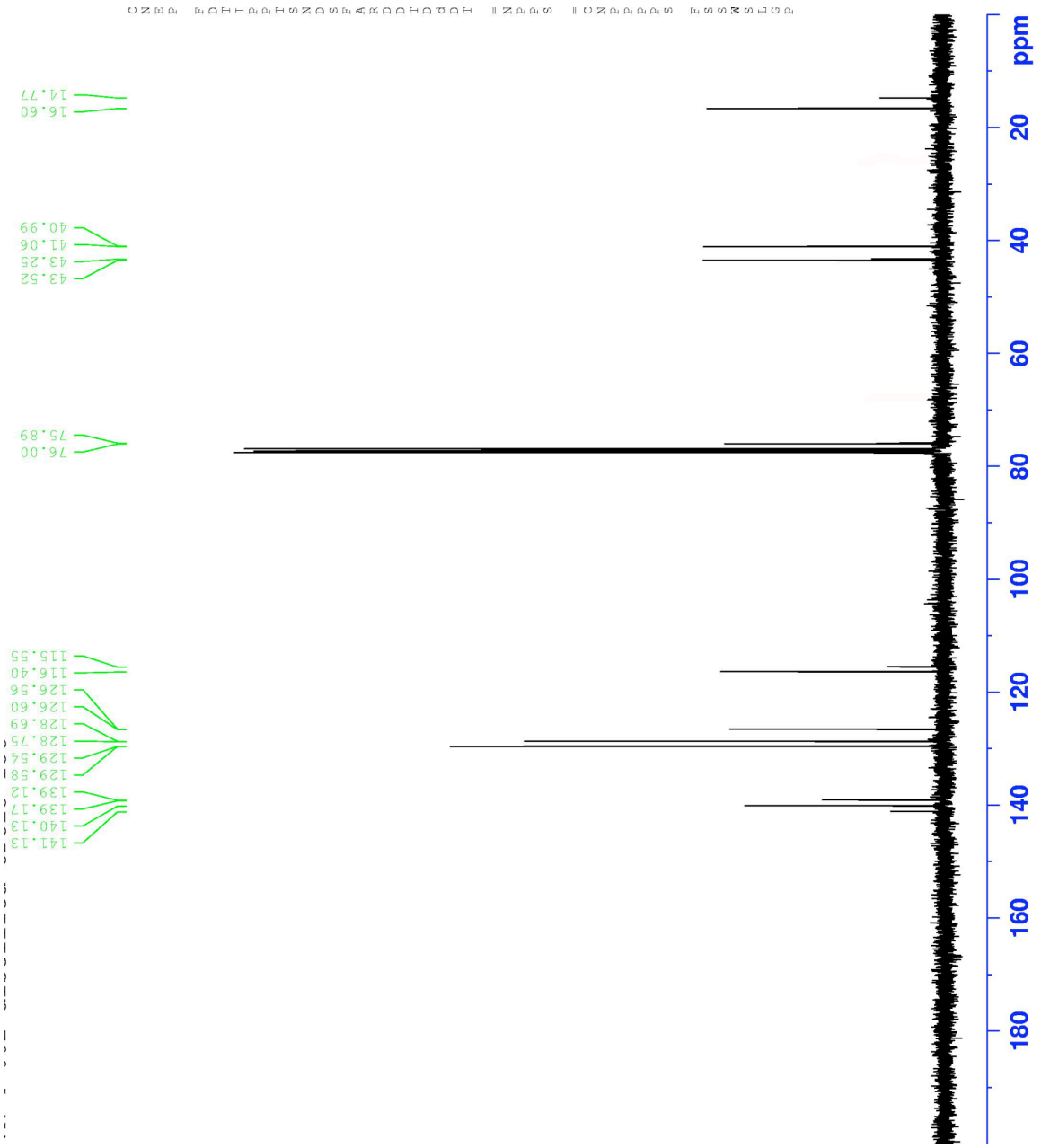


**3-methyl-1-phenyl-4-penten-2-ol (Table 3, entry 2)**


**$^1$H NMR (400 MHz, $CDCl_3$)**

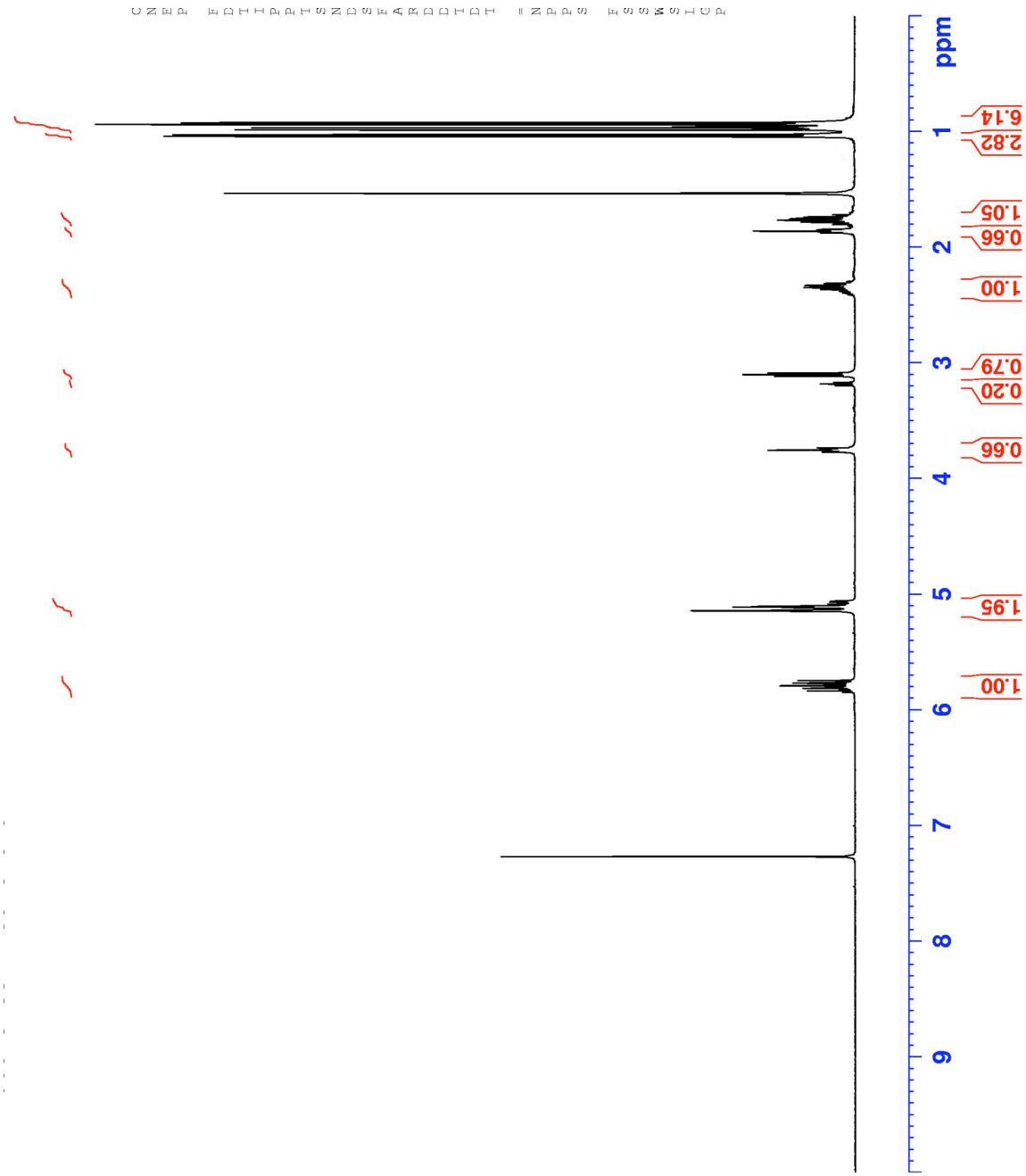


**$^{13}$C NMR (125 MHz, $CDCl_3$)**

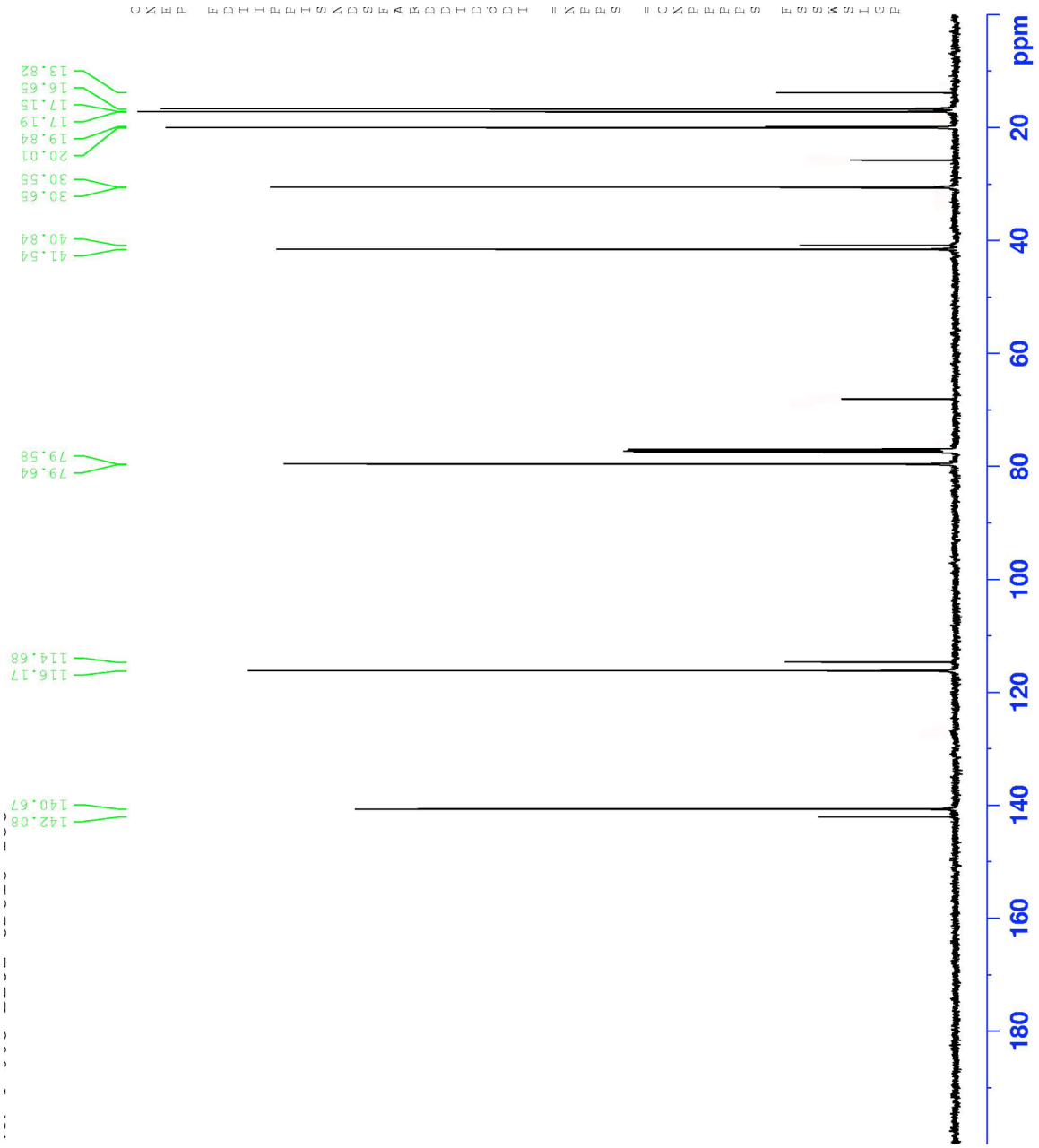


**2,4-dimethyl-5-hexen-3-ol (Table 3, entry 3)**


**$^1$H NMR (400 MHz, $CDCl_3$)**

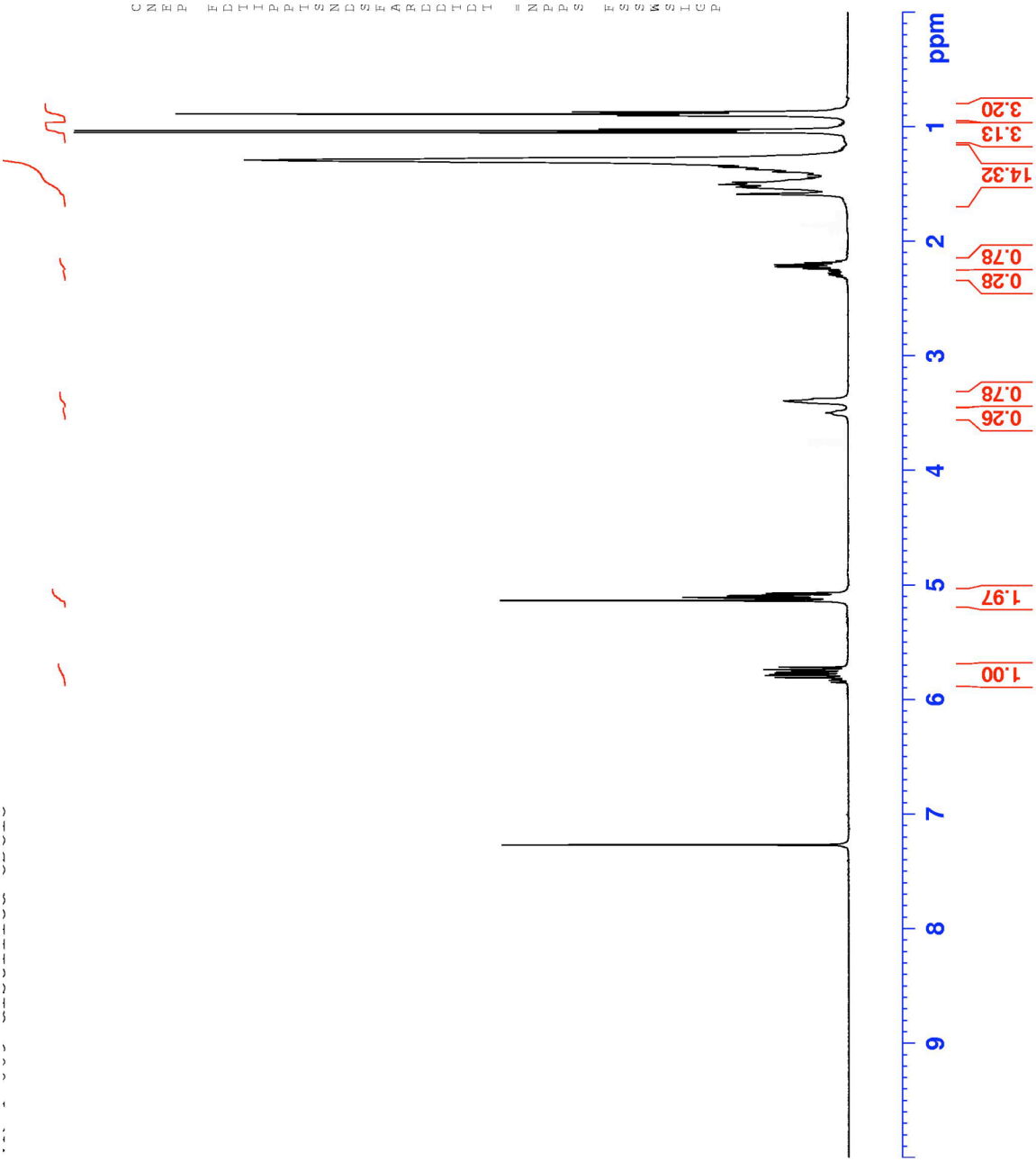


**$^{13}$C NMR (125 MHz, $CDCl_3$)**

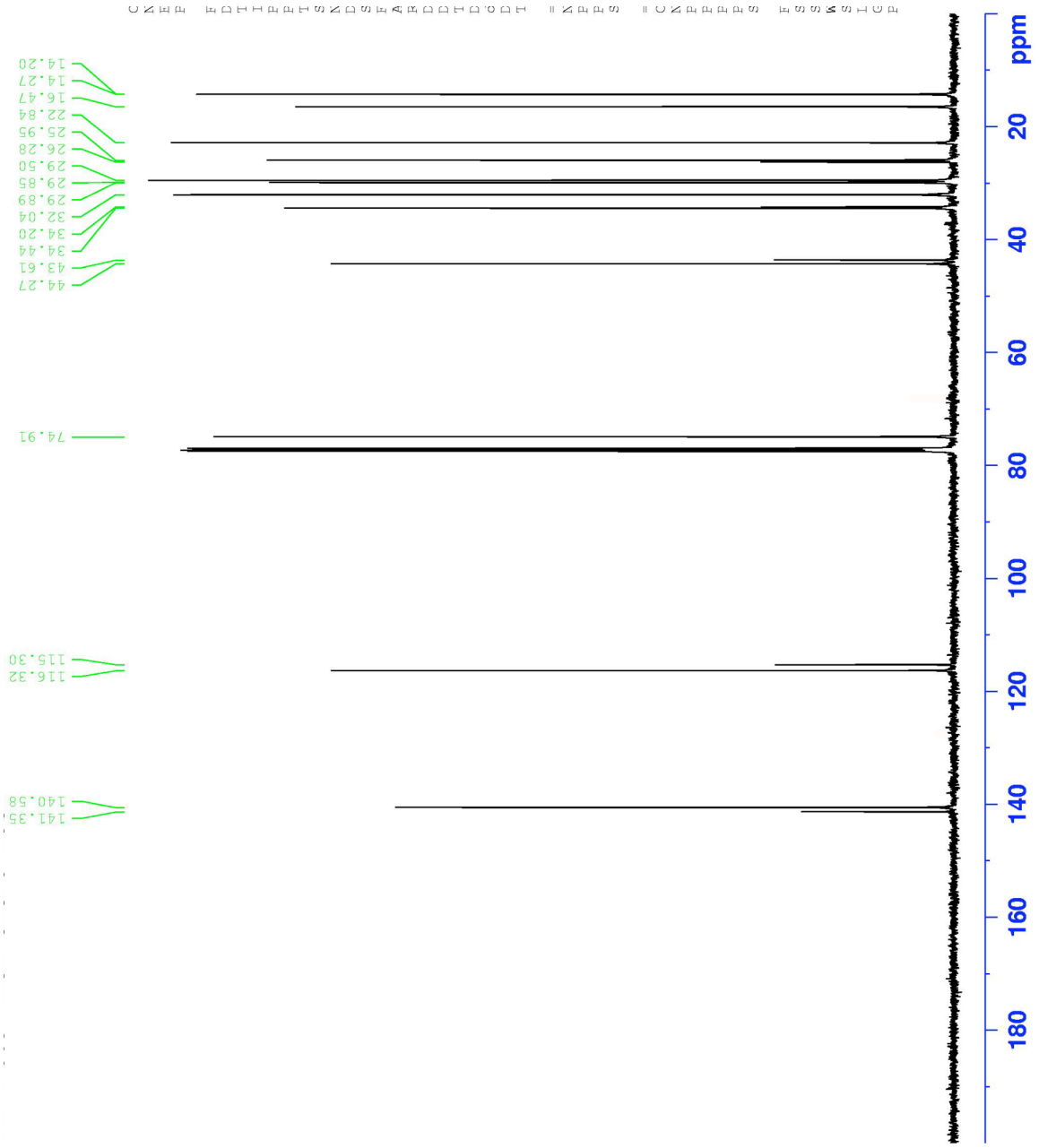


**3-methyl-1-undecen-4-ol (Table 3, entry 4)**

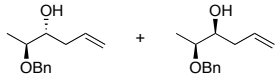

**$^1$H NMR (400 MHz, $CDCl_3$)**



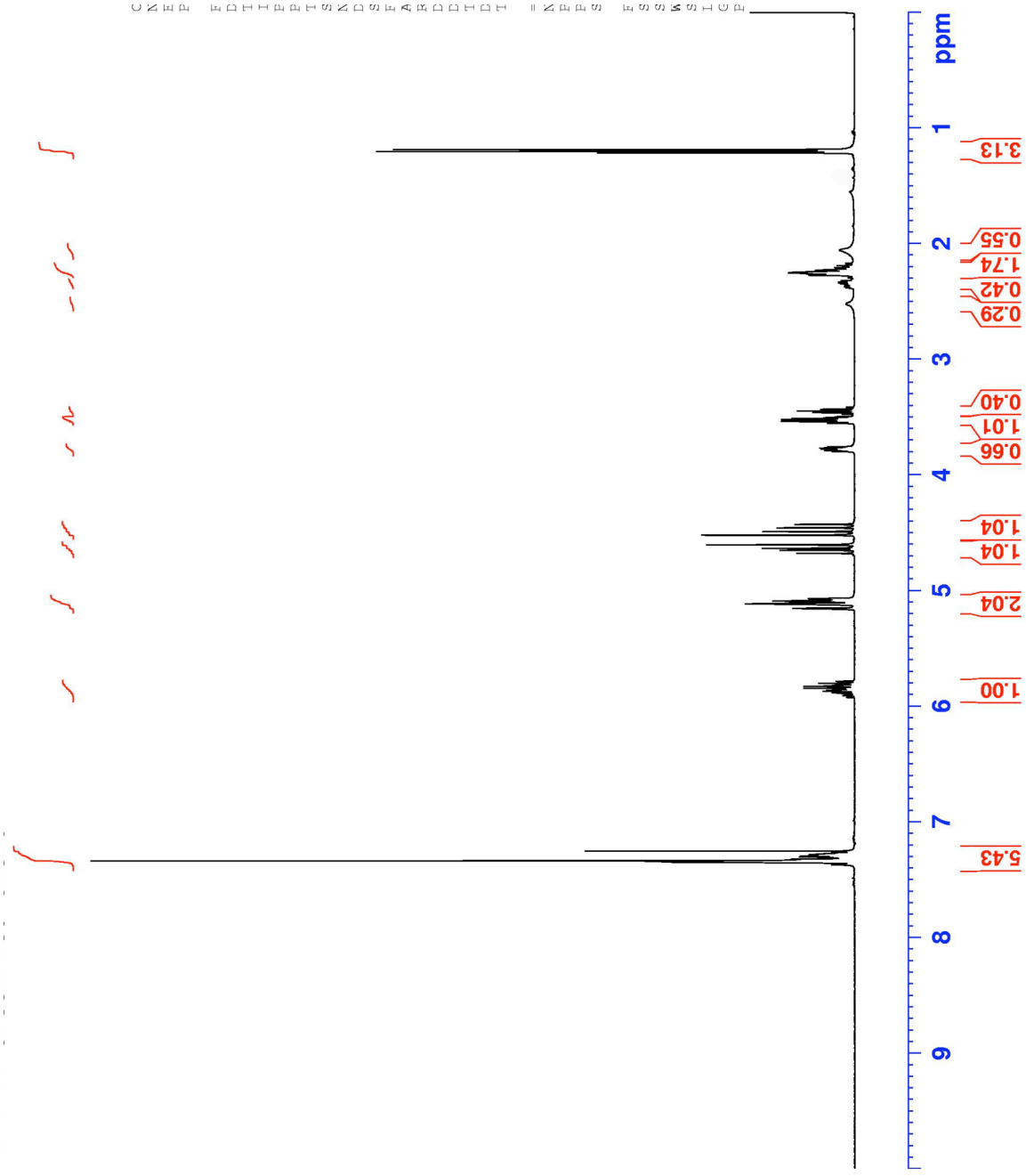
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



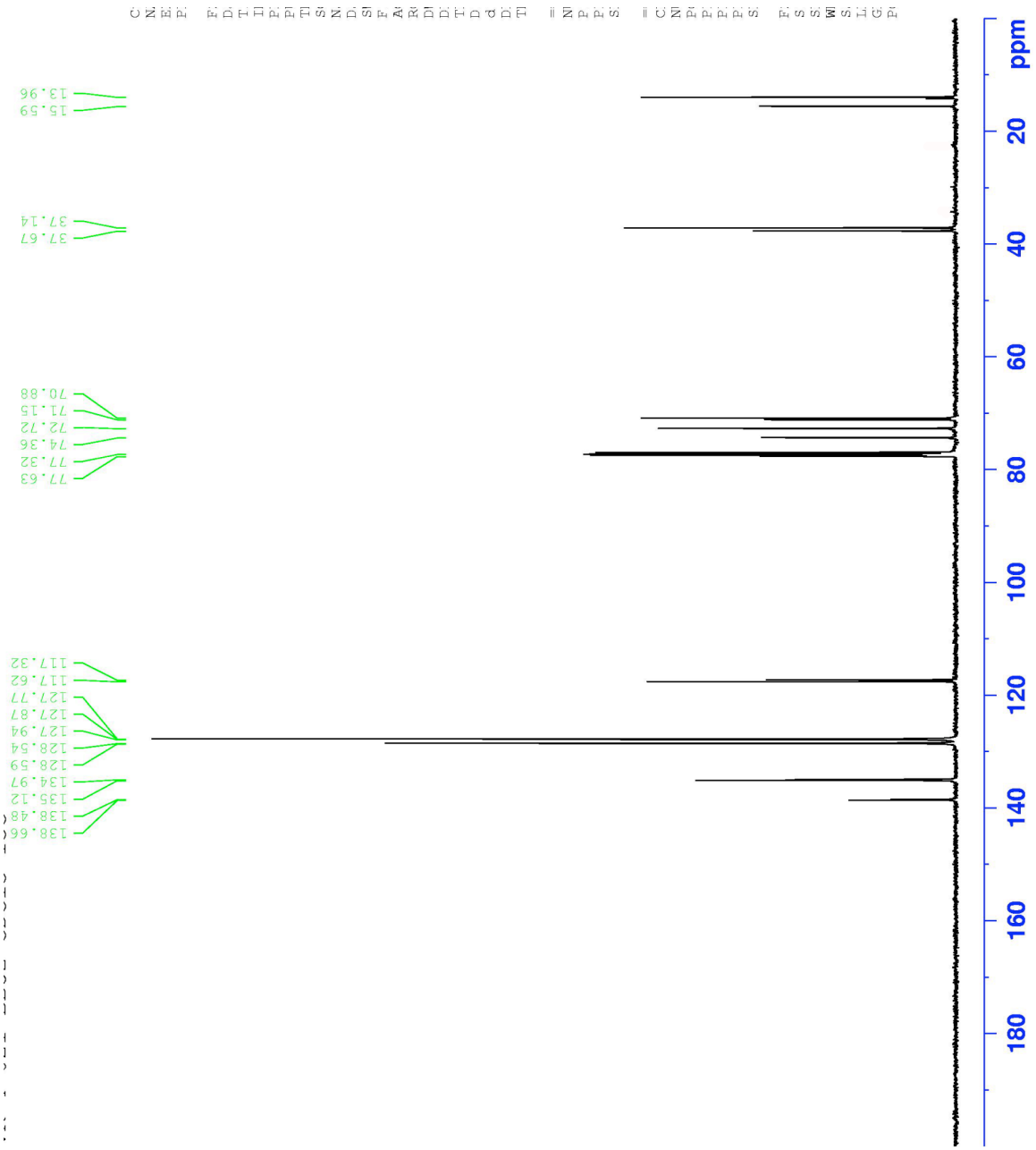
**(S,S)-2-(benzyloxy)hex-5-en-3-ol and (S,R)-2-(benzyloxy)hex-5-en-3-ol**



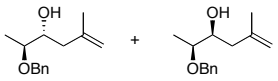

**$^{1}$H NMR (400 MHz, $CDCl_3$)**



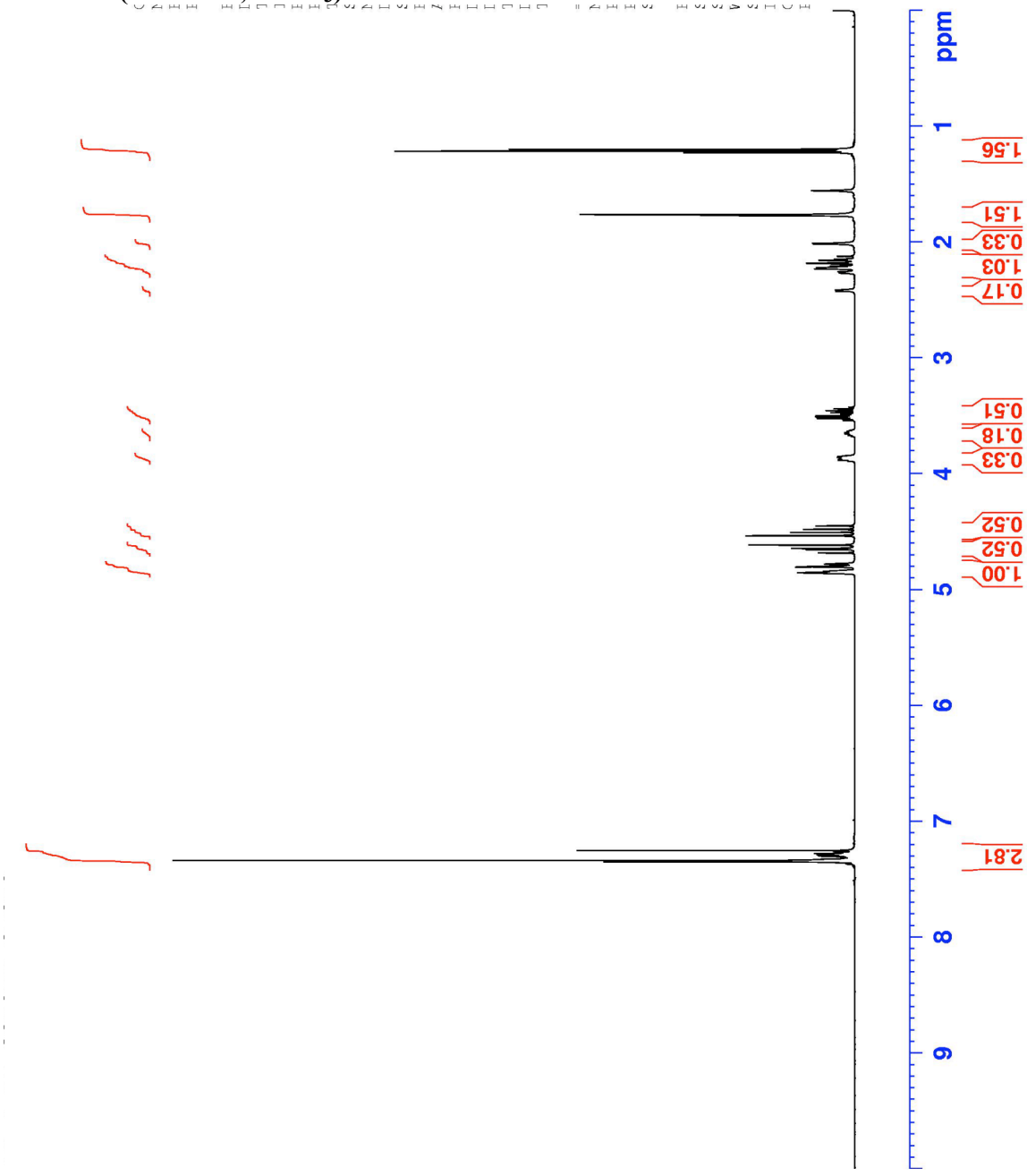
**$^{13}C$ NMR (125 MHz, $CDCl_3$)**



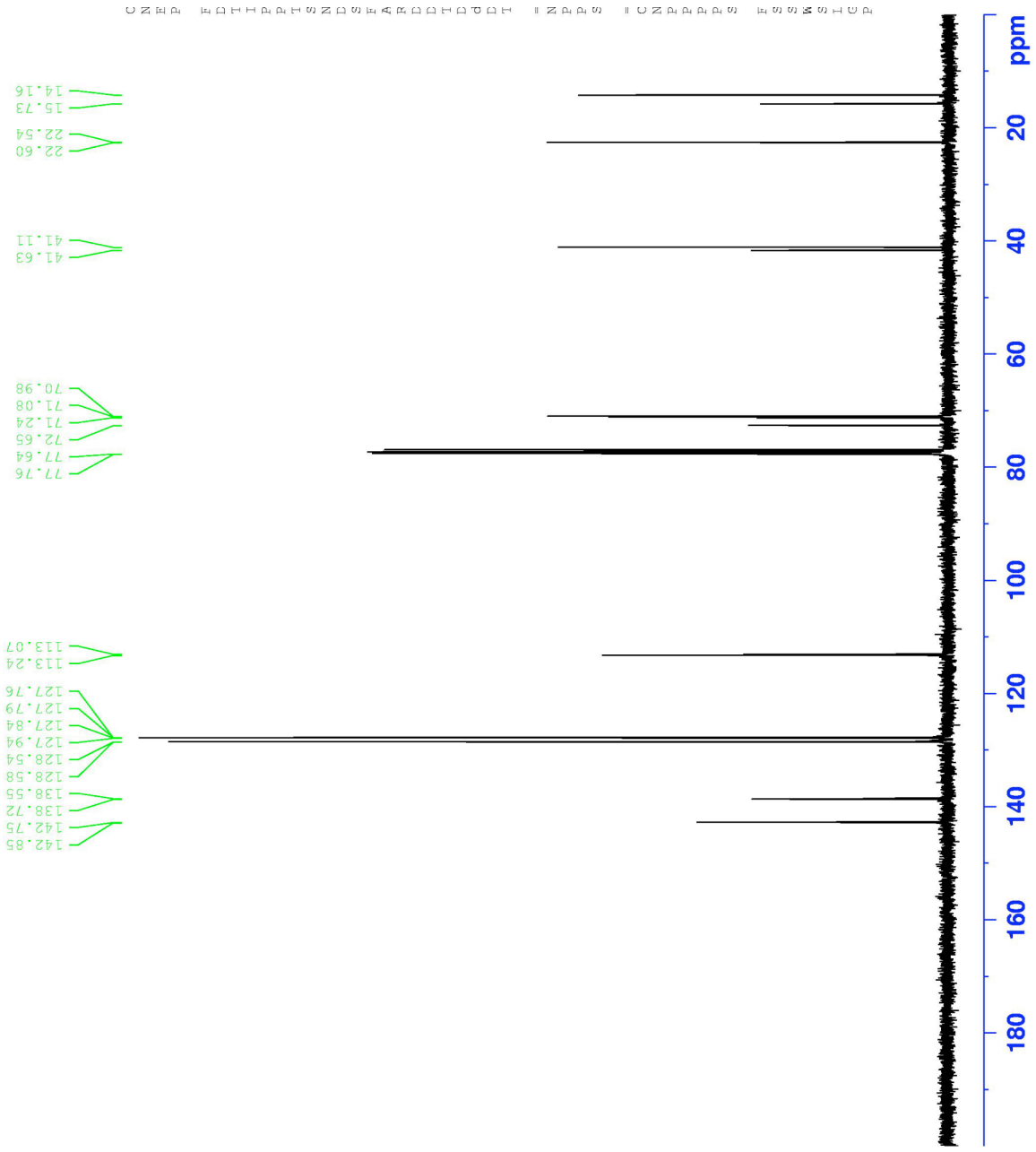
**(S,S)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol and (S,R)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol**



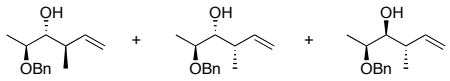

**$^1$H NMR (400 MHz, $CDCl_3$)**



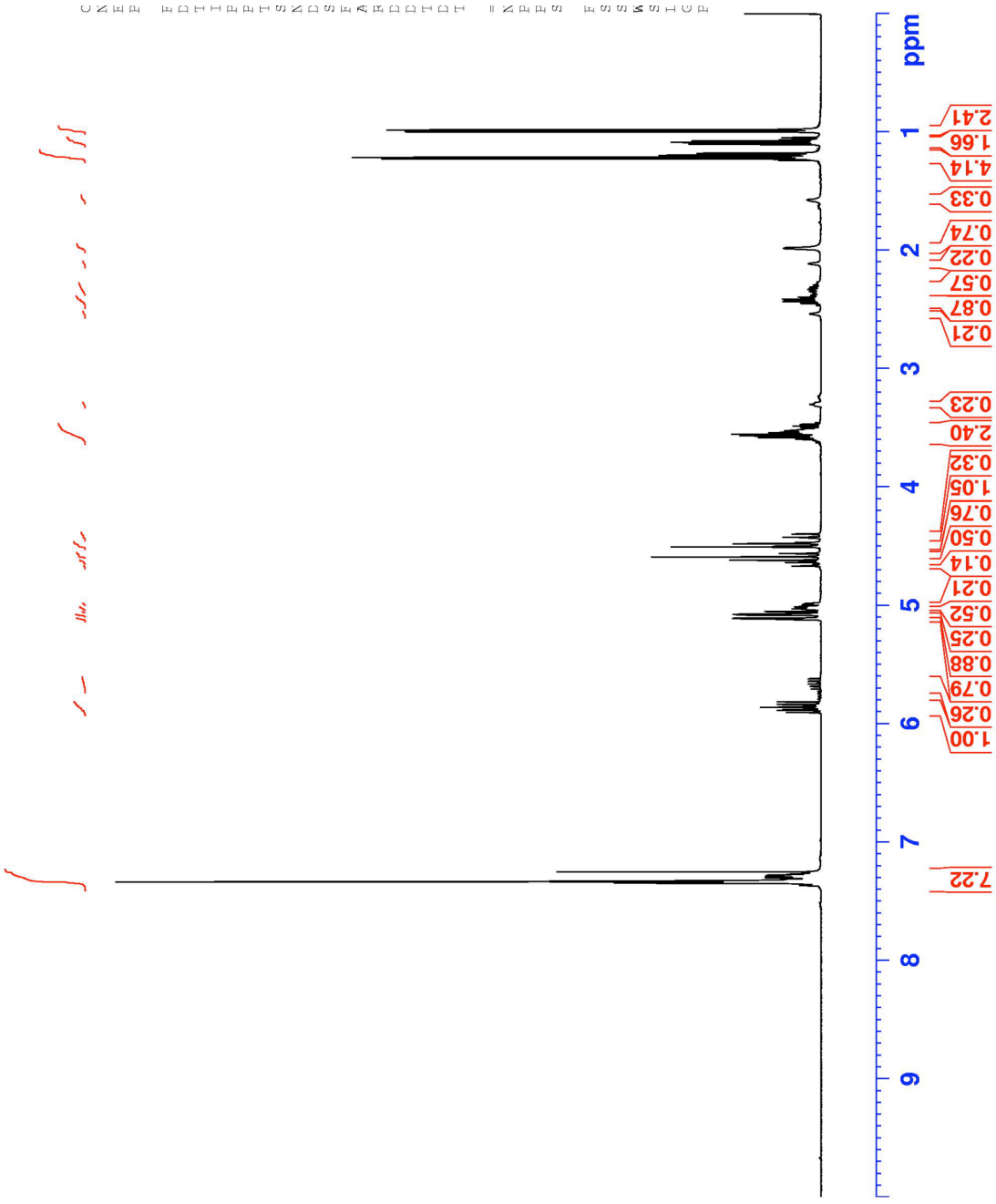
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



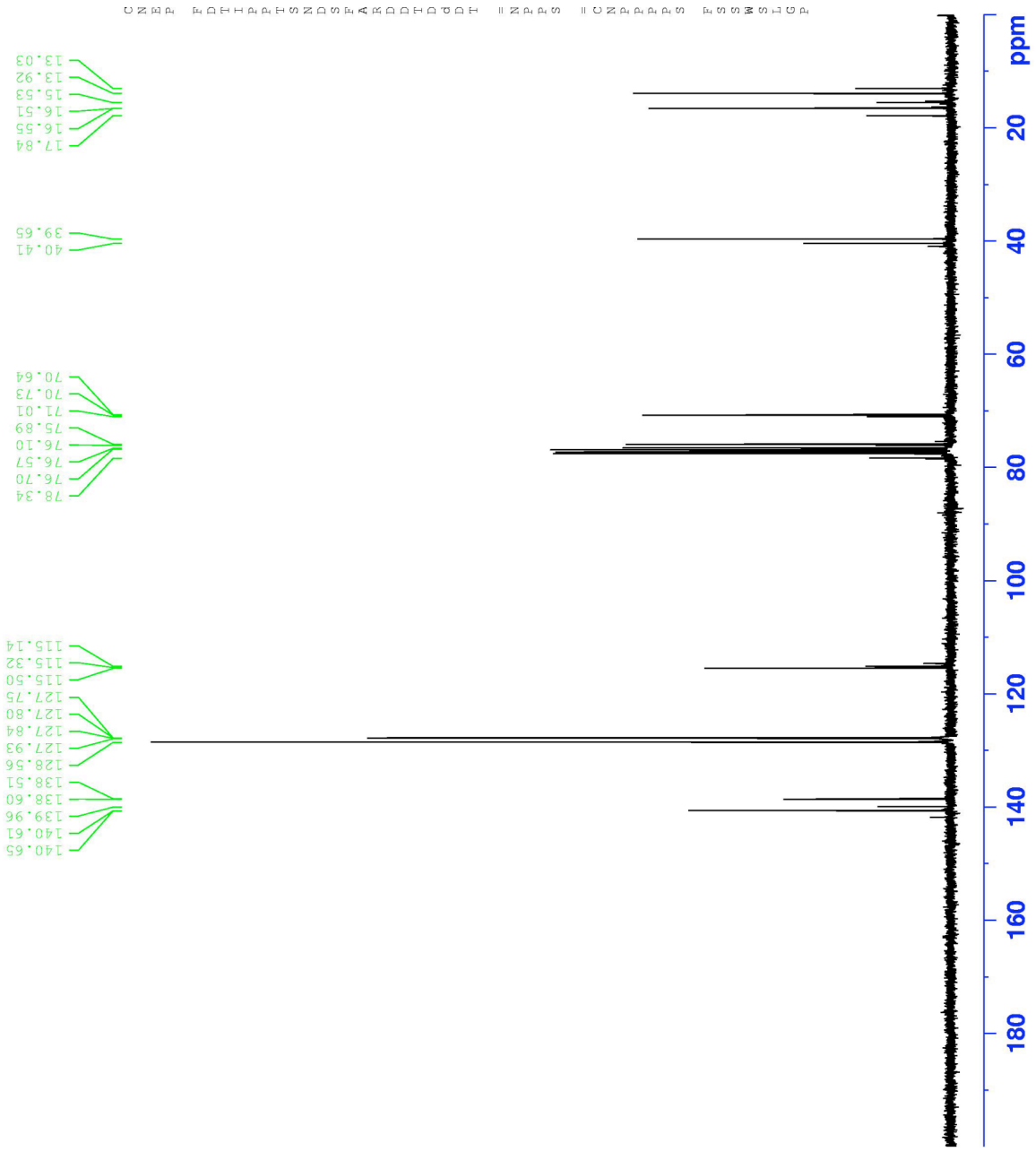
**(2S,3R,4R)-2-(benzyloxy)-4-methyl-5-hexen-3-ol, (2S,3R,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol and (2S,3S,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol.**




**$^1$H NMR (400 MHz, $CDCl_3$)**

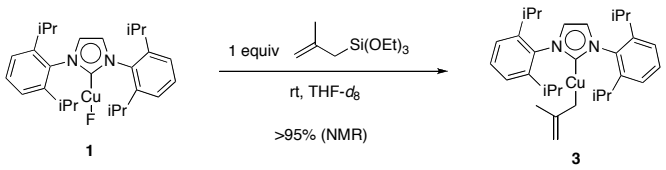


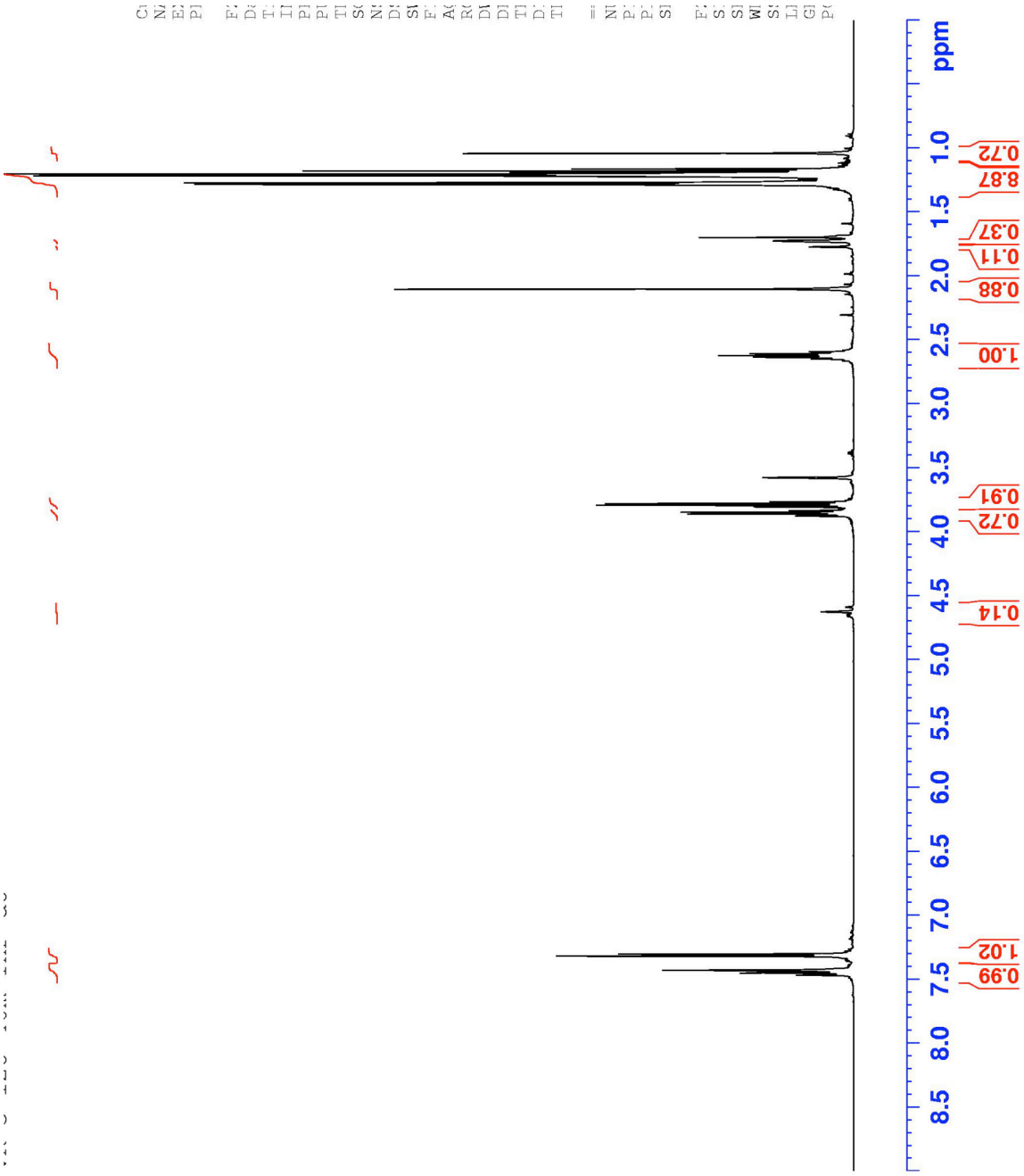
**$^{13}$C NMR (125 MHz, $CDCl_3$)**



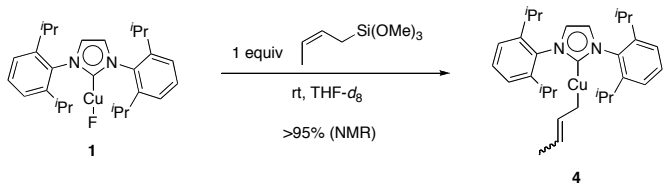
**Scheme 1**

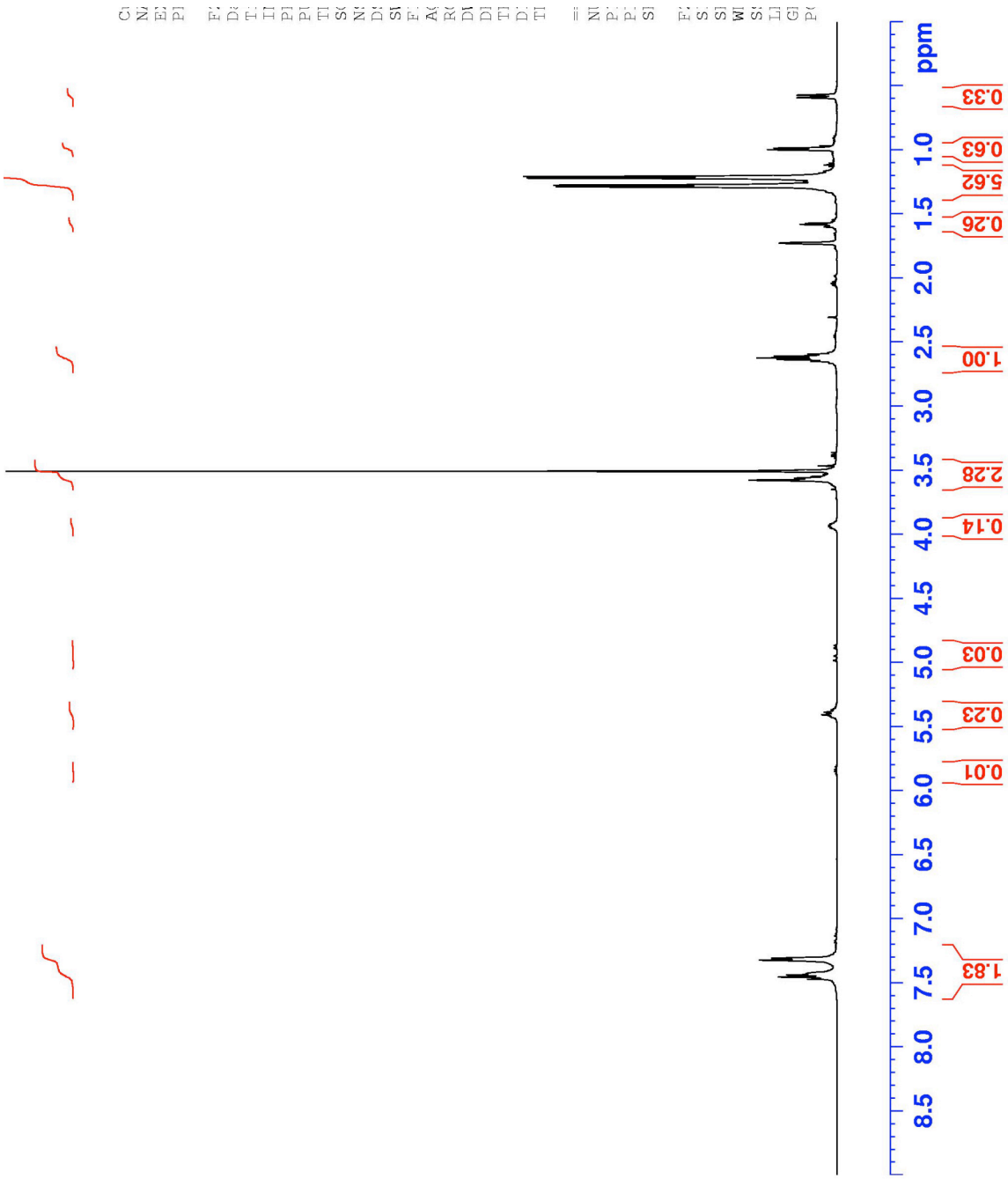
$^1$H NMR (400 MHz, THF-$d_8$) of **3** generated *in situ* from 2-methallyltriethoxysilane and (IPr)CuF



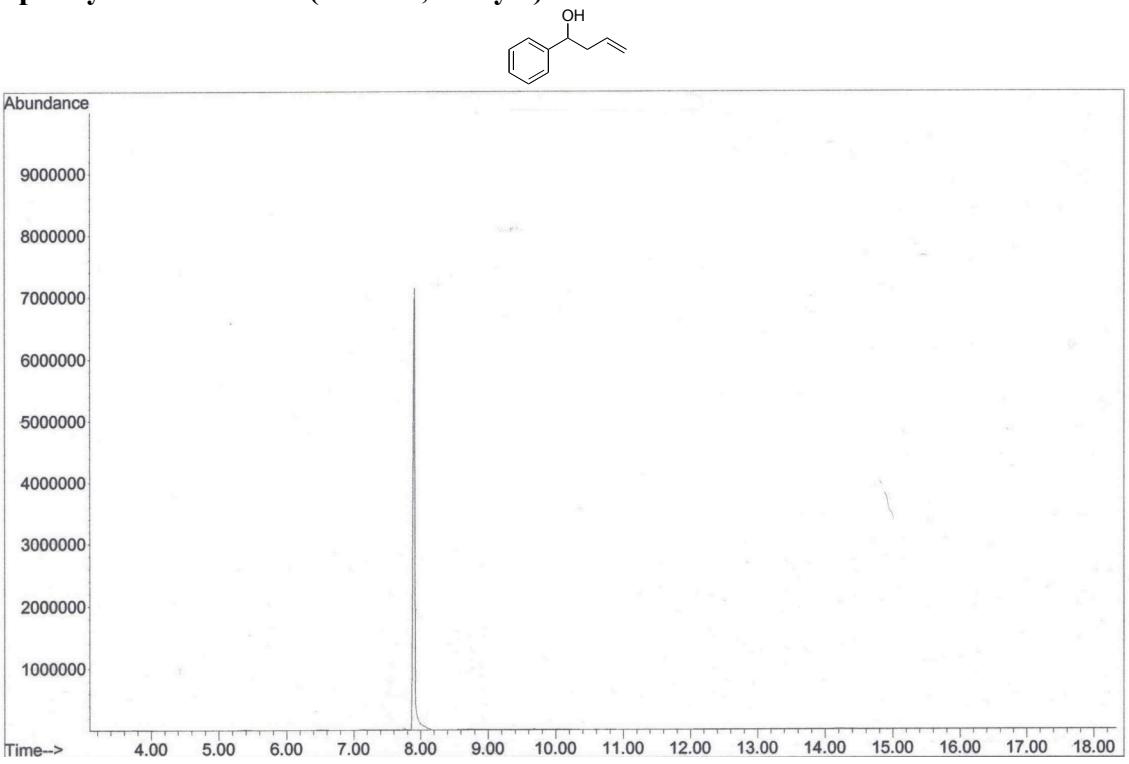
$^1$H NMR (400 MHz, THF-$d_8$) of **4** generated *in situ* from crotyltrimethoxysilane and (IPr)CuF



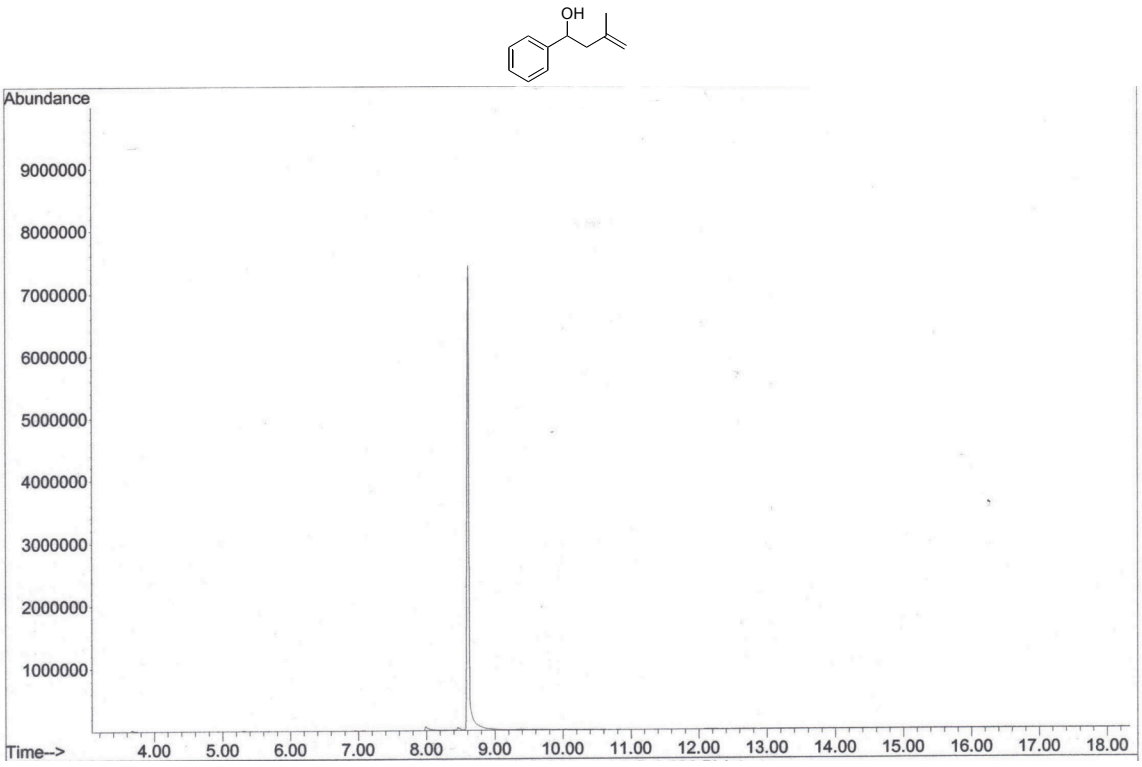



**GC-MS data**

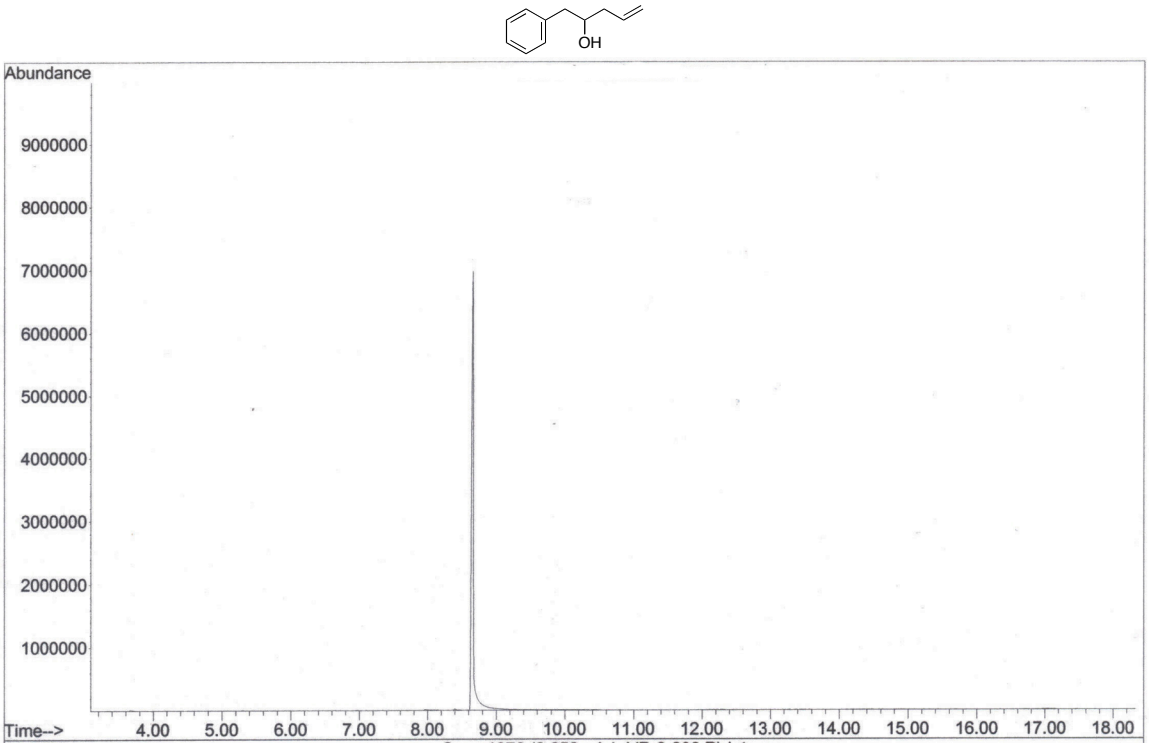
**1-phenyl-but-3-en-1-ol (Table 2, entry 1)**



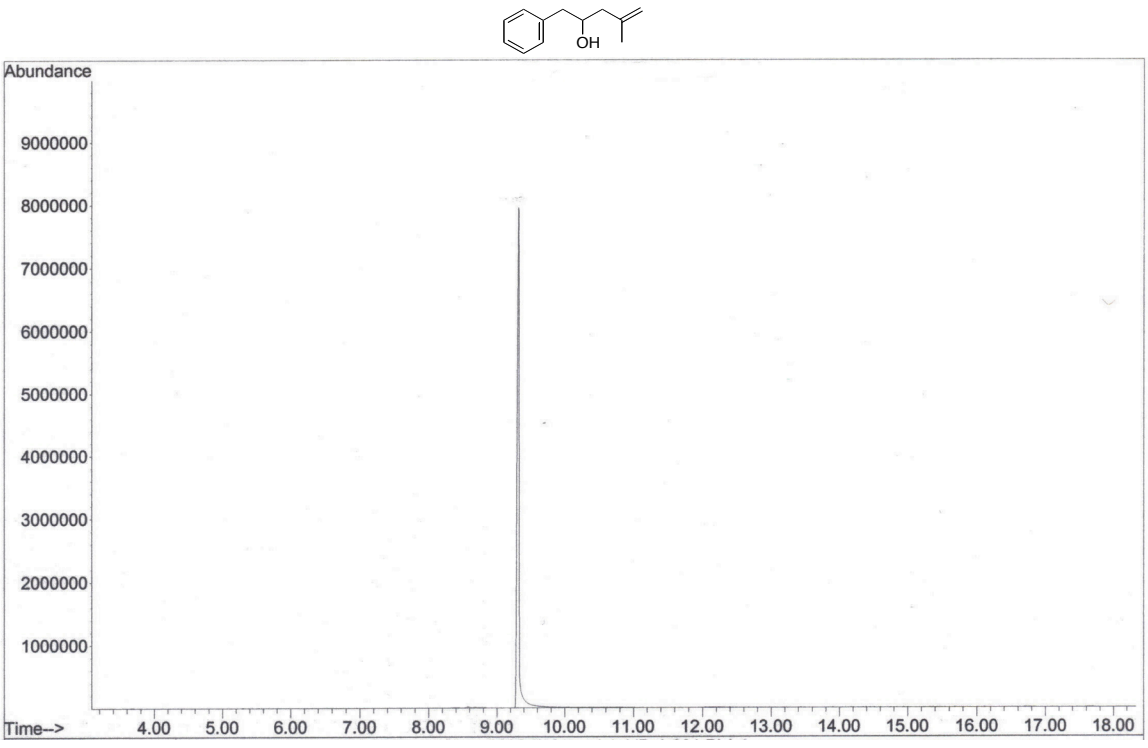

**1-phenyl-3-methyl-3-buten-1-ol (Table 2, entry 2)**



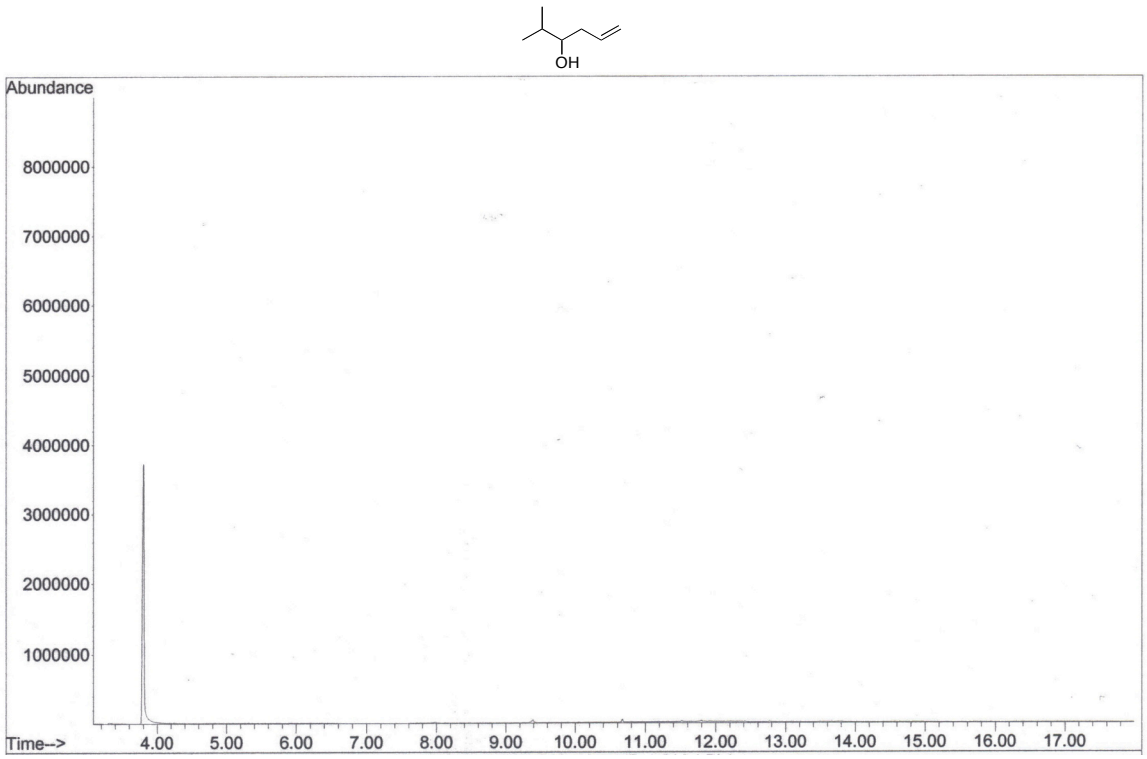
**1-phenyl-4-penten-2-ol (Table 2, entry 3)**



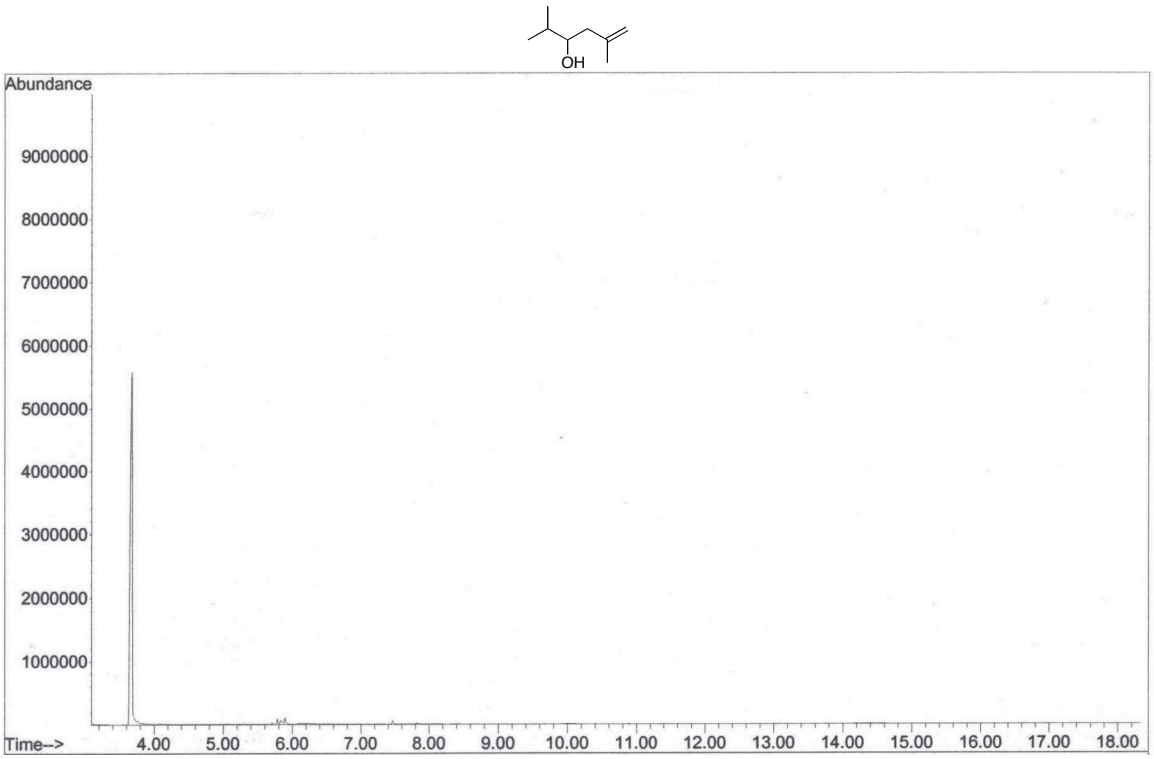

**4-methyl-1-phenyl-4-penten-2-ol (Table 2, entry 4)**



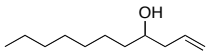
**2-methyl-5-hexen-3-ol (Table 2, entry 5)**

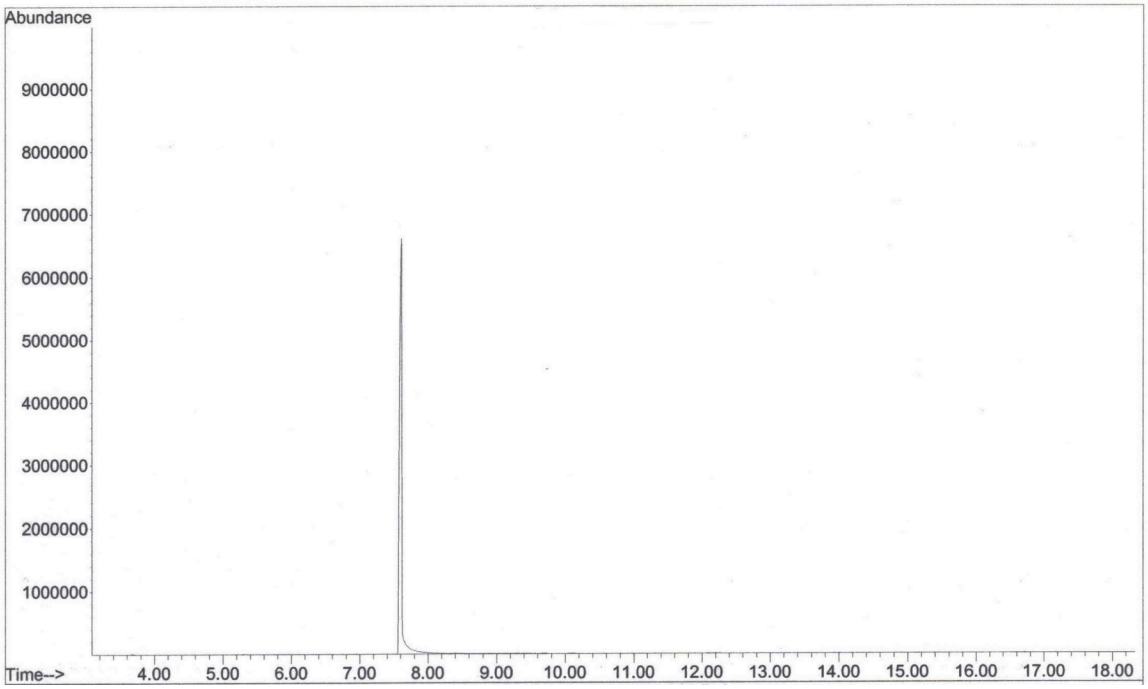



**2,5-dimethyl-5-hexen-3-ol (Table 2, entry 6)**

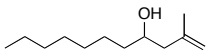


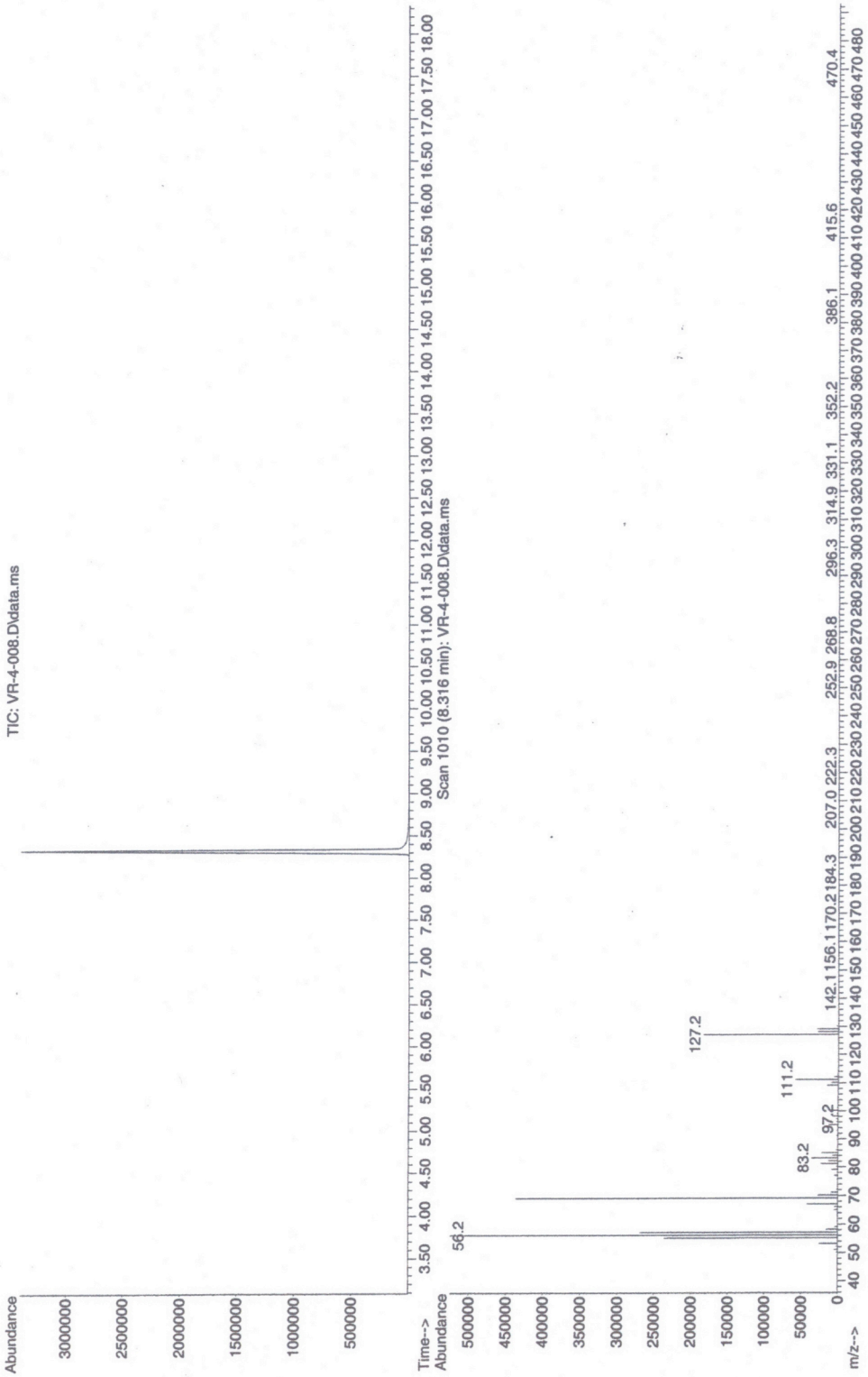
**1-undecen-4-ol (Table 2, entry 7)**



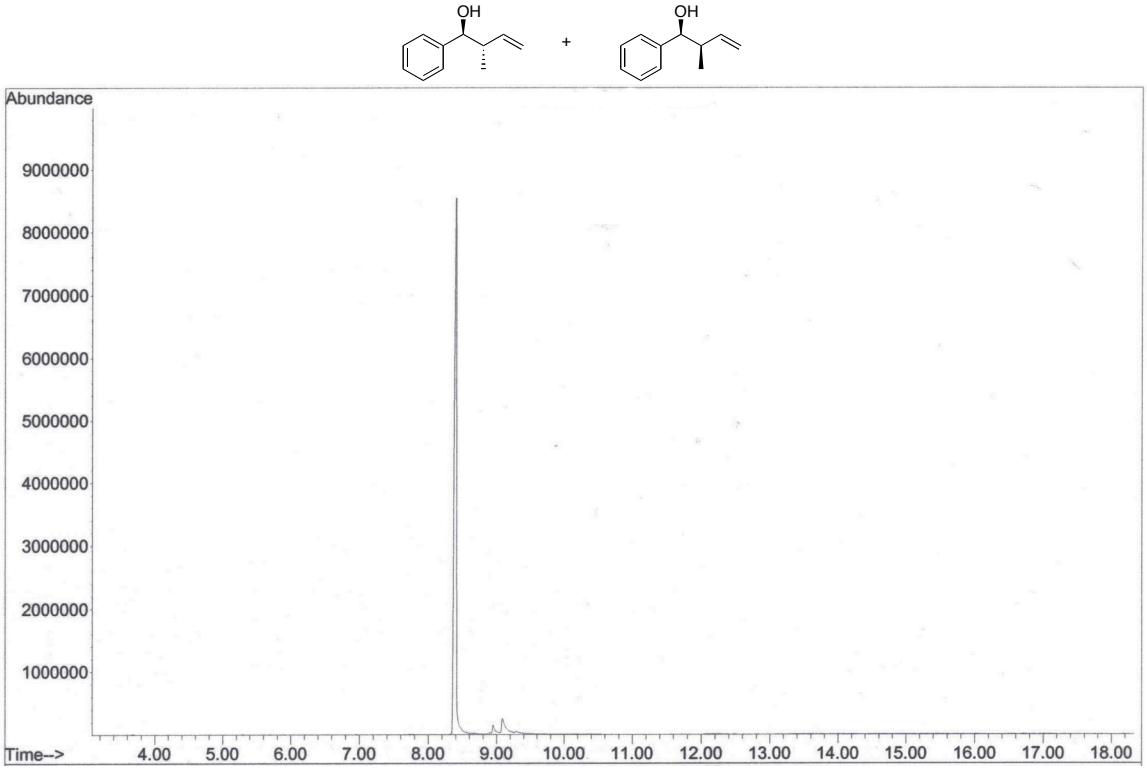



**2-methyl-1-undecen-4-ol (Table 2, entry 8)**

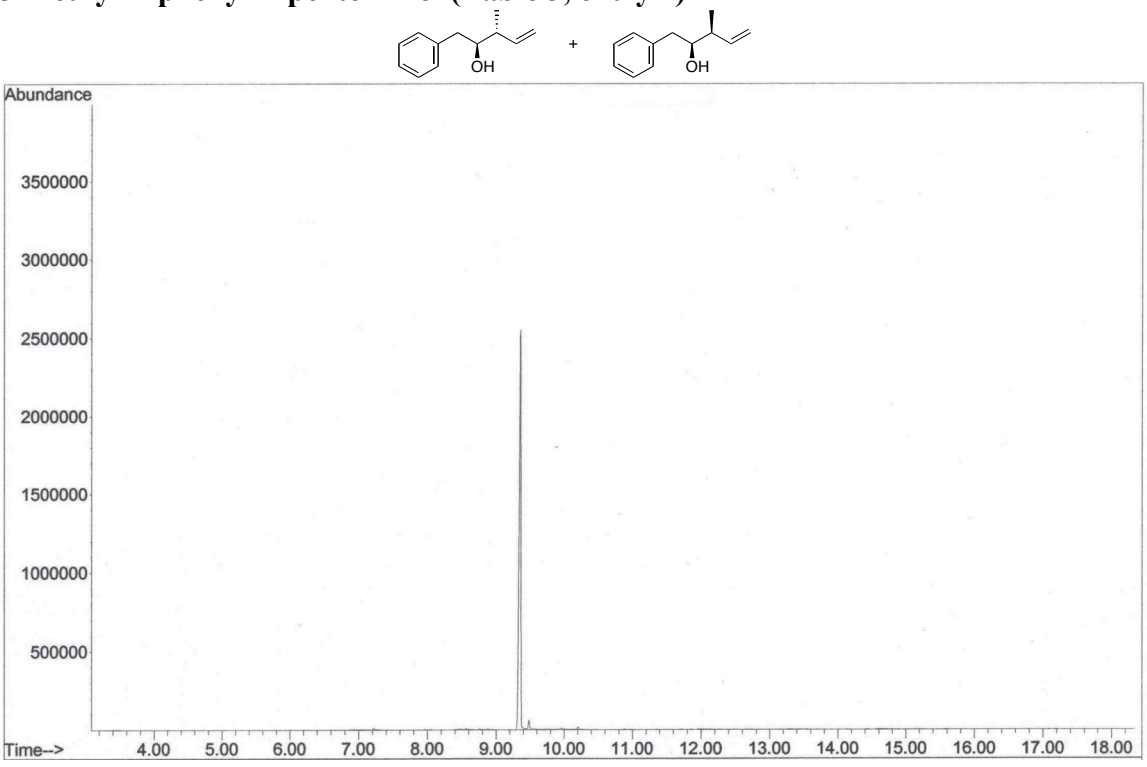


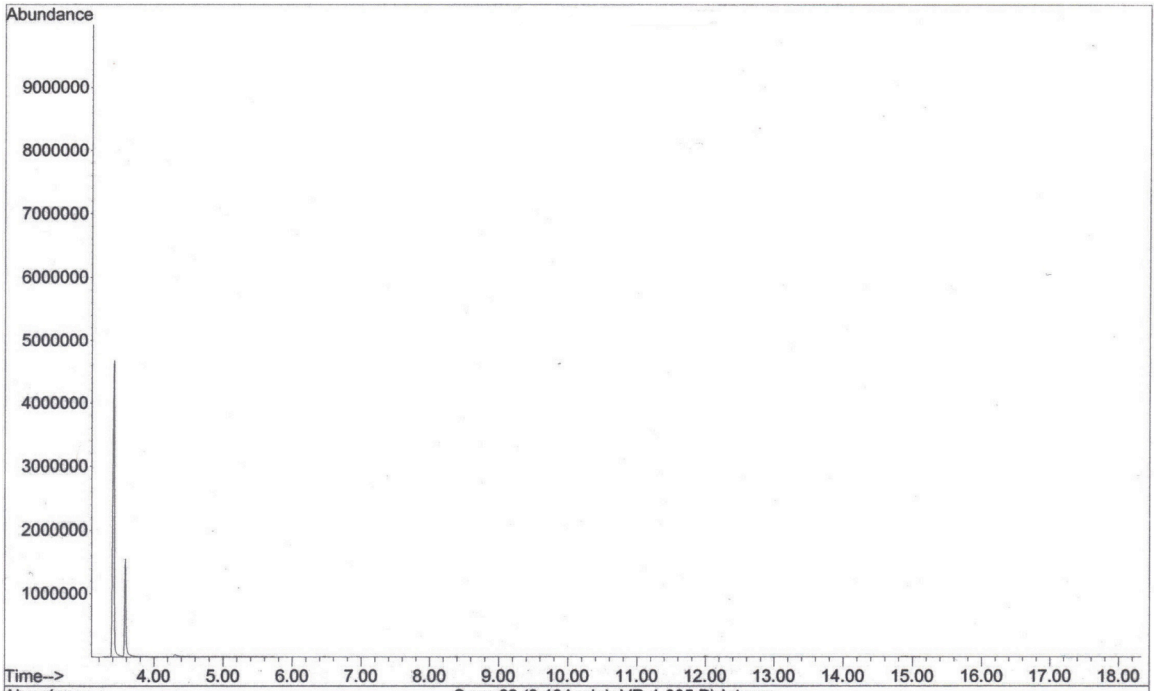
**2-methyl-1-phenyl-3-buten-1-ol (Table 3, entry 1)**



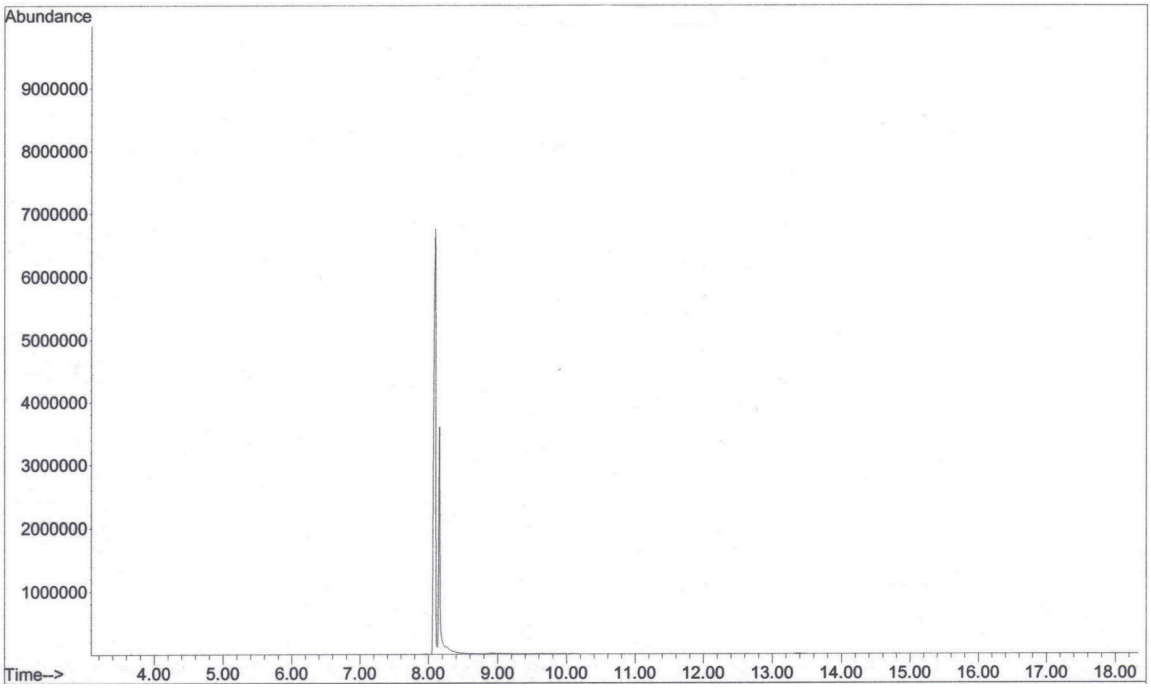

**3-methyl-1-phenyl-4-penten-2-ol (Table 3, entry 2)**



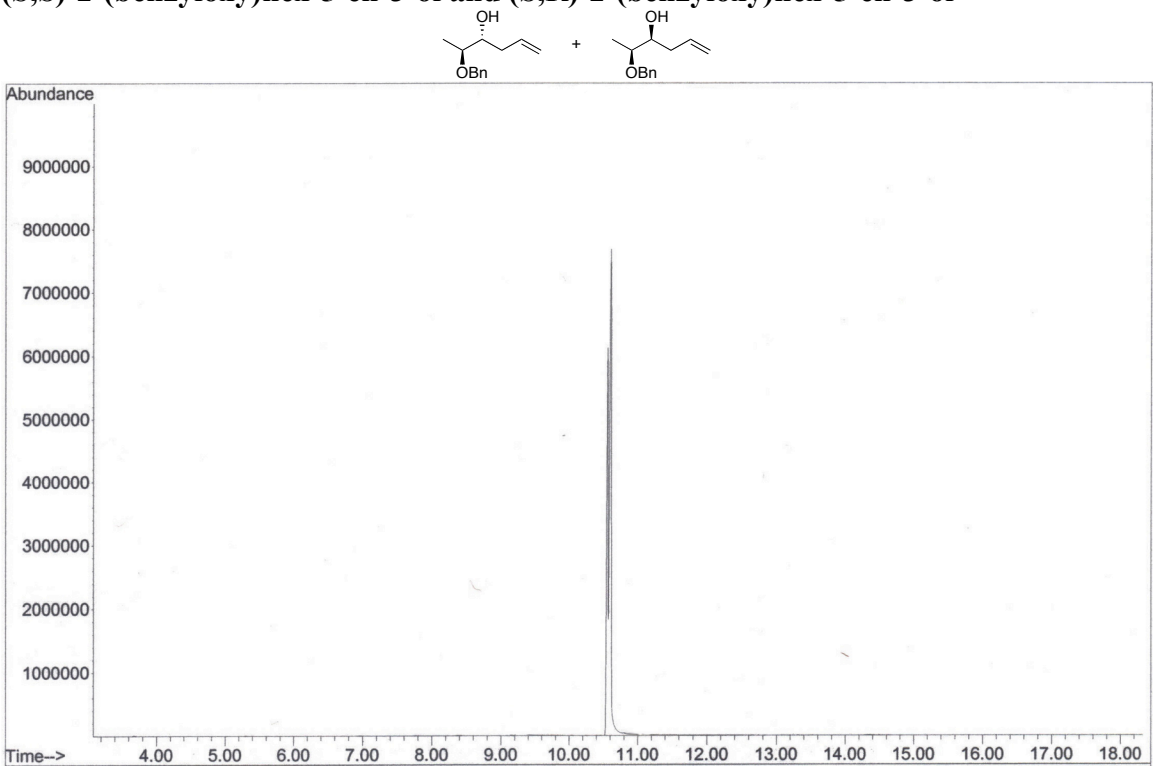
**2,4-dimethyl-5-hexen-3-ol (Table 3, entry 3)**

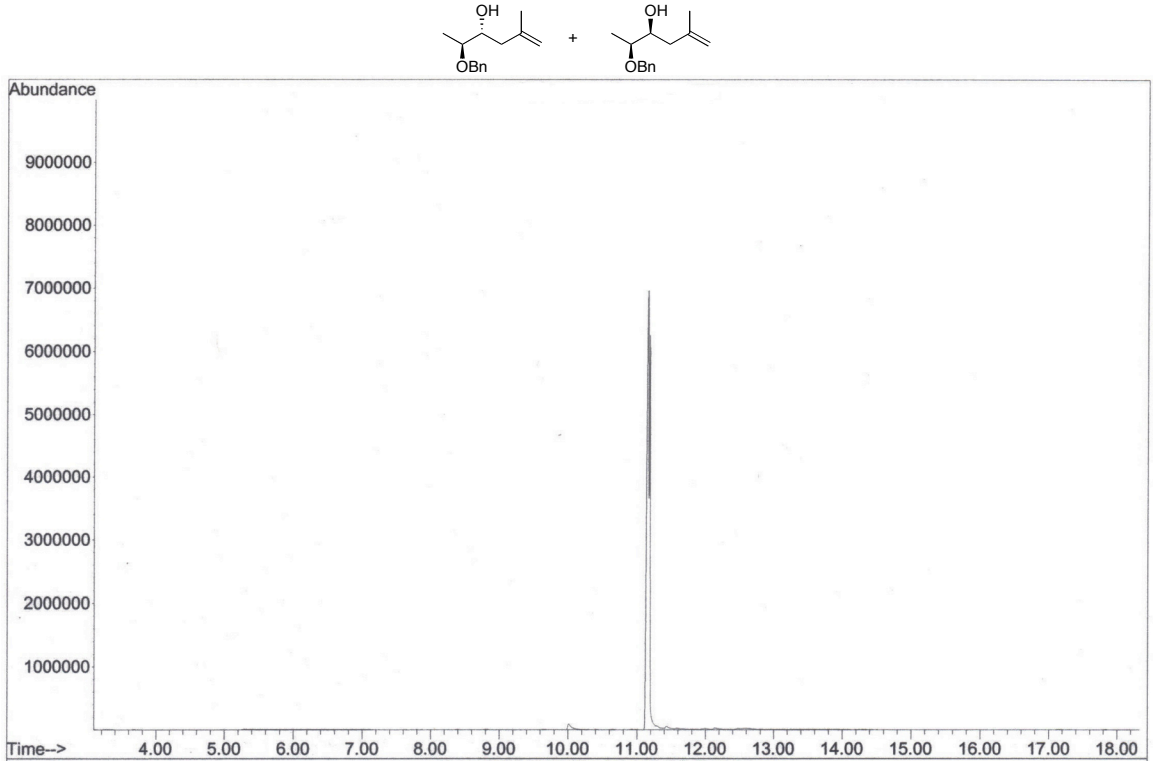

**3-methyl-1-undecen-4-ol (Table 3, entry 4)**

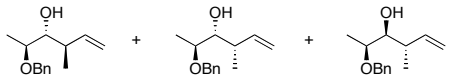
**(S,S)-2-(benzyloxy)hex-5-en-3-ol and (S,R)-2-(benzyloxy)hex-5-en-3-ol**

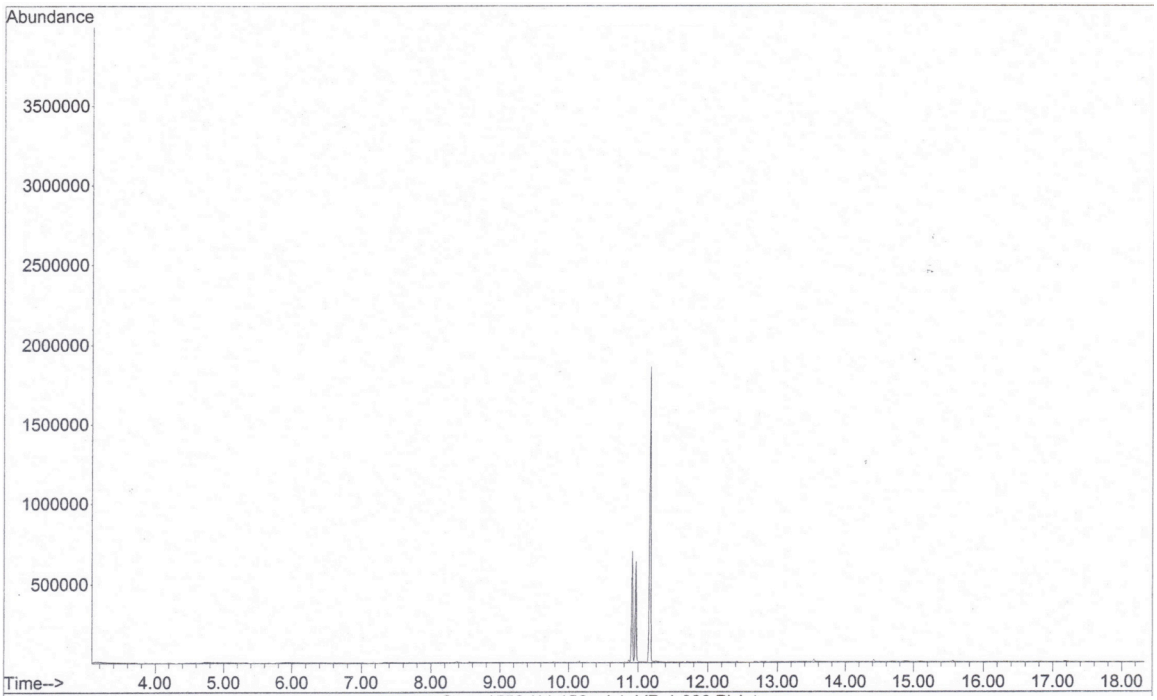



**(S,S)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol and (S,R)-2-methyl-5-(phenylmethoxy)hex-1-en-4-ol**



**(2S,3R,4R)-2-(benzyloxy)-4-methyl-5-hexen-3-ol, (2S,3R,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol and (2S,3S,4S)-2-(benzyloxy)-4-methyl-5-hexen-3-ol.**



## X-Ray Crystallography

**Preparation of the samples.** In the glove box, (IPr)CuF (20.0 mg, 0.042 mmol) was dissolved in dry THF (0.10 mL) in a vial insert, and the insert was the placed into a 4-mL vial, equipped with a septum cap. The vial was sealed and taken out of the box. Allyltrimethoxysilane (6.9 mg, 0.042 mmol) was added via syringe through the septum into the insert, and the solution was let standing for 30 min. The vial was then taken back into the box, and pentane (2 mL) was added on the outside of the insert. The vial was capped and placed in a refrigerator at -36 ˚C. Crystals of compound **2** formed as colorless blocks after 48 h. The same procedure was repeated, using (2-methyl-2-propenyl)triethoxysilane (9.3 mg, 0.042 mmol), to obtain crystals of compound **3**.

### [1,3-bis(2′,6′-diisopropylphenyl)imidazol-2-ylidene]copper(I) allyl (2)

Table 1. Crystal data and structure refinement for K1180.

| | |
|---|---|
| Identification code | k1180 |
| Empirical formula | C30 H41 Cu N2 |
| Formula weight | 493.19 |
| Temperature | 223(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a = 9.3723(6) A alpha = 82.839(1) deg.<br>b = 9.4760(6) A beta = 85.685(1) deg.<br>c = 17.9141(11) A gamma = 64.125(1) deg. |
| Volume | 1419.93(15) A^3 |
| Z, Calculated density | 2, 1.154 Mg/m^3 |
| Absorption coefficient | 0.787 mm^-1 |
| F(000) | 528 |
| Crystal color and shape | Colorless block |
| Crystal size | 0.50 x 0.35 x 0.30 mm |
| Theta range for data collection | 2.40 to 25.09 deg. |
| Limiting indices | -11<=h<=11, -11<=k<=11, 0<=l<=21 |
| Reflections collected / unique | 7232 / 4945 [R(int) = 0.0255] |
| Completeness to theta = 25.09 | 98.2 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.9941 and 0.8268 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4311 / 2 / 289 |
| Goodness-of-fit on F^2 | 1.022 |

| | |
|---|---|
| Final R indices [I>4sigma(I)] | R1 = 0.0328, wR2 = 0.0876 |
| R indices (all data) | R1 = 0.0366, wR2 = 0.0908 |
| Largest diff. peak and hole | 0.489 and -0.330 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for K1180. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cu | 4671(1) | 5600(1) | 7662(1) | 41(1) |
| N(1) | 5241(2) | 8176(2) | 8174(1) | 35(1) |
| N(2) | 4493(2) | 8625(2) | 7037(1) | 34(1) |
| C(1) | 4617(4) | 3644(3) | 7489(1) | 60(1) |
| C(2) | 3844(3) | 4044(3) | 6770(2) | 62(1) |
| C(3) | 2421(4) | 4257(4) | 6614(2) | 77(1) |
| C(4) | 4777(2) | 7552(2) | 7651(1) | 33(1) |
| C(5) | 5252(3) | 9603(2) | 7886(1) | 42(1) |
| C(6) | 4773(3) | 9885(2) | 7174(1) | 43(1) |
| C(7) | 5631(2) | 7431(2) | 8931(1) | 36(1) |
| C(8) | 7105(2) | 6148(2) | 9053(1) | 41(1) |
| C(9) | 7401(3) | 5400(3) | 9783(1) | 52(1) |
| C(10) | 6296(3) | 5913(3) | 10356(1) | 57(1) |
| C(11) | 4863(3) | 7203(3) | 10221(1) | 54(1) |
| C(12) | 4497(2) | 8005(3) | 9505(1) | 44(1) |
| C(13) | 8376(3) | 5581(3) | 8437(1) | 49(1) |
| C(14) | 8831(4) | 3878(4) | 8320(2) | 85(1) |
| C(15) | 9808(4) | 5831(5) | 8605(2) | 89(1) |
| C(16) | 2902(3) | 9415(3) | 9349(1) | 53(1) |
| C(17) | 2383(3) | 10535(4) | 9963(2) | 78(1) |
| C(18) | 1656(3) | 8862(4) | 9219(2) | 72(1) |
| C(19) | 4030(2) | 8374(2) | 6327(1) | 37(1) |
| C(20) | 5224(2) | 7692(2) | 5794(1) | 41(1) |
| C(21) | 4765(3) | 7408(3) | 5127(1) | 53(1) |
| C(22) | 3204(3) | 7775(3) | 5010(1) | 57(1) |
| C(23) | 2051(3) | 8445(3) | 5546(1) | 52(1) |
| C(24) | 2433(2) | 8769(2) | 6225(1) | 43(1) |
| C(25) | 6972(3) | 7179(3) | 5931(1) | 49(1) |
| C(26) | 7776(4) | 7769(4) | 5281(2) | 74(1) |
| C(27) | 7823(3) | 5381(3) | 6075(2) | 76(1) |
| C(28) | 1116(4) | 9470(4) | 6803(3) | 49(2) |
| C(29) | -158(5) | 8879(5) | 6833(3) | 73(1) |
| C(30) | 388(6) | 11253(5) | 6634(3) | 68(1) |
| C(28') | 1205(6) | 9627(7) | 6820(4) | 52(3) |
| C(29') | 423(8) | 8589(7) | 7175(4) | 70(2) |
| C(30') | -44(9) | 11234(7) | 6522(5) | 73(2) |

Table 3. Bond lengths [A] and angles [deg] for K1180.

| | |
|---|---|
| Cu-C(4) | 1.8926(18) |
| Cu-C(1) | 1.940(2) |
| N(1)-C(4) | 1.357(2) |
| N(1)-C(5) | 1.390(2) |
| N(1)-C(7) | 1.442(2) |
| N(2)-C(4) | 1.357(2) |
| N(2)-C(6) | 1.383(2) |
| N(2)-C(19) | 1.453(2) |
| C(1)-C(2) | 1.451(4) |
| C(2)-C(3) | 1.306(4) |
| C(5)-C(6) | 1.340(3) |
| C(7)-C(8) | 1.396(3) |
| C(7)-C(12) | 1.398(3) |
| C(8)-C(9) | 1.393(3) |
| C(8)-C(13) | 1.522(3) |
| C(9)-C(10) | 1.374(3) |
| C(10)-C(11) | 1.378(3) |
| C(11)-C(12) | 1.392(3) |
| C(12)-C(16) | 1.524(3) |
| C(13)-C(15) | 1.517(4) |
| C(13)-C(14) | 1.517(4) |
| C(16)-C(18) | 1.516(3) |
| C(16)-C(17) | 1.528(4) |
| C(19)-C(20) | 1.394(3) |
| C(19)-C(24) | 1.396(3) |
| C(20)-C(21) | 1.396(3) |
| C(20)-C(25) | 1.521(3) |
| C(21)-C(22) | 1.374(3) |
| C(22)-C(23) | 1.375(3) |
| C(23)-C(24) | 1.399(3) |
| C(24)-C(28) | 1.515(4) |
| C(24)-C(28') | 1.528(4) |
| C(25)-C(26) | 1.519(3) |
| C(25)-C(27) | 1.530(3) |
| C(28)-C(29) | 1.5200 |
| C(28)-C(30) | 1.5200 |
| C(28')-C(30') | 1.5199 |
| C(28')-C(29') | 1.5201 |
| | |
| C(4)-Cu-C(1) | 170.19(9) |
| C(4)-N(1)-C(5) | 111.22(15) |
| C(4)-N(1)-C(7) | 122.75(15) |
| C(5)-N(1)-C(7) | 126.02(16) |
| C(4)-N(2)-C(6) | 111.74(15) |
| C(4)-N(2)-C(19) | 121.81(15) |
| C(6)-N(2)-C(19) | 126.38(15) |
| C(2)-C(1)-Cu | 102.65(15) |
| C(3)-C(2)-C(1) | 130.0(3) |
| N(2)-C(4)-N(1) | 103.72(15) |
| N(2)-C(4)-Cu | 124.15(13) |
| N(1)-C(4)-Cu | 131.94(13) |
| C(6)-C(5)-N(1) | 106.80(17) |
| C(5)-C(6)-N(2) | 106.53(17) |
| C(8)-C(7)-C(12) | 123.05(18) |
| C(8)-C(7)-N(1) | 118.59(17) |
| C(12)-C(7)-N(1) | 118.34(17) |
| C(9)-C(8)-C(7) | 116.94(19) |
| C(9)-C(8)-C(13) | 120.00(19) |
| C(7)-C(8)-C(13) | 123.05(18) |
| C(10)-C(9)-C(8) | 121.4(2) |
| C(9)-C(10)-C(11) | 120.4(2) |
| C(10)-C(11)-C(12) | 121.0(2) |
| C(11)-C(12)-C(7) | 117.2(2) |
| C(11)-C(12)-C(16) | 121.3(2) |
| C(7)-C(12)-C(16) | 121.52(19) |
| C(15)-C(13)-C(14) | 111.7(2) |
| C(15)-C(13)-C(8) | 110.61(19) |
| C(14)-C(13)-C(8) | 111.5(2) |

| | |
|---|---|
| C(18)-C(16)-C(12) | 110.3(2) |
| C(18)-C(16)-C(17) | 112.0(2) |
| C(12)-C(16)-C(17) | 112.6(2) |
| C(20)-C(19)-C(24) | 123.56(18) |
| C(20)-C(19)-N(2) | 117.76(17) |
| C(24)-C(19)-N(2) | 118.63(17) |
| C(19)-C(20)-C(21) | 116.98(19) |
| C(19)-C(20)-C(25) | 123.03(18) |
| C(21)-C(20)-C(25) | 119.91(19) |
| C(22)-C(21)-C(20) | 120.9(2) |
| C(21)-C(22)-C(23) | 120.9(2) |
| C(22)-C(23)-C(24) | 121.0(2) |
| C(19)-C(24)-C(23) | 116.68(19) |
| C(19)-C(24)-C(28) | 124.7(2) |
| C(23)-C(24)-C(28) | 118.6(2) |
| C(19)-C(24)-C(28') | 119.2(3) |
| C(23)-C(24)-C(28') | 123.9(3) |
| C(28)-C(24)-C(28') | 7.7(3) |
| C(26)-C(25)-C(20) | 112.3(2) |
| C(26)-C(25)-C(27) | 110.4(2) |
| C(20)-C(25)-C(27) | 109.9(2) |
| C(24)-C(28)-C(29) | 114.3(3) |
| C(24)-C(28)-C(30) | 108.0(3) |
| C(29)-C(28)-C(30) | 110.4 |
| C(30')-C(28')-C(29') | 110.4 |
| C(30')-C(28')-C(24) | 113.8(5) |
| C(29')-C(28')-C(24) | 109.5(5) |

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for K1180. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Cu | 60(1) | 29(1) | 39(1) | 0(1) | -10(1) | -24(1) |
| N(1) | 41(1) | 28(1) | 36(1) | -2(1) | -7(1) | -16(1) |
| N(2) | 43(1) | 26(1) | 34(1) | 1(1) | -8(1) | -15(1) |
| C(1) | 92(2) | 36(1) | 65(2) | -5(1) | -8(1) | -38(1) |
| C(2) | 85(2) | 51(1) | 60(2) | -22(1) | 12(1) | -37(1) |
| C(3) | 75(2) | 80(2) | 82(2) | -34(2) | 2(2) | -33(2) |
| C(4) | 36(1) | 26(1) | 36(1) | -2(1) | -6(1) | -13(1) |
| C(5) | 56(1) | 32(1) | 47(1) | -5(1) | -7(1) | -24(1) |
| C(6) | 59(1) | 28(1) | 45(1) | 3(1) | -7(1) | -22(1) |
| C(7) | 43(1) | 35(1) | 34(1) | -3(1) | -7(1) | -20(1) |
| C(8) | 46(1) | 42(1) | 36(1) | -6(1) | -8(1) | -18(1) |
| C(9) | 57(1) | 50(1) | 41(1) | 2(1) | -14(1) | -16(1) |
| C(10) | 71(2) | 68(2) | 35(1) | 6(1) | -10(1) | -32(1) |
| C(11) | 59(1) | 69(2) | 39(1) | -9(1) | 7(1) | -34(1) |
| C(12) | 44(1) | 46(1) | 45(1) | -8(1) | -1(1) | -23(1) |
| C(13) | 45(1) | 52(1) | 39(1) | -7(1) | -6(1) | -9(1) |
| C(14) | 91(2) | 67(2) | 85(2) | -30(2) | 14(2) | -19(2) |
| C(15) | 68(2) | 140(3) | 76(2) | -43(2) | 16(2) | -55(2) |
| C(16) | 44(1) | 52(1) | 61(1) | -10(1) | 5(1) | -19(1) |
| C(17) | 57(2) | 70(2) | 108(2) | -39(2) | 7(2) | -22(1) |
| C(18) | 49(1) | 74(2) | 96(2) | -22(2) | -7(1) | -23(1) |
| C(19) | 48(1) | 27(1) | 35(1) | 4(1) | -12(1) | -16(1) |
| C(20) | 48(1) | 34(1) | 41(1) | -2(1) | -8(1) | -16(1) |
| C(21) | 58(1) | 54(1) | 44(1) | -12(1) | -5(1) | -19(1) |
| C(22) | 68(2) | 59(1) | 46(1) | -9(1) | -17(1) | -26(1) |
| C(23) | 51(1) | 52(1) | 53(1) | 5(1) | -20(1) | -23(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(24) | 47(1) | 36(1) | 41(1) | 7(1) | -12(1) | -16(1) |
| C(25) | 47(1) | 49(1) | 50(1) | -9(1) | -4(1) | -19(1) |
| C(26) | 73(2) | 75(2) | 86(2) | 0(2) | 1(2) | -45(2) |
| C(27) | 50(1) | 57(2) | 105(2) | 11(2) | -11(1) | -12(1) |

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for K1180.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 5690 | 2790 | 7461 | 72 |
| H(1B) | 4003 | 3330 | 7886 | 72 |
| H(2) | 4464 | 4168 | 6352 | 74 |
| H(3A) | 1730 | 4153 | 7003 | 92 |
| H(3B) | 2086 | 4515 | 6113 | 92 |
| H(5) | 5539 | 10245 | 8141 | 51 |
| H(6) | 4652 | 10768 | 6833 | 52 |
| H(9) | 8378 | 4525 | 9886 | 62 |
| H(10) | 6519 | 5381 | 10842 | 69 |
| H(11) | 4121 | 7546 | 10619 | 65 |
| H(13) | 7926 | 6235 | 7962 | 59 |
| H(14A) | 7892 | 3766 | 8205 | 128 |
| H(14B) | 9296 | 3205 | 8774 | 128 |
| H(14C) | 9595 | 3573 | 7905 | 128 |
| H(15A) | 9477 | 6934 | 8665 | 134 |
| H(15B) | 10575 | 5528 | 8191 | 134 |
| H(15C) | 10286 | 5190 | 9064 | 134 |
| H(16) | 3029 | 10013 | 8876 | 63 |
| H(17A) | 3203 | 10873 | 10025 | 117 |
| H(17B) | 2211 | 9997 | 10434 | 117 |
| H(17C) | 1406 | 11448 | 9821 | 117 |
| H(18A) | 2023 | 8163 | 8823 | 109 |
| H(18B) | 676 | 9766 | 9071 | 109 |
| H(18C) | 1470 | 8303 | 9679 | 109 |
| H(21) | 5534 | 6959 | 4751 | 64 |
| H(22) | 2921 | 7567 | 4558 | 68 |
| H(23) | 990 | 8688 | 5455 | 62 |
| H(25) | 7050 | 7627 | 6388 | 59 |
| H(26A) | 7234 | 8910 | 5201 | 112 |
| H(26B) | 7734 | 7324 | 4829 | 112 |
| H(26C) | 8874 | 7450 | 5400 | 112 |
| H(27A) | 7300 | 5021 | 6492 | 114 |
| H(27B) | 8918 | 5066 | 6198 | 114 |
| H(27C) | 7791 | 4917 | 5628 | 114 |
| H(28) | 1598 | 9196 | 7304 | 59 |
| H(29A) | 323 | 7740 | 6941 | 110 |
| H(29B) | -676 | 9169 | 6352 | 110 |
| H(29C) | -935 | 9349 | 7225 | 110 |
| H(30A) | 1214 | 11613 | 6617 | 102 |
| H(30B) | -387 | 11732 | 7026 | 102 |
| H(30C) | -128 | 11553 | 6153 | 102 |
| H(28') | 1776 | 9789 | 7220 | 62 |
| H(29D) | -272 | 9084 | 7588 | 104 |
| H(29E) | 1234 | 7568 | 7362 | 104 |
| H(29F) | -190 | 8452 | 6801 | 104 |
| H(30D) | -715 | 11757 | 6937 | 109 |
| H(30E) | -688 | 11104 | 6161 | 109 |
| H(30F) | 472 | 11868 | 6280 | 109 |

Table 6. Torsion angles [deg] for K1180.

| | |
|---|---|
| C(4)-Cu-C(1)-C(2) | -35.2(7) |
| Cu-C(1)-C(2)-C(3) | -108.0(3) |
| C(6)-N(2)-C(4)-N(1) | 0.0(2) |
| C(19)-N(2)-C(4)-N(1) | 177.17(16) |
| C(6)-N(2)-C(4)-Cu | -175.36(14) |
| C(19)-N(2)-C(4)-Cu | 1.8(2) |
| C(5)-N(1)-C(4)-N(2) | -0.4(2) |
| C(7)-N(1)-C(4)-N(2) | 178.46(16) |
| C(5)-N(1)-C(4)-Cu | 174.50(15) |
| C(7)-N(1)-C(4)-Cu | -6.7(3) |
| C(1)-Cu-C(4)-N(2) | 21.9(7) |
| C(1)-Cu-C(4)-N(1) | -152.0(5) |
| C(4)-N(1)-C(5)-C(6) | 0.6(2) |
| C(7)-N(1)-C(5)-C(6) | -178.20(18) |
| N(1)-C(5)-C(6)-N(2) | -0.5(2) |
| C(4)-N(2)-C(6)-C(5) | 0.3(2) |
| C(19)-N(2)-C(6)-C(5) | -176.67(18) |
| C(4)-N(1)-C(7)-C(8) | 77.7(2) |
| C(5)-N(1)-C(7)-C(8) | -103.7(2) |
| C(4)-N(1)-C(7)-C(12) | -100.8(2) |
| C(5)-N(1)-C(7)-C(12) | 77.9(3) |
| C(12)-C(7)-C(8)-C(9) | 2.1(3) |
| N(1)-C(7)-C(8)-C(9) | -176.25(18) |
| C(12)-C(7)-C(8)-C(13) | -176.4(2) |
| N(1)-C(7)-C(8)-C(13) | 5.2(3) |
| C(7)-C(8)-C(9)-C(10) | -0.5(3) |
| C(13)-C(8)-C(9)-C(10) | 178.0(2) |
| C(8)-C(9)-C(10)-C(11) | -0.8(4) |
| C(9)-C(10)-C(11)-C(12) | 0.5(4) |
| C(10)-C(11)-C(12)-C(7) | 1.0(3) |
| C(10)-C(11)-C(12)-C(16) | 178.9(2) |
| C(8)-C(7)-C(12)-C(11) | -2.4(3) |
| N(1)-C(7)-C(12)-C(11) | 176.02(18) |
| C(8)-C(7)-C(12)-C(16) | 179.75(19) |
| N(1)-C(7)-C(12)-C(16) | -1.9(3) |
| C(9)-C(8)-C(13)-C(15) | -64.6(3) |
| C(7)-C(8)-C(13)-C(15) | 113.8(3) |
| C(9)-C(8)-C(13)-C(14) | 60.4(3) |
| C(7)-C(8)-C(13)-C(14) | -121.2(2) |
| C(11)-C(12)-C(16)-C(18) | -83.0(3) |
| C(7)-C(12)-C(16)-C(18) | 94.8(3) |
| C(11)-C(12)-C(16)-C(17) | 42.9(3) |
| C(7)-C(12)-C(16)-C(17) | -139.3(2) |
| C(4)-N(2)-C(19)-C(20) | -93.9(2) |
| C(6)-N(2)-C(19)-C(20) | 82.8(2) |
| C(4)-N(2)-C(19)-C(24) | 83.8(2) |
| C(6)-N(2)-C(19)-C(24) | -99.5(2) |
| C(24)-C(19)-C(20)-C(21) | 0.3(3) |
| N(2)-C(19)-C(20)-C(21) | 177.78(17) |
| C(24)-C(19)-C(20)-C(25) | -176.32(19) |
| N(2)-C(19)-C(20)-C(25) | 1.2(3) |
| C(19)-C(20)-C(21)-C(22) | -0.6(3) |
| C(25)-C(20)-C(21)-C(22) | 176.1(2) |
| C(20)-C(21)-C(22)-C(23) | 0.5(4) |
| C(21)-C(22)-C(23)-C(24) | 0.0(4) |
| C(20)-C(19)-C(24)-C(23) | 0.2(3) |
| N(2)-C(19)-C(24)-C(23) | -177.31(17) |
| C(20)-C(19)-C(24)-C(28) | 178.2(2) |
| N(2)-C(19)-C(24)-C(28) | 0.7(3) |
| C(20)-C(19)-C(24)-C(28') | -175.4(3) |
| N(2)-C(19)-C(24)-C(28') | 7.1(4) |
| C(22)-C(23)-C(24)-C(19) | -0.3(3) |
| C(22)-C(23)-C(24)-C(28) | -178.5(3) |
| C(22)-C(23)-C(24)-C(28') | 175.0(3) |
| C(19)-C(20)-C(25)-C(26) | -131.6(2) |
| C(21)-C(20)-C(25)-C(26) | 51.9(3) |
| C(19)-C(20)-C(25)-C(27) | 105.2(2) |
| C(21)-C(20)-C(25)-C(27) | -71.3(3) |
| C(19)-C(24)-C(28)-C(29) | -142.8(3) |

| | |
|---|---|
| C(23)-C(24)-C(28)-C(29) | 35.2(4) |
| C(28')-C(24)-C(28)-C(29) | 171(3) |
| C(19)-C(24)-C(28)-C(30) | 93.9(3) |
| C(23)-C(24)-C(28)-C(30) | -88.1(3) |
| C(28')-C(24)-C(28)-C(30) | 48(3) |
| C(19)-C(24)-C(28')-C(30') | 119.4(4) |
| C(23)-C(24)-C(28')-C(30') | -55.8(5) |
| C(28)-C(24)-C(28')-C(30') | -103(3) |
| C(19)-C(24)-C(28')-C(29') | -116.5(4) |
| C(23)-C(24)-C(28')-C(29') | 68.3(5) |
| C(28)-C(24)-C(28')-C(29') | 21(2) |

**[1,3-bis(2′,6′-diisopropylphenyl)imidazol-2-ylidene]copper(I) 2-methallyl (3)**

Table 1. Crystal data and structure refinement for K1179.

| | |
|---|---|
| Identification code | k1179 |
| Empirical formula | C31 H43 Cu N2 |
| Formula weight | 507.21 |
| Temperature | 223(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a = 9.3636(5) A alpha = 81.497(1) deg.<br>b = 9.4808(5) A beta = 76.013(1) deg.<br>c = 19.0262(11) A gamma = 63.904(1) deg. |
| Volume | 1470.21(14) A^3 |
| Z, Calculated density | 2, 1.146 Mg/m^3 |
| Absorption coefficient | 0.762 mm^-1 |
| F(000) | 544 |
| Crystal color and shape | Colorless block |
| Crystal size | 0.50 x 0.45 x 0.40 mm |
| Theta range for data collection | 2.21 to 25.07 deg. |
| Limiting indices | -10<=h<=11, -11<=k<=11, 0<=l<=22 |
| Reflections collected / unique | 7479 / 5133 [R(int) = 0.0324] |
| Completeness to theta = 25.07 | 98.3 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.9973 and 0.8144 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4391 / 10 / 283 |
| Goodness-of-fit on F^2 | 0.986 |
| Final R indices [I>4sigma(I)] | R1 = 0.0447, wR2 = 0.1181 |
| R indices (all data) | R1 = 0.0498, wR2 = 0.1229 |
| Largest diff. peak and hole | 0.635 and -0.408 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for K1179. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cu | 5833 | 5549 | 2654 | 34(1) |
| C(1) | 5832(9) | 3583(8) | 2494(3) | 41(2) |
| C(2) | 5676(7) | 3652(7) | 1734(3) | 39(2) |
| C(3) | 6943(8) | 2900(9) | 1270(4) | 60(2) |
| C(4) | 4087(10) | 4664(10) | 1466(5) | 79(2) |
| Cu' | 5414 | 5737 | 2696 | 31(1) |
| C(1') | 5330(9) | 3813(8) | 2528(4) | 42(2) |
| C(2') | 5198(8) | 3845(8) | 1776(3) | 41(2) |
| C(3') | 3808(8) | 4107(9) | 1671(5) | 67(2) |
| C(4') | 6575(9) | 3699(11) | 1129(4) | 75(2) |
| N(1) | 5985(2) | 8143(2) | 3289(1) | 35(1) |
| N(2) | 5668(3) | 8680(2) | 2192(1) | 36(1) |
| C(5) | 5737(3) | 7565(3) | 2740(1) | 35(1) |
| C(6) | 6070(3) | 9576(3) | 3083(1) | 42(1) |
| C(7) | 5864(3) | 9911(3) | 2396(1) | 43(1) |
| C(8) | 6077(3) | 7378(3) | 4001(1) | 37(1) |
| C(9) | 4702(3) | 7956(3) | 4554(1) | 43(1) |
| C(10) | 4812(4) | 7175(4) | 5234(2) | 55(1) |
| C(11) | 6205(4) | 5906(4) | 5352(2) | 61(1) |
| C(12) | 7541(4) | 5379(4) | 4798(2) | 55(1) |
| C(13) | 7516(3) | 6094(3) | 4104(1) | 44(1) |
| C(14) | 3155(3) | 9329(4) | 4414(2) | 52(1) |
| C(15) | 1993(4) | 8742(5) | 4264(2) | 74(1) |
| C(16) | 2357(4) | 10481(5) | 5024(2) | 76(1) |
| C(17) | 8980(5) | 5550(7) | 3490(4) | 48(6) |
| C(18) | 10370(9) | 5754(9) | 3672(5) | 75(2) |
| C(19) | 9492(9) | 3842(7) | 3348(5) | 77(2) |
| C(17') | 9054(5) | 5488(7) | 3520(4) | 56(7) |
| C(18') | 10029(9) | 6432(7) | 3486(4) | 67(2) |
| C(19') | 10126(10) | 3738(6) | 3586(5) | 82(2) |
| C(20) | 5470(3) | 8515(3) | 1482(1) | 40(1) |
| C(21) | 3906(3) | 8984(3) | 1369(1) | 51(1) |
| C(22) | 3774(4) | 8734(4) | 686(2) | 61(1) |
| C(23) | 5120(4) | 8073(4) | 155(2) | 59(1) |
| C(24) | 6642(4) | 7641(4) | 284(2) | 59(1) |
| C(25) | 6859(3) | 7862(3) | 952(1) | 48(1) |
| C(26) | 2403(5) | 9954(7) | 1933(3) | 56(2) |
| C(27) | 1404(10) | 11642(7) | 1698(6) | 86(2) |
| C(28) | 1325(10) | 9089(9) | 2206(6) | 108(3) |
| C(29) | 8535(4) | 7191(6) | 1116(3) | 51(2) |
| C(30) | 9269(8) | 5407(6) | 1205(4) | 70(2) |
| C(31) | 9622(9) | 7726(8) | 518(4) | 75(2) |
| C(26') | 2431(6) | 9508(8) | 1965(3) | 51(2) |
| C(27') | 1350(12) | 11173(9) | 1735(7) | 90(3) |
| C(28') | 1511(13) | 8481(11) | 2117(8) | 109(4) |
| C(29') | 8536(5) | 7575(8) | 1069(4) | 52(2) |
| C(30') | 9575(11) | 5822(8) | 1159(5) | 86(3) |
| C(31') | 9467(11) | 8342(10) | 507(5) | 81(3) |

Table 3. Bond lengths [A] and angles [deg] for K1179.

| | |
|---|---|
| Cu-C(5) | 1.903(2) |
| Cu-C(1) | 1.933(6) |
| C(1)-C(2) | 1.477(9) |
| C(2)-C(3) | 1.278(7) |
| C(2)-C(4) | 1.537(8) |
| Cu'-C(5) | 1.902(2) |
| Cu'-C(1') | 1.936(6) |
| C(1')-C(2') | 1.462(9) |
| C(2')-C(3') | 1.274(7) |
| C(2')-C(4') | 1.524(8) |
| N(1)-C(5) | 1.358(3) |
| N(1)-C(6) | 1.389(3) |
| N(1)-C(8) | 1.442(3) |
| N(2)-C(5) | 1.362(3) |
| N(2)-C(7) | 1.380(3) |
| N(2)-C(20) | 1.447(3) |
| C(6)-C(7) | 1.338(4) |
| C(8)-C(13) | 1.396(4) |
| C(8)-C(9) | 1.400(4) |
| C(9)-C(10) | 1.396(4) |
| C(9)-C(14) | 1.513(4) |
| C(10)-C(11) | 1.372(5) |
| C(11)-C(12) | 1.377(4) |
| C(12)-C(13) | 1.392(4) |
| C(13)-C(17) | 1.514(4) |
| C(13)-C(17') | 1.525(4) |
| C(14)-C(15) | 1.518(4) |
| C(14)-C(16) | 1.528(4) |
| C(17)-C(19) | 1.5199 |
| C(17)-C(18) | 1.5199 |
| C(17')-C(18') | 1.5200 |
| C(17')-C(19') | 1.5200 |
| C(20)-C(25) | 1.390(4) |
| C(20)-C(21) | 1.392(4) |
| C(21)-C(22) | 1.398(4) |
| C(21)-C(26') | 1.498(4) |
| C(21)-C(26) | 1.549(4) |
| C(22)-C(23) | 1.371(5) |
| C(23)-C(24) | 1.372(5) |
| C(24)-C(25) | 1.395(4) |
| C(25)-C(29) | 1.504(4) |
| C(25)-C(29') | 1.538(4) |
| C(26)-C(28) | 1.5199 |
| C(26)-C(27) | 1.5200 |
| C(29)-C(30) | 1.5200 |
| C(29)-C(31) | 1.5201 |
| C(26')-C(27') | 1.5199 |
| C(26')-C(28') | 1.5200 |
| C(29')-C(30') | 1.5200 |
| C(29')-C(31') | 1.5201 |

| | |
|---|---|
| C(5)-Cu-C(1) | 174.8(2) |
| C(2)-C(1)-Cu | 107.2(4) |
| C(3)-C(2)-C(1) | 118.4(6) |
| C(3)-C(2)-C(4) | 118.3(6) |
| C(1)-C(2)-C(4) | 123.2(6) |
| C(5)-Cu'-C(1') | 171.8(2) |
| C(2')-C(1')-Cu' | 109.2(4) |
| C(3')-C(2')-C(1') | 116.3(7) |
| C(3')-C(2')-C(4') | 119.8(7) |
| C(1')-C(2')-C(4') | 123.8(6) |
| C(5)-N(1)-C(6) | 111.4(2) |
| C(5)-N(1)-C(8) | 123.42(19) |
| C(6)-N(1)-C(8) | 125.1(2) |
| C(5)-N(2)-C(7) | 111.8(2) |
| C(5)-N(2)-C(20) | 122.32(19) |
| C(7)-N(2)-C(20) | 125.9(2) |
| N(1)-C(5)-N(2) | 103.38(19) |

| | |
|---|---|
| N(1)-C(5)-Cu' | 131.55(17) |
| N(2)-C(5)-Cu' | 124.98(17) |
| N(1)-C(5)-Cu | 130.15(17) |
| N(2)-C(5)-Cu | 125.65(17) |
| Cu'-C(5)-Cu | 10.424(13) |
| C(7)-C(6)-N(1) | 106.8(2) |
| C(6)-C(7)-N(2) | 106.7(2) |
| C(13)-C(8)-C(9) | 123.3(2) |
| C(13)-C(8)-N(1) | 118.8(2) |
| C(9)-C(8)-N(1) | 117.9(2) |
| C(10)-C(9)-C(8) | 116.8(3) |
| C(10)-C(9)-C(14) | 121.7(3) |
| C(8)-C(9)-C(14) | 121.5(2) |
| C(11)-C(10)-C(9) | 121.3(3) |
| C(10)-C(11)-C(12) | 120.3(3) |
| C(11)-C(12)-C(13) | 121.5(3) |
| C(12)-C(13)-C(8) | 116.7(2) |
| C(12)-C(13)-C(17) | 122.3(4) |
| C(8)-C(13)-C(17) | 120.9(3) |
| C(12)-C(13)-C(17') | 118.9(4) |
| C(8)-C(13)-C(17') | 124.3(3) |
| C(17)-C(13)-C(17') | 3.5(4) |
| C(9)-C(14)-C(15) | 110.3(3) |
| C(9)-C(14)-C(16) | 112.7(3) |
| C(15)-C(14)-C(16) | 111.7(3) |
| C(13)-C(17)-C(19) | 110.3(5) |
| C(13)-C(17)-C(18) | 110.1(5) |
| C(19)-C(17)-C(18) | 110.4 |
| C(18')-C(17')-C(19') | 110.4 |
| C(18')-C(17')-C(13) | 110.2(5) |
| C(19')-C(17')-C(13) | 115.3(6) |
| C(25)-C(20)-C(21) | 123.6(2) |
| C(25)-C(20)-N(2) | 118.0(2) |
| C(21)-C(20)-N(2) | 118.4(2) |
| C(20)-C(21)-C(22) | 116.5(3) |
| C(20)-C(21)-C(26') | 123.1(3) |
| C(22)-C(21)-C(26') | 119.7(4) |
| C(20)-C(21)-C(26) | 120.9(3) |
| C(22)-C(21)-C(26) | 122.0(3) |
| C(26')-C(21)-C(26) | 15.3(4) |
| C(23)-C(22)-C(21) | 121.4(3) |
| C(22)-C(23)-C(24) | 120.3(3) |
| C(23)-C(24)-C(25) | 121.2(3) |
| C(20)-C(25)-C(24) | 116.9(3) |
| C(20)-C(25)-C(29) | 122.2(3) |
| C(24)-C(25)-C(29) | 120.3(3) |
| C(20)-C(25)-C(29') | 121.4(3) |
| C(24)-C(25)-C(29') | 121.3(4) |
| C(29)-C(25)-C(29') | 13.6(3) |
| C(28)-C(26)-C(27) | 110.4 |
| C(28)-C(26)-C(21) | 110.5(6) |
| C(27)-C(26)-C(21) | 116.3(5) |
| C(25)-C(29)-C(30) | 112.4(4) |
| C(25)-C(29)-C(31) | 109.4(5) |
| C(30)-C(29)-C(31) | 110.4 |
| C(21)-C(26')-C(27') | 105.5(6) |
| C(21)-C(26')-C(28') | 115.0(7) |
| C(27')-C(26')-C(28') | 110.4 |
| C(30')-C(29')-C(31') | 110.4 |
| C(30')-C(29')-C(25) | 110.2(6) |
| C(31')-C(29')-C(25) | 116.4(6) |

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for K1179. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Cu | 37(1) | 29(1) | 36(1) | -3(1) | -7(1) | -14(1) |
| Cu' | 36(1) | 30(1) | 30(1) | -2(1) | -6(1) | -15(1) |
| N(1) | 48(1) | 34(1) | 29(1) | -1(1) | -12(1) | -20(1) |
| N(2) | 52(1) | 32(1) | 30(1) | 2(1) | -13(1) | -20(1) |
| C(5) | 46(1) | 34(1) | 29(1) | 0(1) | -11(1) | -19(1) |
| C(6) | 58(2) | 39(1) | 40(1) | -3(1) | -14(1) | -27(1) |
| C(7) | 61(2) | 34(1) | 39(1) | 2(1) | -13(1) | -26(1) |
| C(8) | 50(1) | 41(1) | 28(1) | -1(1) | -12(1) | -24(1) |
| C(9) | 49(2) | 50(2) | 38(1) | -4(1) | -9(1) | -27(1) |
| C(10) | 62(2) | 72(2) | 34(1) | -4(1) | -1(1) | -35(2) |
| C(11) | 79(2) | 70(2) | 31(1) | 10(1) | -15(1) | -32(2) |
| C(12) | 68(2) | 55(2) | 39(2) | 6(1) | -21(1) | -19(2) |
| C(13) | 55(2) | 47(1) | 33(1) | -2(1) | -14(1) | -21(1) |
| C(14) | 47(2) | 58(2) | 51(2) | -7(1) | -6(1) | -24(1) |
| C(15) | 57(2) | 81(2) | 94(3) | -19(2) | -25(2) | -26(2) |
| C(16) | 60(2) | 74(2) | 91(3) | -32(2) | -15(2) | -17(2) |
| C(20) | 61(2) | 34(1) | 30(1) | 5(1) | -17(1) | -24(1) |
| C(21) | 63(2) | 61(2) | 37(1) | 8(1) | -18(1) | -34(2) |
| C(22) | 76(2) | 79(2) | 47(2) | 10(2) | -30(2) | -45(2) |
| C(23) | 92(2) | 60(2) | 38(2) | 0(1) | -27(2) | -37(2) |
| C(24) | 79(2) | 53(2) | 37(2) | -8(1) | -17(1) | -17(2) |
| C(25) | 64(2) | 42(1) | 36(1) | -2(1) | -17(1) | -16(1) |

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for K1179.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 6844 | 2700 | 2579 | 49 |
| H(1B) | 4921 | 3439 | 2826 | 49 |
| H(3A) | 7944 | 2320 | 1415 | 72 |
| H(3B) | 6875 | 2926 | 783 | 72 |
| H(4A) | 4310 | 4737 | 940 | 119 |
| H(4B) | 3616 | 5709 | 1649 | 119 |
| H(4C) | 3332 | 4185 | 1639 | 119 |
| H(1'A) | 6315 | 2906 | 2625 | 50 |
| H(1'B) | 4393 | 3712 | 2856 | 50 |
| H(3'A) | 2938 | 4265 | 2068 | 80 |
| H(3'B) | 3652 | 4141 | 1198 | 80 |
| H(4'A) | 6161 | 3944 | 684 | 113 |
| H(4'B) | 7417 | 2634 | 1124 | 113 |
| H(4'C) | 7022 | 4428 | 1166 | 113 |
| H(6) | 6240 | 10192 | 3370 | 51 |
| H(7) | 5855 | 10810 | 2108 | 51 |
| H(10) | 3913 | 7527 | 5619 | 66 |
| H(11) | 6249 | 5393 | 5814 | 73 |
| H(12) | 8492 | 4517 | 4889 | 66 |
| H(14) | 3449 | 9910 | 3968 | 62 |
| H(15A) | 2536 | 8022 | 3873 | 112 |
| H(15B) | 1055 | 9627 | 4127 | 112 |

| | | | | |
|---|---|---|---|---|
| H(15C) | 1644 | 8201 | 4698 | 112 |
| H(16A) | 3128 | 10840 | 5100 | 114 |
| H(16B) | 2016 | 9959 | 5466 | 114 |
| H(16C) | 1419 | 11375 | 4892 | 114 |
| H(17) | 8685 | 6203 | 3046 | 57 |
| H(18A) | 10026 | 6849 | 3761 | 112 |
| H(18B) | 11289 | 5438 | 3268 | 112 |
| H(18C) | 10682 | 5106 | 4101 | 112 |
| H(19A) | 8594 | 3729 | 3233 | 115 |
| H(19B) | 9801 | 3187 | 3776 | 115 |
| H(19C) | 10408 | 3518 | 2943 | 115 |
| H(17') | 8705 | 5688 | 3050 | 67 |
| H(18D) | 10993 | 6050 | 3107 | 101 |
| H(18E) | 10342 | 6317 | 3948 | 101 |
| H(18F) | 9372 | 7533 | 3380 | 101 |
| H(19D) | 11064 | 3459 | 3191 | 122 |
| H(19E) | 9515 | 3148 | 3563 | 122 |
| H(19F) | 10482 | 3489 | 4045 | 122 |
| H(22) | 2741 | 9025 | 589 | 73 |
| H(23) | 5000 | 7915 | -300 | 71 |
| H(24) | 7554 | 7189 | -86 | 71 |
| H(26) | 2819 | 10010 | 2355 | 67 |
| H(27A) | 490 | 12134 | 2086 | 128 |
| H(27B) | 1008 | 11651 | 1270 | 128 |
| H(27C) | 2075 | 12218 | 1587 | 128 |
| H(28A) | 397 | 9706 | 2562 | 161 |
| H(28B) | 1937 | 8077 | 2428 | 161 |
| H(28C) | 954 | 8931 | 1803 | 161 |
| H(29) | 8458 | 7613 | 1576 | 61 |
| H(30A) | 8564 | 5083 | 1588 | 105 |
| H(30B) | 10325 | 5031 | 1331 | 105 |
| H(30C) | 9387 | 4969 | 754 | 105 |
| H(31A) | 9138 | 8865 | 467 | 113 |
| H(31B) | 9741 | 7295 | 65 | 113 |
| H(31C) | 10679 | 7358 | 641 | 113 |
| H(26') | 2764 | 9545 | 2415 | 61 |
| H(27D) | 1952 | 11814 | 1640 | 135 |
| H(27E) | 409 | 11614 | 2120 | 135 |
| H(27F) | 997 | 11152 | 1299 | 135 |
| H(28D) | 2215 | 7424 | 2263 | 164 |
| H(28E) | 1159 | 8450 | 1682 | 164 |
| H(28F) | 571 | 8912 | 2503 | 164 |
| H(29') | 8349 | 8027 | 1538 | 63 |
| H(30D) | 10615 | 5657 | 1249 | 129 |
| H(30E) | 9742 | 5316 | 720 | 129 |
| H(30F) | 9029 | 5375 | 1565 | 129 |
| H(31D) | 10495 | 8096 | 635 | 122 |
| H(31E) | 8836 | 9473 | 492 | 122 |
| H(31F) | 9663 | 7948 | 34 | 122 |

Table 6. Torsion angles [deg] for K1179.

| | |
|---|---|
| C(5)-Cu-C(1)-C(2) | 23(3) |
| Cu-C(1)-C(2)-C(3) | 103.0(7) |
| Cu-C(1)-C(2)-C(4) | -73.2(8) |
| C(5)-Cu'-C(1')-C(2') | -50.8(18) |
| Cu'-C(1')-C(2')-C(3') | -104.9(7) |
| Cu'-C(1')-C(2')-C(4') | 70.8(8) |
| C(6)-N(1)-C(5)-N(2) | -0.1(3) |
| C(8)-N(1)-C(5)-N(2) | 177.5(2) |
| C(6)-N(1)-C(5)-Cu' | -176.63(19) |
| C(8)-N(1)-C(5)-Cu' | 1.0(4) |
| C(6)-N(1)-C(5)-Cu | 169.70(19) |
| C(8)-N(1)-C(5)-Cu | -12.7(4) |
| C(7)-N(2)-C(5)-N(1) | -0.1(3) |
| C(20)-N(2)-C(5)-N(1) | 177.8(2) |
| C(7)-N(2)-C(5)-Cu' | 176.70(18) |
| C(20)-N(2)-C(5)-Cu' | -5.4(3) |
| C(7)-N(2)-C(5)-Cu | -170.55(18) |
| C(20)-N(2)-C(5)-Cu | 7.4(3) |
| C(1')-Cu'-C(5)-N(1) | -129.0(15) |
| C(1')-Cu'-C(5)-N(2) | 55.1(15) |
| C(1')-Cu'-C(5)-Cu | -42.2(15) |
| C(1)-Cu-C(5)-N(1) | 166(2) |
| C(1)-Cu-C(5)-N(2) | -26(3) |
| C(1)-Cu-C(5)-Cu' | 64(3) |
| C(5)-N(1)-C(6)-C(7) | 0.3(3) |
| C(8)-N(1)-C(6)-C(7) | -177.2(2) |
| N(1)-C(6)-C(7)-N(2) | -0.4(3) |
| C(5)-N(2)-C(7)-C(6) | 0.3(3) |
| C(20)-N(2)-C(7)-C(6) | -177.5(2) |
| C(5)-N(1)-C(8)-C(13) | 78.7(3) |
| C(6)-N(1)-C(8)-C(13) | -104.1(3) |
| C(5)-N(1)-C(8)-C(9) | -100.6(3) |
| C(6)-N(1)-C(8)-C(9) | 76.6(3) |
| C(13)-C(8)-C(9)-C(10) | -0.5(4) |
| N(1)-C(8)-C(9)-C(10) | 178.8(2) |
| C(13)-C(8)-C(9)-C(14) | -178.6(2) |
| N(1)-C(8)-C(9)-C(14) | 0.7(4) |
| C(8)-C(9)-C(10)-C(11) | 0.2(4) |
| C(14)-C(9)-C(10)-C(11) | 178.3(3) |
| C(9)-C(10)-C(11)-C(12) | 0.5(5) |
| C(10)-C(11)-C(12)-C(13) | -0.9(5) |
| C(11)-C(12)-C(13)-C(8) | 0.6(4) |
| C(11)-C(12)-C(13)-C(17) | 179.0(4) |
| C(11)-C(12)-C(13)-C(17') | 178.0(4) |
| C(9)-C(8)-C(13)-C(12) | 0.2(4) |
| N(1)-C(8)-C(13)-C(12) | -179.1(2) |
| C(9)-C(8)-C(13)-C(17) | -178.3(3) |
| N(1)-C(8)-C(13)-C(17) | 2.4(4) |
| C(9)-C(8)-C(13)-C(17') | -177.1(4) |
| N(1)-C(8)-C(13)-C(17') | 3.6(5) |
| C(10)-C(9)-C(14)-C(15) | -82.4(4) |
| C(8)-C(9)-C(14)-C(15) | 95.6(3) |
| C(10)-C(9)-C(14)-C(16) | 43.3(4) |
| C(8)-C(9)-C(14)-C(16) | -138.7(3) |
| C(12)-C(13)-C(17)-C(19) | 59.6(5) |
| C(8)-C(13)-C(17)-C(19) | -122.0(4) |
| C(17')-C(13)-C(17)-C(19) | 74(6) |
| C(12)-C(13)-C(17)-C(18) | -62.4(5) |
| C(8)-C(13)-C(17)-C(18) | 115.9(4) |
| C(17')-C(13)-C(17)-C(18) | -48(6) |
| C(12)-C(13)-C(17')-C(18') | -93.6(5) |
| C(8)-C(13)-C(17')-C(18') | 83.6(5) |
| C(17)-C(13)-C(17')-C(18') | 100(7) |
| C(12)-C(13)-C(17')-C(19') | 32.1(6) |
| C(8)-C(13)-C(17')-C(19') | -150.7(4) |
| C(17)-C(13)-C(17')-C(19') | -134(7) |
| C(5)-N(2)-C(20)-C(25) | -93.4(3) |
| C(7)-N(2)-C(20)-C(25) | 84.2(3) |
| C(5)-N(2)-C(20)-C(21) | 85.2(3) |

| | |
|---|---|
| C(7)-N(2)-C(20)-C(21) | -97.2(3) |
| C(25)-C(20)-C(21)-C(22) | 1.5(4) |
| N(2)-C(20)-C(21)-C(22) | -177.0(2) |
| C(25)-C(20)-C(21)-C(26') | 172.6(4) |
| N(2)-C(20)-C(21)-C(26') | -6.0(5) |
| C(25)-C(20)-C(21)-C(26) | -169.6(3) |
| N(2)-C(20)-C(21)-C(26) | 11.8(4) |
| C(20)-C(21)-C(22)-C(23) | -0.6(5) |
| C(26')-C(21)-C(22)-C(23) | -171.9(4) |
| C(26)-C(21)-C(22)-C(23) | 170.5(4) |
| C(21)-C(22)-C(23)-C(24) | -0.1(5) |
| C(22)-C(23)-C(24)-C(25) | -0.1(5) |
| C(21)-C(20)-C(25)-C(24) | -1.7(4) |
| N(2)-C(20)-C(25)-C(24) | 176.9(2) |
| C(21)-C(20)-C(25)-C(29) | -172.5(3) |
| N(2)-C(20)-C(25)-C(29) | 6.0(4) |
| C(21)-C(20)-C(25)-C(29') | 171.4(4) |
| N(2)-C(20)-C(25)-C(29') | -10.0(5) |
| C(23)-C(24)-C(25)-C(20) | 0.9(4) |
| C(23)-C(24)-C(25)-C(29) | 171.9(3) |
| C(23)-C(24)-C(25)-C(29') | -172.2(4) |
| C(20)-C(21)-C(26)-C(28) | -121.2(5) |
| C(22)-C(21)-C(26)-C(28) | 68.2(6) |
| C(26')-C(21)-C(26)-C(28) | -18.1(16) |
| C(20)-C(21)-C(26)-C(27) | 112.0(5) |
| C(22)-C(21)-C(26)-C(27) | -58.6(6) |
| C(26')-C(21)-C(26)-C(27) | -144.9(19) |
| C(20)-C(25)-C(29)-C(30) | 100.8(4) |
| C(24)-C(25)-C(29)-C(30) | -69.8(5) |
| C(29')-C(25)-C(29)-C(30) | -168.3(19) |
| C(20)-C(25)-C(29)-C(31) | -136.2(4) |
| C(24)-C(25)-C(29)-C(31) | 53.2(5) |
| C(29')-C(25)-C(29)-C(31) | -45.3(17) |
| C(20)-C(21)-C(26')-C(27') | 121.2(5) |
| C(22)-C(21)-C(26')-C(27') | -68.1(6) |
| C(26)-C(21)-C(26')-C(27') | 34.7(16) |
| C(20)-C(21)-C(26')-C(28') | -117.0(6) |
| C(22)-C(21)-C(26')-C(28') | 53.8(7) |
| C(26)-C(21)-C(26')-C(28') | 156.6(19) |
| C(20)-C(25)-C(29')-C(30') | 109.8(5) |
| C(24)-C(25)-C(29')-C(30') | -77.3(6) |
| C(29)-C(25)-C(29')-C(30') | 12.3(16) |
| C(20)-C(25)-C(29')-C(31') | -123.5(5) |
| C(24)-C(25)-C(29')-C(31') | 49.3(6) |
| C(29)-C(25)-C(29')-C(31') | 139(2) |