

Silver-Catalyzed Vinylcarbene Insertion into Si-H Bonds with Vinyl-N-Triftosylhydrazones Leading to Allylsilanes

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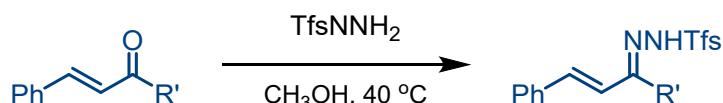
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I. General information.

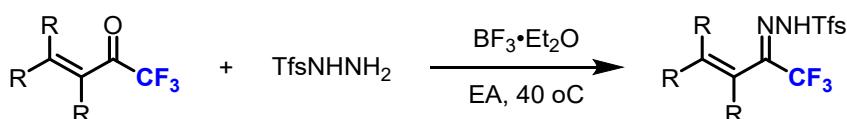
All reagents were purchased from commercial sources and used without purification unless otherwise mentioned. The products were purified by column chromatography over silica gel (300-400). NMR spectra were recorded on a Brüker Advance 600 (¹H: 600 MHz, ¹³C: 150 MHz) and Brüker Advance 500 (¹H: 500 MHz, ¹³C: 125 MHz, ¹⁹F: 471 MHz) at ambient temperature. Data were reported as chemical shifts in ppm relative to TMS (0.00 ppm) for ¹H and CDCl₃ (77.0 ppm) for ¹³C. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Mass spectra were recorded on BRUKER AutoflexIII Smartbeam MS-spectrometer. High-resolution mass spectra (HRMS) were recorded on Bruker microTof by using ESI method.

II. General Procedures for Synthesis of Vinyl-N-sulfonylhydrazones.



Vinyl-N-sulfonylhydrazones were prepared according to literature procedure. To a stirred solution of 2-(trifluoromethyl) benzenesulfonohydrazide (2.0 mmol, 1.0 equiv) in methanol (2 mL) were added carbonyl compounds (2.0 mmol, 1.0 equiv) and the mixture was stirred for 1-2 h at room temperature. If the hydrazone precipitated, the mixture was filtered and the resulting solid was washed with ice cold diethyl ether and dried under reduced pressure to give pure vinyl-N-sulfonylhydrazones. If not, the solvent was removed and the residue was purified by flash chromatography on silica gel to obtain the N-Sulfonylhydrazone. The yields were around 70%-90% in general. (Reference: Yang et al., the merger of vinyl-N-triftosylhydrazones and silver catalysis to enable stereoselective vinylcyclopropanation of alkenes. *Chem. Catal.* **2022**, 2, 563–577.)

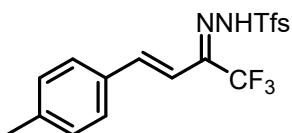
III. General procedures for the synthesis of trifluoromethyl vinyl-N- sulfonylhydrazones.



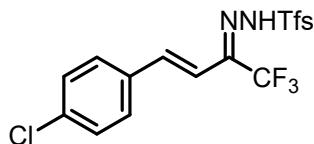
To a stirred solution of TfsNNH₂ (2.2 mmol, 1.1 equiv) in ethyl acetate (2.0 mL) were added carbonyl compounds (2.2 mmol, 1.1 equiv) and boron trifluoride etherate. The mixture was stirred at 40 °C for 5 h. After the complete consumption of ketones, the solvent was removed

under reduced pressure, and the resultant residue was purified by flash chromatography on silica gel to obtain the trifluoromethyl vinyl-*N*- sulfonylhydrazones (**Reference:** Zhang *et al.*, A Carbene Strategy for Progressive (Deutero)Hydrodefluorination of Fluoroalkyl Ketones. *Angew. Chem. Int. Ed.* **2023**, *61*, e202116190)

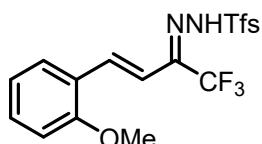
Part of select examples:



Yield 80 %. **¹H NMR** (500 MHz, DMSO) δ 12.76 (s, 1H), 8.18 (d, *J* = 7.5 Hz, 1H), 8.06 (d, *J* = 7.5 Hz, 1H), 7.99 (t, *J* = 7.5 Hz, 1H), 7.94 (t, *J* = 7.5 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 16.5 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 16.5 Hz, 1H), 2.37 (s, 3H). **¹³C NMR** (150 MHz, DMSO) δ 140.96, 139.13, 138.22 (q, *J* = 33.0 Hz), 137.61, 134.67, 134.01, 132.99, 132.28, 130.13, 129.16 (q, *J* = 5.5 Hz), 128.70, 127.12 (q, *J* = 32.8 Hz), 123.27 (q, *J* = 275.0 Hz), 121.11 (q, *J* = 275.5 Hz), 111.70, 60.34, 21.55, 14.60. **¹⁹F NMR** (565 MHz, DMSO) δ -56.46 (s, 3F), -64.18 (s, 3F). **HRMS** (ESI) m/z calculated C₁₈H₁₄F₆N₂NaO₂S [M+Na]⁺ 459.0572, found 459.0566.



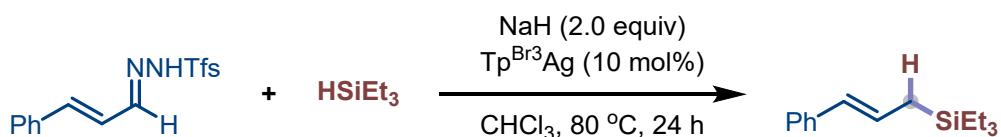
Yield 88 %. 189-190 °C. **¹H NMR** (500 MHz, DMSO) δ 12.72 (s, 1H), 8.13 (d, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.96-7.88 (m, 2H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 16.5 Hz, 1H), 7.12 (d, *J* = 16.5 Hz, 1H). **¹³C NMR** (125 MHz, DMSO) δ 141.5, 141.4 (q, *J* = 33.0 Hz) 141.3, 138.8, 138.5, 137.8, 136.3, 136.2, 134.4, 133.0 (q, *J* = 6.5 Hz), 131.0 (q, *J* = 33.0 Hz), 128.1, 126.4 (q, *J* = 272.5 Hz), 125.9, 117.3. **¹⁹F NMR** (470 MHz, DMSO) δ -56.47 (s, 3F), -64.25 (s, 3F). **HRMS** (ESI) m/z calculated C₁₇H₁₁ClF₆N₂NaO₂S [M+Na]⁺ 479.0026, found 479.0021.



Yield 72 %. **¹H NMR** (600 MHz, DMSO) δ 12.72 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 8.0

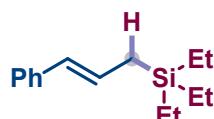
Hz, 1H), 7.96 (t, J = 7.5 Hz, 1H), 7.92 (t, J = 7.5 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 16.5 Hz, 1H), 7.44 (t, J = 8.0 Hz, 1H), 7.37 (d, J = 16.5 Hz, 1H), 7.09 (d, J = 8.0 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, DMSO) δ 157.85, 138.23 (q, J = 32.0 Hz), 137.47, 134.55, 133.92, 132.80, 132.49, 132.07, 129.05 (q, J = 6.5 Hz), 126.90 (q, J = 32.0 Hz) 127.17, 123.74, 123.11 (q, J = 274.0 Hz), 121.14, 121.01 (q, J = 276.0 Hz), 112.25, 112.07, 56.26. ^{19}F NMR (564 MHz, DMSO) δ -56.38 (s, 3F), -64.08 (s, 3F). HRMS (ESI) m/z calculated C₁₈H₁₄F₆N₂NaO₃S [M+Na]⁺ 475.0521, found 475.0526.

IV. General procedures for synthesis of allylsilanes.

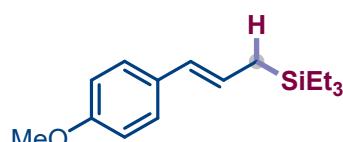


General procedure (with 3 as an example): In the glove box, a sealed tube was charged with alkynyl *N*-nosylhydrazone **1a** (0.3 mmol), NaH (14.0 mg, 60 wt.% dispersion in mineral oil, 1.2 equiv), **2a** (0.6 mmol, 2.0 equiv), Tp^{Br3}Ag (5 mol%) and dry CHCl₃ (5.0 mL). The resulting mixture was stirred at 80 °C for 24 h. When the reaction was completed, the reaction was allowed to cool to room temperature, and filtered through a short pad of silica gel with EtOAc as an eluent. After removal of the solvent under vacuum, the residue was purified by flash chromatography on silica gel (using PE and EA as eluent) to obtain the final product **3**.

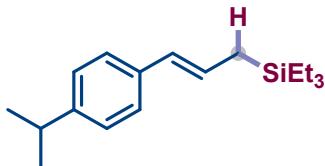
V. Characterization data of prepared compounds.



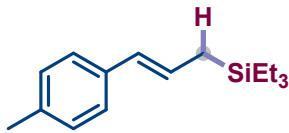
3. Colorless oil. ^1H NMR (500 MHz, CDCl₃) δ 7.30-7.24 (m, 4H), 7.16-7.12 (m, 1H), 6.26-6.23 (m, 2H), 1.71-1.69 (m 2H), 0.96 (t, J = 8.0 Hz, 9H), 0.57 (q, J = 8.0 Hz, 6H). ^{13}C NMR (125 MHz, CDCl₃) δ 138.6, 128.4, 128.1, 128.0, 126.1, 125.4, 18.8, 7.4, 3.2. HRMS (ESI) m/z calculated for C₁₅H₂₅Si [M+H]⁺ 233.1720, found 233.1721.



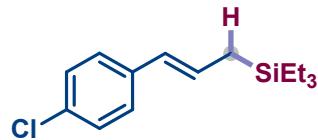
4. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.22 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 6.19 (d, *J* = 15.5 Hz, 1H), 6.12-6.06 (m, 1H), 3.79 (s, 3H), 1.68-1.66 (m, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.56 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 158.2, 131.5, 127.4, 126.5, 125.8, 113.9, 55.3, 18.6, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₆H₂₇OSi [M+H]⁺ 263.1826, found 263.1823.



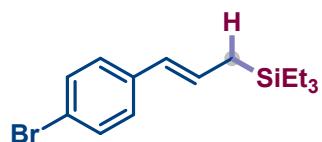
5. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.22 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.24-6.16 (m, 2H), 2.91-2.83 (m, 1H), 1.68 (d, *J* = 7.0 Hz, 2H), 1.23 (d, *J* = 7.0 Hz, 6H), 0.96 (t, *J* = 7.5Hz, 9H), 0.56 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 146.8, 136.2, 127.9, 127.0, 126.5, 125.4, 33.8, 24.0, 18.7, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₈H₃₀Si [M+H]⁺ 275.2190, found 275.2181.



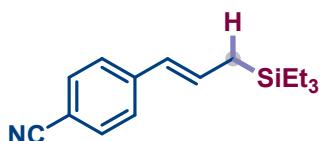
6. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.19 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.23-6.15 (m, 2H), 2.31 (s, 3H), 1.68 (d, *J* = 7.0 Hz, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.56 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 135.8, 129.1, 127.8, 126.9, 125.3, 21.1, 18.7, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₆H₂₆Si [M+H]⁺ 245.1731, found 275.1715.



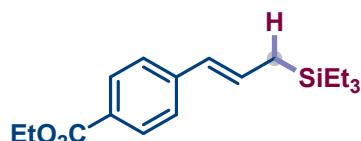
7. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.22-7.15 (m, 4H), 6.23-6.14 (m, 2H), 1.67 (d, *J* = 7.0 Hz, 2H), 0.93 (t, *J* = 8.0 Hz, 9H), 0.54 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 137.0, 131.6, 128.9, 128.5, 126.8, 126.6, 18.9, 7.3, 3.2. **HRMS** (ESI) m/z calculated for C₁₅H₂₂ClSi [M-H]⁻ 265.1185, found 265.1183.



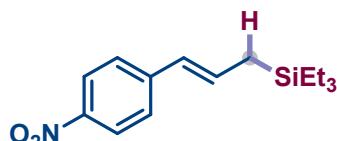
8. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.37 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 6.30-6.20 (m, 1H), 6.17 (d, *J* = 15.5 Hz, 1H), 1.69 (d, *J* = 7.5 Hz, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.56 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 137.4, 131.5, 129.1, 127.0, 126.8, 119.6, 19.0, 7.3, 3.2. **HRMS** (ESI) m/z calculated for C₁₅H₂₂BrSi [M-H]⁻ 309.0680, found 309.0653.



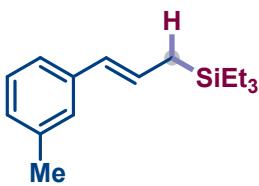
9. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.45-6.39 (m, 1H), 6.24 (d, *J* = 16.0 Hz, 1H), 1.76 (dd, *J* = 8.0, 1.0 Hz, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.57 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 142.9, 133.1, 132.3, 126.6, 125.8, 119.3, 109.1, 19.7, 7.3, 3.2. **HRMS** (ESI) m/z calculated for C₁₆H₂₂NSi [M-H]⁻ 256.1527, found 256.1503.



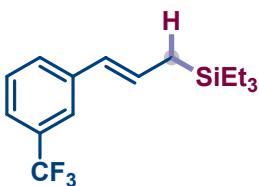
10. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.95 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 6.44-6.38 (m, 1H), 6.28 (d, *J* = 15.5 Hz, 1H), 4.36 (q, *J* = 7.0 Hz, 2H), 1.75 (dd, *J* = 8.5, 1.0 Hz, 2H), 1.39 (t, *J* = 7.0 Hz, 3H), 0.97 (t, *J* = 8.0 Hz, 9H), 0.58 (q, *J* = 7.5 Hz, 6H). **¹³C NMR** (125MHz, CDCl₃) δ 166.6, 142.9, 131.4, 129.8, 127.9, 127.3, 125.1, 60.7, 19.4, 14.3, 7.3, 3.2. **HRMS** (ESI) m/z calculated for C₁₈H₂₉O₂Si [M+H]⁻ 305.1931, found 305.1909.



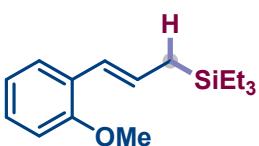
11. Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 8.13 (d, *J* = 9.0 Hz, 2H), 7.38 (d, *J* = 9.0 Hz, 2H), 6.53-6.48 (m, 1H), 6.30 (d, *J* = 15.6 Hz, 1H), 1.80 (d, *J* = 9.0 Hz, 2H), 0.97 (t, *J* = 7.8 Hz, 9H), 0.59 (q, *J* = 7.8 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 145.9, 145.0, 134.4, 126.2, 125.6, 124.0, 20.0, 7.3, 3.3. **HRMS** (ESI) m/z calculated for C₁₅H₂₄NO₂Si [M+H]⁻ 278.1576, found 278.1580.



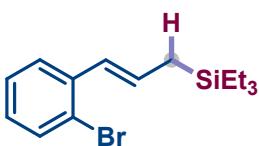
12. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.16 (t, *J* = 7.0 Hz, 1H), 7.12-7.04 (m, 2H), 6.96 (d, *J* = 7.0 Hz, 1H), 6.27-6.19 (m, 2H), 2.32 (s, 3H), 1.70-1.68 (m, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.57 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.5, 137.9, 128.3, 128.1, 127.8, 126.9, 126.2, 122.6, 21.4, 18.8, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₆H₂₅Si [M-H]⁻ 245.1731, found 245.1715.



13. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.51 (s, 1H), 7.46 (d, *J* = 7.0 Hz, 1H), 7.41-7.36 (m, 2H), 6.41-6.30 (m, 1H), 6.27 (d, *J* = 16.0 Hz, 1H), 1.74 (d, *J* = 7.5 Hz, 2H), 0.98 (t, *J* = 8.0 Hz, 9H), 0.59 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 139.3, 130.8 (q, *J* = 30.0 Hz), 130.4, 128.8, 128.4, 126.8, 124.3 (q, *J* = 270.0 Hz), 122.7 (q, *J* = 4.5 Hz), 122.1 (q, *J* = 4.5 Hz), 19.1, 7.3, 3.2. **¹⁹F NMR** (564 MHz, CDCl₃). δ -62.8 (s). **HRMS** (ESI) m/z calculated for C₁₆H₂₄F₃Si [M+H]⁺ 301.1599, found 301.1593.



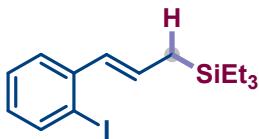
14. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.35 (d, *J* = 7.5 Hz, 1H), 7.16-7.13 (m, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 1H), 6.55 (d, *J* = 16.0 Hz, 1H), 6.26-6.19 (m, 1H), 3.83 (s, 3H), 1.73 (d, *J* = 8.5 Hz, 2H), 0.97 (t, *J* = 8.0 Hz, 9H), 0.57 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 156.0, 128.8, 127.8, 127.1, 126.0, 122.6, 120.6, 110.8, 55.5, 19.3, 7.4, 3.3. **HRMS** (ESI) m/z calculated for C₁₆H₂₅OSi [M-H]⁻ 261.1680, found 261.1655.



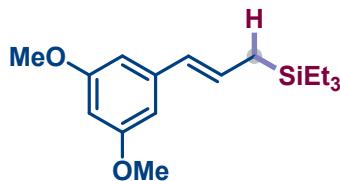
15. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.51 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.43 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.04-7.00 (m, 1H), 6.58 (d, *J* = 16.0 Hz, 1H), 6.23-6.16 (m, 1H), 1.78 (dd, *J* = 8.5, 1.0 Hz, 2H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.60 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.3, 132.7, 131.4, 127.5, 127.3, 127.0, 126.5, 122.7, 19.2, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₅H₂₂BrSi [M-H]⁻ 309.0680, found 309.0652.



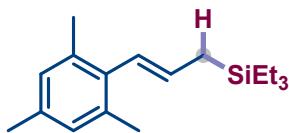
16. Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.85 (d, *J* = 8.4 Hz, 1H), 7.54-7.48 (m, 2H), 7.30-7.26 (m, 1H), 6.70 (d, *J* = 15.0 Hz, 1H), 6.32-6.27 (m, 1H), 1.80 (d, *J* = 8.4 Hz, 2H), 0.98 (t, *J* = 7.8 Hz, 9H), 0.60 (q, *J* = 7.8 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 147.3, 134.5, 133.8, 132.7, 127.9, 126.6, 124.4, 122.8, 19.8, 7.3, 3.2. **HRMS** (ESI) m/z calculated for C₁₅H₂₄NO₂Si [M-H]⁻ 278.1576, found 278.1581.



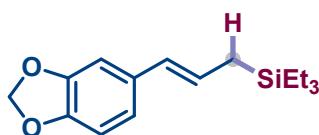
17. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.79 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.37 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.25 (t, *J* = 8.0 Hz, 1H), 6.86-6.83 (m, 1H), 6.41 (d, *J* = 15.0 Hz, 1H), 6.14-5.99 (m, 1H), 1.76 (dd, *J* = 8.5, 1.0 Hz, 2H), 0.98 (t, *J* = 8.0 Hz, 9H), 0.60 (q, *J* = 8.0, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 141.6, 139.3, 131.9, 131.6, 128.2, 127.7, 126.0, 99.1, 19.0, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₅H₂₂ISi [M-H]⁻ 357.0541, found 357.0510.



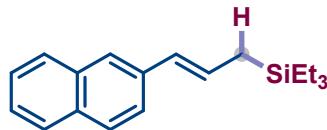
18. Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 6.46 (d, *J* = 2.4 Hz, 2H), 6.30 (t, *J* = 2.4 Hz, 1H), 6.26-6.21 (m, 1H), 6.17 (d, *J* = 15.6 Hz, 1H), 3.79 (s, 6H), 1.69 (d, *J* = 8.0 Hz, 2H), 0.96 (t, *J* = 7.8 Hz, 9H), 0.57 (q, *J* = 7.8 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 160.8, 140.6, 128.8, 127.9, 103.7, 98.3, 55.3, 18.8, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₇H₂₉O₂Si [M+H]⁻ 293.1931, found 293.1910.



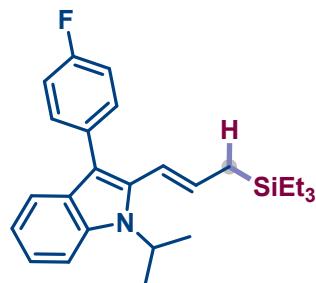
19. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 6.85 (s, 2H), 6.15 (d, *J* = 16.0 Hz, 1H), 5.68-5.61 (m, 1H), 2.27 (s, 6H), 2.25 (s, 3H), 1.71 (dd, *J* = 8.0, 1.0 Hz, 2H), 0.97 (t, *J* = 8.0 Hz, 9H), 0.58 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 135.8, 135.3, 135.2, 131.9, 128.4, 125.6, 21.1, 20.8, 18.8, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₈H₂₉Si [M-H]⁻ 273.2044, found 273.2023.



20. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 6.85 (s, 1H), 6.78-6.66 (m, 2H), 6.16 (d, *J* = 16.0 Hz, 1H), 6.09-6.03 (m, 1H), 5.92 (s, 2H), 1.66 (d, *J* = 8.0 Hz, 2H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.56 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 147.9, 146.0, 133.2, 127.6, 126.3, 119.5, 108.2, 105.0, 100.8, 18.6, 7.4, 3.2. **HRMS** (ESI) m/z calculated for C₁₆H₂₅O₂Si [M+H]⁻ 277.1618, found 277.1601.

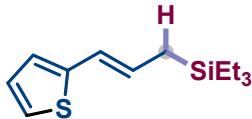


21. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.81-7.70 (m, 3H), 7.60 (s, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.43-7.36 (m, 2H), 6.43-6.38 (m, 2H), 1.76 (d, *J* = 7.0 Hz, 2H), 0.98 (t, *J* = 8.0 Hz, 9H), 0.59 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 136.0, 133.8, 132.3, 128.6, 128.2, 128.0, 127.7, 127.6, 126.0, 125.1, 124.4, 123.4, 19.1, 7.4, 3.3. **HRMS** (ESI) m/z calculated for C₁₉H₂₅Si [M-H]⁻ 281.1731, found 281.1706.



22. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.55-7.46 (m, 2H), 7.44-7.36 (m, 2H), 7.16-7.13 (m, 1H), 7.10-7.03 (m, 3H), 6.22 (d, *J* = 16.0 Hz, 1H), 5.80-5.73 (m, 1H), 4.89-4.83 (m, 1H), 1.68-1.62 (m,

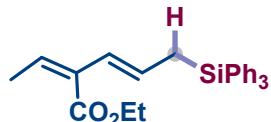
8H), 0.90 (t, J = 8.0 Hz, 9H), 0.46 (q, J = 8.0 Hz, 6H). **^{13}C NMR** (125 MHz, CDCl_3) δ 161.3 (d, J = 242.5 Hz), 136.3, 135.4, 134.5, 132.1 (d, J = 3.3 Hz), 132.0 (d, J = 8.8 Hz), 128.6, 121.1, 119.3, 119.1, 117.3, 115.1 (d, J = 20.3 Hz), 113.2, 111.6, 47.5, 21.6, 19.6, 7.3, 3.2. **^{19}F NMR** (470 MHz, CDCl_3) δ -117.4--117.5 (m). **HRMS** (ESI) m/z calculated for $\text{C}_{26}\text{H}_{35}\text{FNSi}$ [M+H]⁻ 408.2523, found 408.2529.



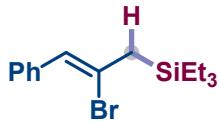
23. Colorless oil. **^1H NMR** (500 MHz, CDCl_3) δ 7.24-7.22 (m, 1H), 7.16-7.15 (m, 1H), 6.96 (d, J = 2.0 Hz, 1H), 6.27 (d, J = 15.5 Hz, 1H), 6.13-6.07 (m, 1H), 1.66 (dd, J = 7.5, 1.0 Hz, 2H), 0.97 (t, J = 8.0 Hz, 9H), 0.57 (q, J = 8.0 Hz, 6H). **^{13}C NMR** (125 MHz, CDCl_3) δ 141.0, 128.0, 125.5, 124.8, 122.5, 118.9, 18.5, 7.4, 3.2. **HRMS** (ESI) m/z calculated for $\text{C}_{13}\text{H}_{23}\text{SSi}$ [M+H]⁻ 239.1284, found 239.1270.



24. Colorless oil. **^1H NMR** (500 MHz, CDCl_3) δ 7.28-7.23 (m, 4H), 7.21-7.17 (m, 1H), 5.66-5.60 (m, 1H), 5.42-5.36 (m, 1H), 4.40 (s, 2H), 3.88 (d, J = 6.0 Hz, 2H), 1.47 (d, J = 8.0 Hz, 2H), 0.86 (t, J = 8.0 Hz, 9H), 0.46 (q, J = 8.0 Hz, 6H). **^{13}C NMR** (125 MHz, CDCl_3) δ 138.6, 132.0, 128.3, 127.7, 127.4, 124.5, 71.3, 71.2, 17.6, 7.3, 3.1. **HRMS** (ESI) m/z calculated for $\text{C}_{17}\text{H}_{27}\text{OSi}$ [M-H]⁻ 277.1982, found 277.1963.



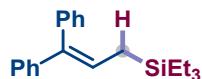
25. Colorless oil. **^1H NMR** (500 MHz, CDCl_3) δ 7.50-7.48 (m, 6H), 7.42-7.39 (m, 3H), 7.37-7.32 (m, 6H), 6.20-6.14 (m, 1H), 5.98 (d, J = 15.5 Hz, 1H), 5.54 (s, 1H), 4.12 (q, J = 7.2 Hz, 2H), 2.50 (d, J = 8.0 Hz, 2H), 2.15 (s, 3H), 1.25 (t, J = 7.2 Hz, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 167.3, 152.6, 135.6, 133.9, 133.8, 133.2, 129.7, 127.9, 116.6, 59.5, 21.0, 14.3, 13.7. **HRMS** (ESI) m/z calculated for $\text{C}_{27}\text{H}_{27}\text{O}_2\text{Si}$ [M-H]⁻ 411.1786, found 411.1748.



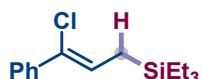
26. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.41 (d, *J* = 7.5 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 7.0 Hz, 1H), 6.46 (s, 1H), 2.22 (s, 2H), 0.91 (t, *J* = 8.0 Hz, 9H), 0.59 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 136.9, 128.7, 128.0, 127.0, 124.9, 30.1, 7.3, 3.5. **HRMS** (ESI) m/z calculated for C₁₅H₂₄BrSi [M+H]⁻ 311.0825, found 311.0868.



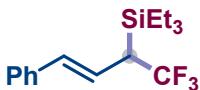
27. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.53 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.23-7.20 (m, 1H), 6.30 (s, 1H), 2.08 (s, 2H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.67 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 135.9, 133.4, 128.7, 128.1, 126.8, 121.9, 27.7, 7.3, 3.5. **HRMS** (ESI) m/z calculated for C₁₅H₂₂ClSi [M-H]⁻ 265.1185, found 265.1183.



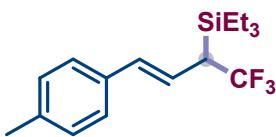
28. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.36 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 7.25-7.22 (m, 2H), 7.20-7.15 (m, 5H), 6.15 (t, *J* = 9.0 Hz, 1H), 1.68 (d, *J* = 9.0 Hz, 2H), 0.87 (t, *J* = 8.0 Hz, 9H), 0.52 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 143.5, 140.5, 139.3, 130.3, 128.2, 128.0, 126.9, 126.7, 126.5, 126.3, 15.9, 7.3, 3.4. **HRMS** (ESI) m/z calculated for C₂₁H₂₇Si [M-H]⁻ 309.2033, found 309.2013.



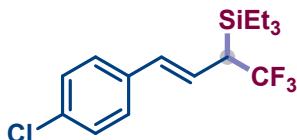
29. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.54-7.53 (m, 2H), 7.33 (t, *J* = 7.0 Hz, 2H), 7.28-7.25 (m, 1H), 6.21 (t, *J* = 8.5 Hz, 1H), 1.92 (d, *J* = 9.0 Hz, 2H), 1.00 (t, *J* = 8.0 Hz, 9H), 0.62 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.8, 129.7, 128.2, 127.6, 126.0, 125.3, 16.7, 7.4, 3.6. **HRMS** (ESI) m/z calculated for C₁₅H₂₂ClSi [M-H]⁻ 265.1185, found 265.1183.



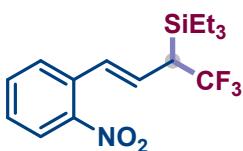
30. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.35-7.29 (m, 4H), 7.24-7.21 (m, 1H), 6.40 (d, *J* = 15.5 Hz, 1H), 6.11 (dd, *J* = 15.5, 10.5 Hz, 1H), 2.75-2.65 (m, 1H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.71 (q, *J* = 8.0 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 137.0, 132.5, 128.6, 128.3 (q, *J* = 275.0 Hz), 127.5, 126.1, 121.5 (q, *J* = 4.2 Hz), 38.5 (q, *J* = 28.0 Hz), 7.1, 2.7. **¹⁹F NMR** (470 MHz, CDCl₃) δ -59.0 (d, *J* = 11.5 Hz). **HRMS** (ESI) m/z calculated for C₁₆H₂₄F₃Si [M+H]⁻ 301.4482, found 301.4488.



31. Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.24 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.36 (d, *J* = 15.6 Hz, 1H), 6.05 (dd, *J* = 15.6, 10.8 Hz, 1H), 2.71-2.63 (m, 1H), 2.33 (s, 3H), 0.98 (t, *J* = 7.8 Hz, 9H), 0.70 (q, *J* = 7.8 Hz, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 137.3, 134.2, 132.4, 129.3, 128.3 (q, *J* = 275.0 Hz), 126.0, 120.4 (q, *J* = 4.5 Hz), 38.4 (q, *J* = 28.5 Hz), 21.1, 7.1, 2.7. **¹⁹F NMR** (565 MHz, CDCl₃) δ -59.0 (d, *J* = 13.0 Hz). **HRMS** (ESI) m/z calculated for C₁₇H₂₄F₃Si [M-H]⁻ 313.1605, found 313.1620.

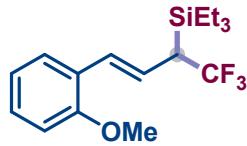


32. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.29-7.24 (m, 4H), 6.35 (d, *J* = 16.0 Hz, 1H), 6.09 (dd, *J* = 16.0, 10.5 Hz, 1H), 2.74-2.65 (m, 1H), 0.98 (t, *J* = 7.5 Hz, 9H), 0.70 (q, *J* = 7.5 Hz, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 135.4, 133.1, 131.2, 128.8, 128.2 (q, *J* = 275.0 Hz), 127.3, 122.4 (q, *J* = 4.5 Hz), 38.6 (q, *J* = 28.4 Hz), 7.1, 2.7. **¹⁹F NMR** (470 MHz, CDCl₃) δ -59.0 (d, *J* = 12.5 Hz). **HRMS** (ESI) m/z calculated for C₁₆H₂₃F₃ClSi [M+H]⁻ 335.1210, found 335.1217.

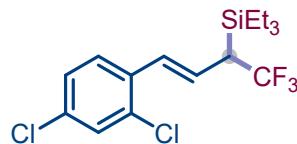


33. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.95 (d, *J* = 8.5 Hz, 1H), 7.59-7.56 (m, 2H), 7.42-7.38 (m, 1H), 6.91 (d, *J* = 15.5 Hz, 1H), 6.13 (dd, *J* = 15.5, 10.5 Hz, 1H), 2.87-2.78 (m, 1H), 1.01 (t, *J* = 8.0 Hz, 9H).

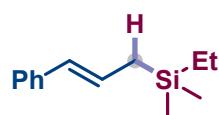
Hz, 9H), 0.74 (q, $J = 8.0$ Hz, 6H). **^{13}C NMR** (125 MHz, CDCl_3) δ 147.5, 133.2, 132.6, 128.5, 128.039 (q, $J = 278.0$ Hz), 128.038, 127.7, 127.3 (q, $J = 4.2$ Hz), 124.6, 38.9 (q, $J = 28.0$ Hz), 7.1, 2.6. **^{19}F NMR** (470 MHz, CDCl_3) δ -58.8 (d, $J = 11.0$ Hz). **HRMS** (ESI) m/z calculated for $\text{C}_{16}\text{H}_{21}\text{F}_3\text{NO}_2\text{Si}$ [M-H]⁻ 344.1299, found 344.1267.



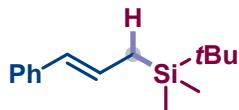
34. Colorless oil. **^1H NMR** (500 MHz, CDCl_3) δ 7.38 (dd, $J = 7.5, 1.0$ Hz, 1H), 7.24-7.19 (m, 1H), 6.92 (t, $J = 7.0$ Hz, 1H), 6.86 (d, $J = 7.5$ Hz, 1H), 6.70 (d, $J = 16.0$ Hz, 1H), 6.13 (dd, $J = 16.0, 10.5$ Hz, 1H), 3.83 (s, 3H), 2.77-2.68 (m, 1H), 0.99 (t, $J = 8.0$ Hz, 9H), 0.71 (q, $J = 8.0$ Hz, 6H). **^{13}C NMR** (150 MHz, CDCl_3) δ 156.5, 128.44, 128.41 (q, $J = 277.0$ Hz), 127.5, 126.5, 126.1, 121.9 (q, $J = 4.0$ Hz), 120.6, 110.9, 55.4, 38.9 (q, $J = 28.5$ Hz), 7.1, 2.7. **^{19}F NMR** (565 MHz, CDCl_3) δ -59.0 (d, $J = 12.4$ Hz). **HRMS** (ESI) m/z calculated for $\text{C}_{17}\text{H}_{25}\text{F}_3\text{OSi}$ [M-H]⁻ 329.1554, found 329.1525.



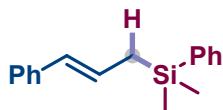
35. Colorless oil. **^1H NMR** (600 MHz, CDCl_3) δ 7.39 (d, $J = 8.4$ Hz, 1H), 7.36 (d, $J = 1.8$ Hz, 1H), 7.19 (dd, $J = 8.4, 1.8$ Hz, 1H), 6.70 (d, $J = 15.6$ Hz, 1H), 6.08 (dd, $J = 15.6, 10.4$ Hz, 1H), 2.86-2.73 (m, 1H), 0.99 (t, $J = 7.8$ Hz, 9H), 0.72 (q, $J = 7.8$ Hz, 6H). **^{13}C NMR** (150 MHz, CDCl_3) δ 133.8, 133.5, 133.3, 129.4, 128.1 (q, $J = 274.5$ Hz), 127.7, 127.4, 127.3, 125.2 (q, $J = 4.5$ Hz), 38.9 (q, $J = 28.5$ Hz), 7.1, 2.7. **^{19}F NMR** (565 MHz, CDCl_3) δ -58.9 (d, $J = 12.5$ Hz). **HRMS** (ESI) m/z calculated for $\text{C}_{16}\text{H}_{22}\text{F}_3\text{Cl}_2\text{Si}$ [M+H]⁻ 369.0820, found 369.0825.



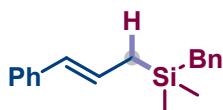
36. Colorless oil. **^1H NMR** (500 MHz, CDCl_3) δ 7.43-7.34 (m, 4H), 7.26 (t, $J = 7.0$ Hz, 1H), 6.40-6.30 (m, 2H), 1.78 (d, $J = 6.5$ Hz, 2H), 1.06 (t, $J = 8.0$ Hz, 3H), 0.65 (q, $J = 8.0$ Hz, 2H), 0.12 (s, 6H). **^{13}C NMR** (125 MHz, CDCl_3) δ 138.5, 128.4, 128.1, 127.9, 126.2, 125.5, 22.2, 7.3, 6.7, -4.1. **HRMS** (ESI) m/z calculated for $\text{C}_{13}\text{H}_{21}\text{Si}$ [M+H]⁻ 205.1413, found 205.1420.



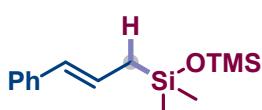
37. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.44-7.39 (m, 4H), 7.28 (t, *J* = 7.0 Hz, 1H), 6.42-6.35 (m, 2H), 1.84-1.80 (m, 2H), 1.05 (s, 9H), 0.12 (s, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 135.8, 128.4, 128.3, 128.2, 126.1, 125.5, 26.6, 20.0, 16.8, -6.4. **HRMS** (ESI) m/z calculated for C₁₅H₂₃Si [M-H]⁻ 234.1575, found 234.1551.



38. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.58-7.56 (m, 2H), 7.42-7.39 (m, 3H), 7.33-7.27 (m, 4H), 7.22-7.17 (m, 1H), 6.30-6.22 (m, 2H), 1.94 (d, *J* = 6.5 Hz, 2H), 0.36 (s, 6H). **¹³C NMR** (150 MHz, CDCl₃) δ 138.5, 138.4, 133.6, 129.1, 128.9, 128.4, 127.8, 127.1, 126.3, 125.5, 23.0, -3.3. **HRMS** (ESI) m/z calculated for C₁₇H₂₁Si [M+H]⁻ 253.1413, found 253.1419.



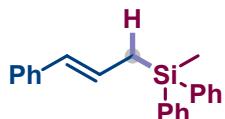
39. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.39-7.35 (m, 4H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.27-7.24 (m, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 2H), 6.34-6.24 (m, 2H), 2.24 (s, 2H), 1.77 (d, *J* = 7.5 Hz, 2H), 0.12 (s, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 139.8, 138.3, 128.7, 128.4, 128.2, 128.1, 127.1, 126.3, 125.5, 124.1, 25.3, 22.0, -3.8. **HRMS** (ESI) m/z calculated for C₁₈H₂₁Si [M-H]⁻ 265.1418, found 265.1456.



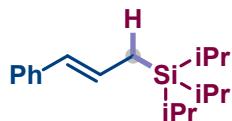
40. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.23-7.17 (m, 4H), 7.09-7.05 (m, 1H), 6.20-6.15 (m, 2H), 1.63-1.61 (m, 2H), 0.03 (s, 6H), 0.00 (s, 9H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.5, 128.8, 128.4, 126.9, 126.2, 125.5, 25.6, 2.0, 0.1. **HRMS** (ESI) m/z calculated for C₁₄H₂₅OSi₂ [M+H]⁻ 265.1444, found 265.1438.



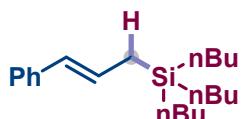
41. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.34-7.29 (m, 4H), 7.20-7.17 (m, 1H), 6.37-6.20 (m, 2H), 1.68 (d, *J* = 7.5 Hz, 2H), 0.14 (s, 18H), 0.10 (s, 3H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.4, 129.2, 128.4, 126.5, 126.2, 125.5, 24.8, 1.9, -0.6. **HRMS** (ESI) m/z calculated for C₁₆H₂₉O₂Si₃ [M-H]- 337.1481, found 337.1448.



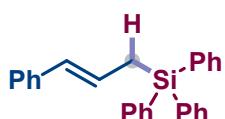
42. Colorless oil. **¹H NMR** (600 MHz, CDCl₃) δ 7.56-7.51 (m, 4H), 7.39-7.33 (m, 6H), 7.24-7.21 (m, 4H), 7.15-7.11 (m, 1H), 6.28-6.18 (m, 2H), 2.21 (d, *J* = 7.2 Hz, 2H), 0.58 (s, 3H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.2, 136.4, 134.5, 129.6, 129.4, 128.4, 127.9, 126.5, 126.4, 125.6, 21.4, -4.6. **HRMS** (ESI) m/z calculated for C₂₂H₂₁Si [M-H]- 313.1418, found 313.1391.



43. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.29-7.25 (m, 4H), 7.16-7.13 (m, 1H), 6.30-6.26 (m, 2H), 1.81-1.78 (m, 2H), 1.10-1.05 (m, 21H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.6, 128.7, 128.4, 128.1, 126.1, 125.4, 18.7, 16.7, 11.1. **HRMS** (ESI) m/z calculated for C₁₈H₃₀Si [M-H]- 330.0723, found 330.0724. **HRMS** (ESI) m/z calculated for C₁₈H₂₉Si [M-H]- 273.2044, found 273.2050.



44. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.29-7.25 (m, 4H), 7.16-7.12 (m, 1H), 6.24-6.22 (m, 2H), 1.72-1.65 (m, 2H), 1.35-1.28 (m, 12H), 0.88 (t, *J* = 7.0 Hz, 9H), 0.58-0.54 (m, 6H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.6, 128.4, 128.2, 128.1, 126.1, 125.4, 26.8, 26.1, 19.9, 13.8, 12.0. **HRMS** (ESI) m/z calculated for C₂₁H₃₅Si [M-H]- 315.2514, found 315.2485.

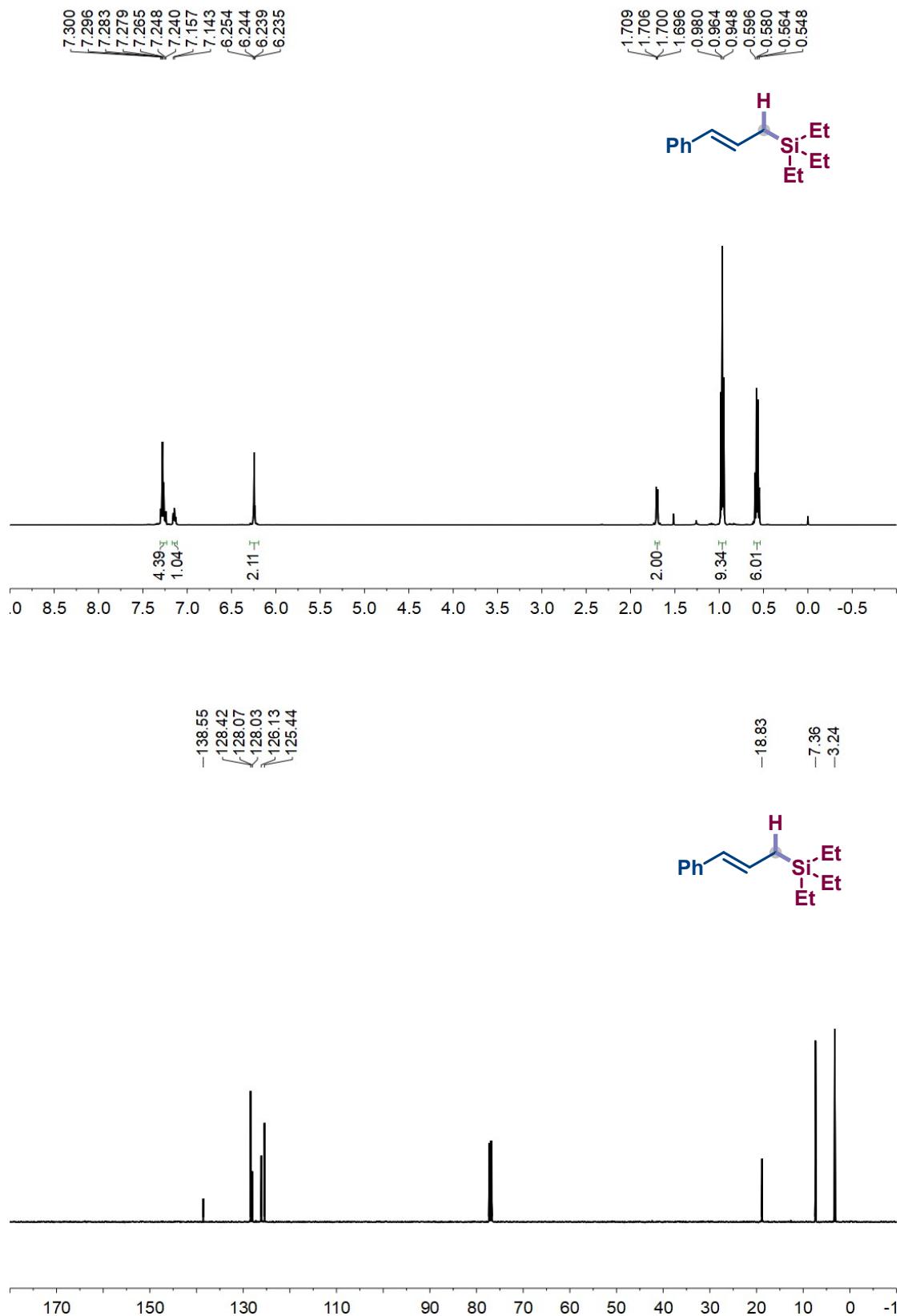


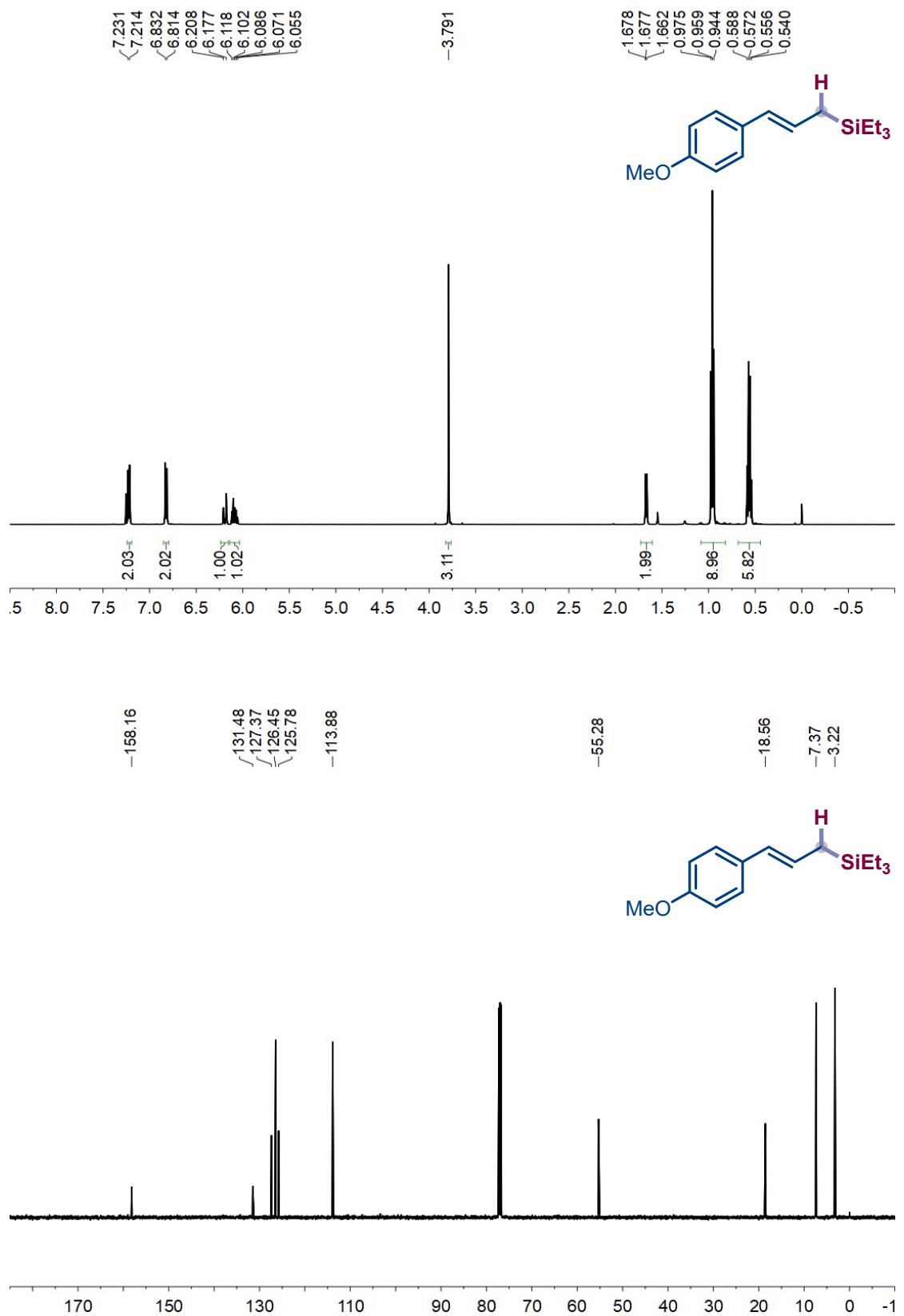
45. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.56-7.51 (m, 6H), 7.43-7.38 (m, 3H), 7.37-7.32 (m, 6H), 7.24-7.16 (m, 4H), 7.14-7.10 (m, 1H), 6.29-6.22 (m, 2H), 2.55-2.52 (m, 2H). **¹³C NMR** (125 MHz, CDCl₃) δ 138.2, 135.7, 134.4, 130.3, 129.6, 128.4, 127.9, 126.4, 126.1, 125.6, 20.4. **HRMS** (ESI) m/z calculated for C₂₇H₂₃Si [M-H]⁻ 375.1575, found 375.1543.

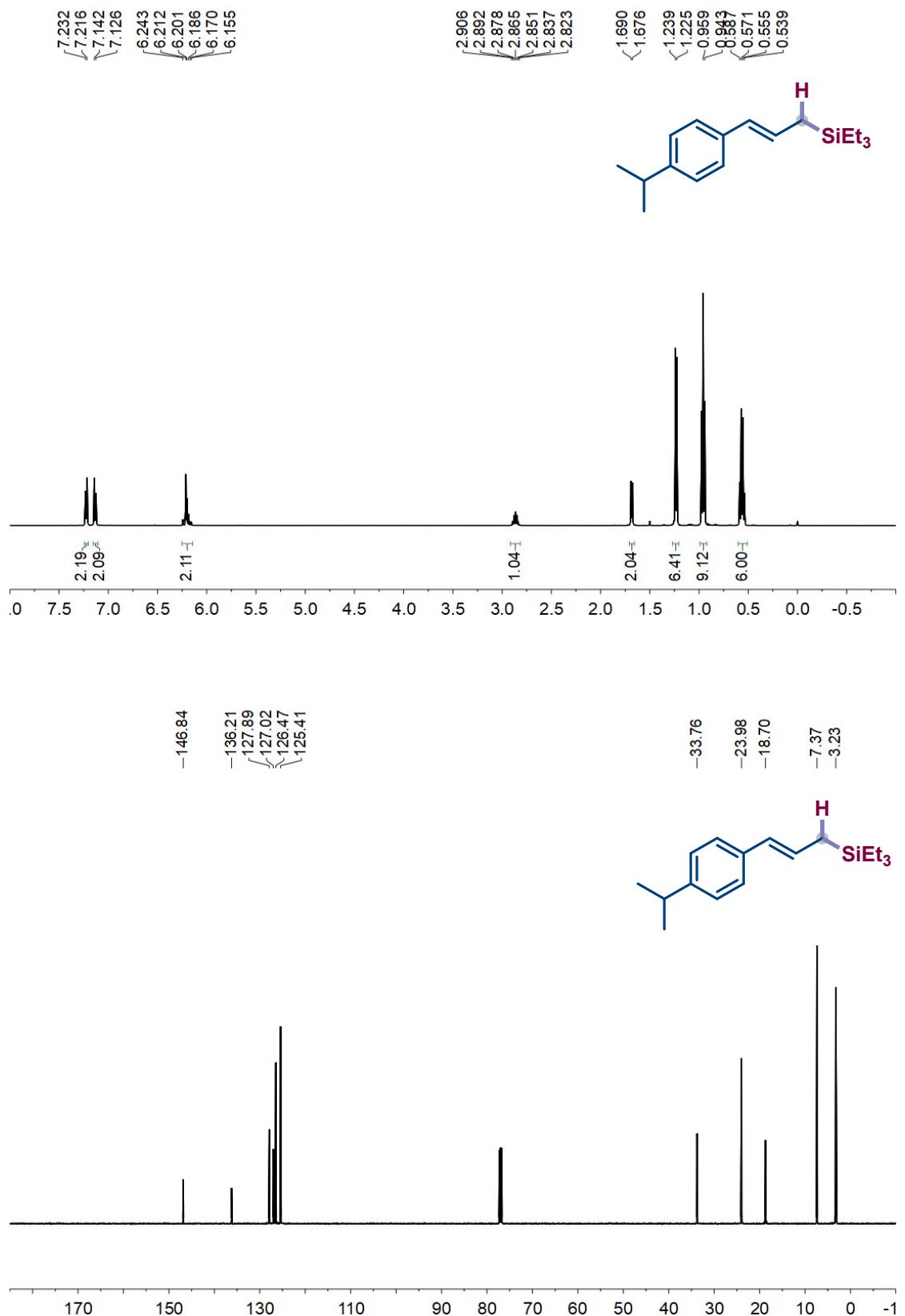


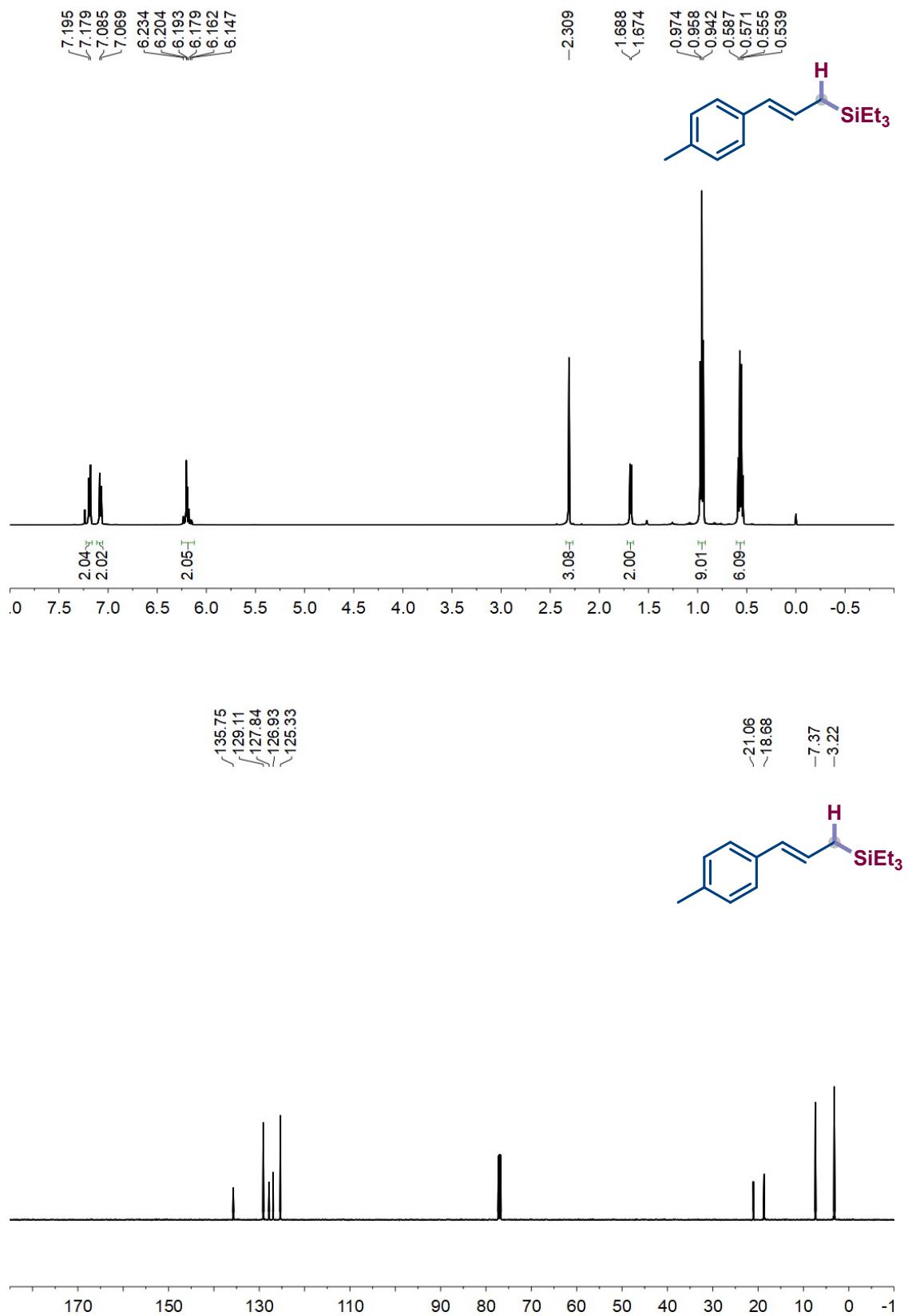
46. Colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.30-7.20 (m, 8H), 7.18-7.15 (m, 3H), 7.12 (t, *J* = 7.0 Hz, 3H), 6.99 (d, *J* = 7.5 Hz, 6H), 6.14 (d, *J* = 16.0 Hz, 1H), 5.86-5.79 (m, 1H), 2.17 (s, 6H), 1.63 (d, *J* = 8.0 Hz, 2H). **¹³C NMR** (150 MHz, CDCl₃) δ 138.9, 138.0, 129.8, 128.6, 128.43, 128.40, 126.4, 126.2, 125.6, 124.5, 21.8, 19.1. **HRMS** (ESI) m/z calculated for C₃₀H₂₉Si [M-H]⁻ 417.2044, found 417.2010.

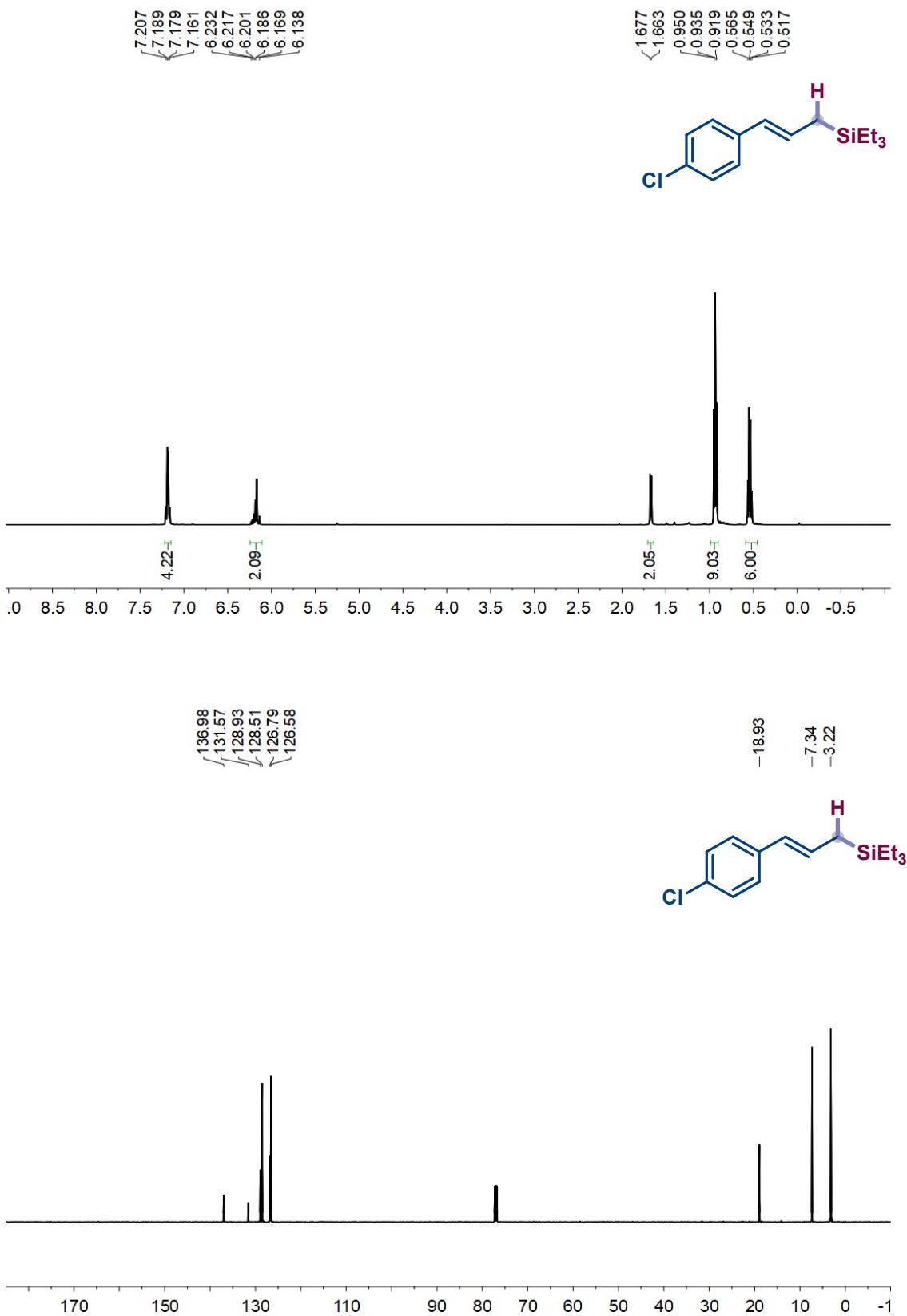
VI. Copies of NMR spectra.

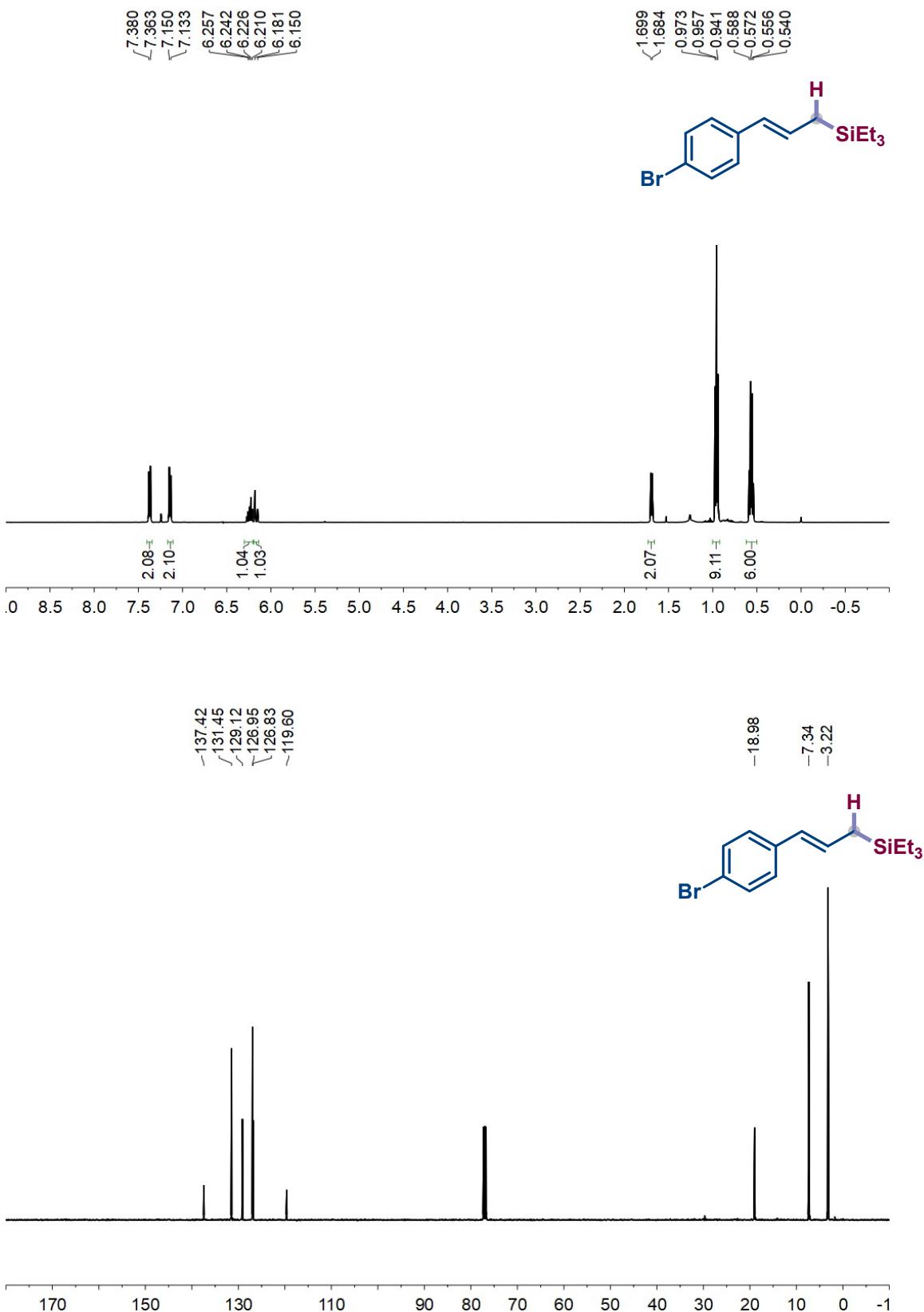


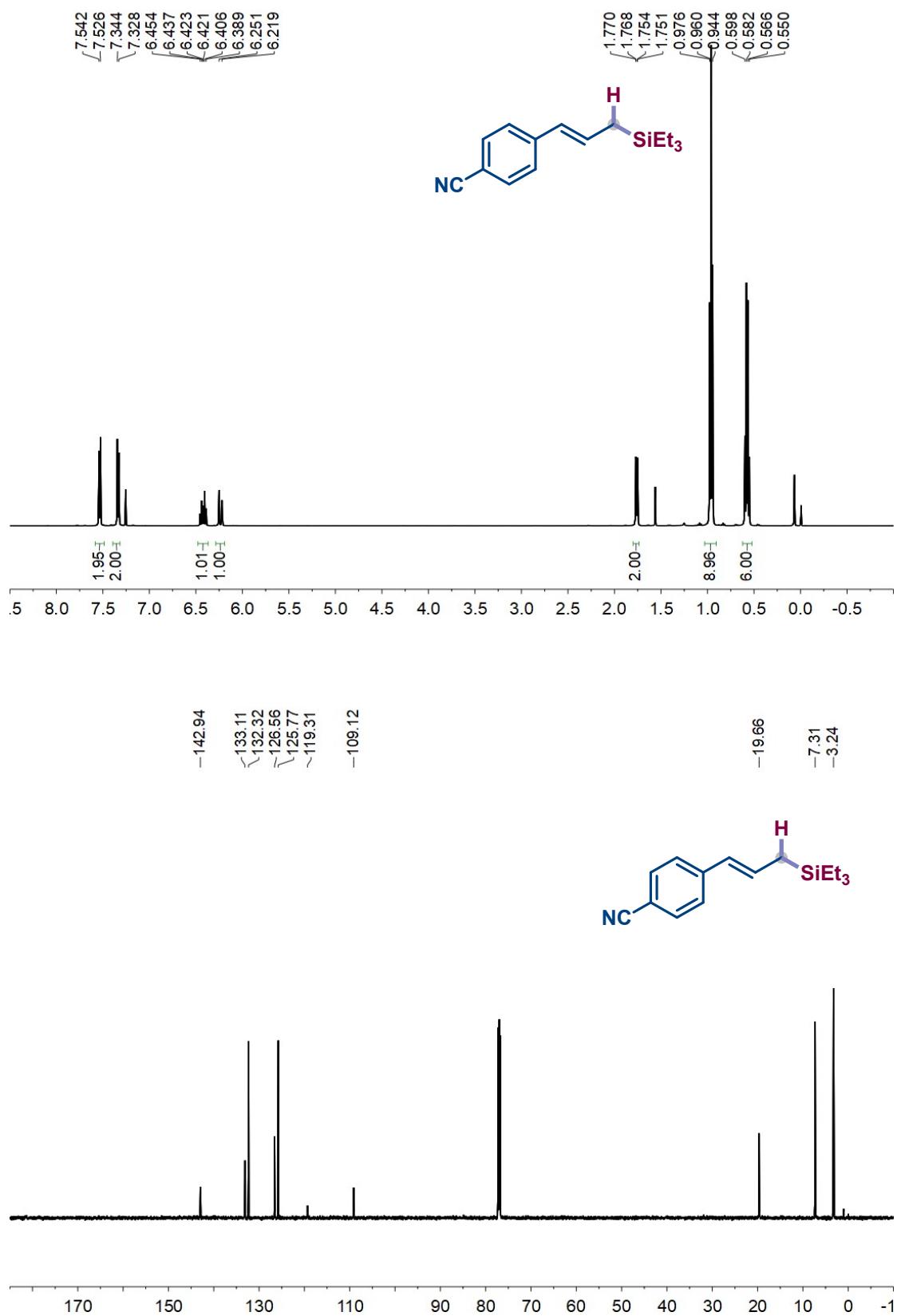


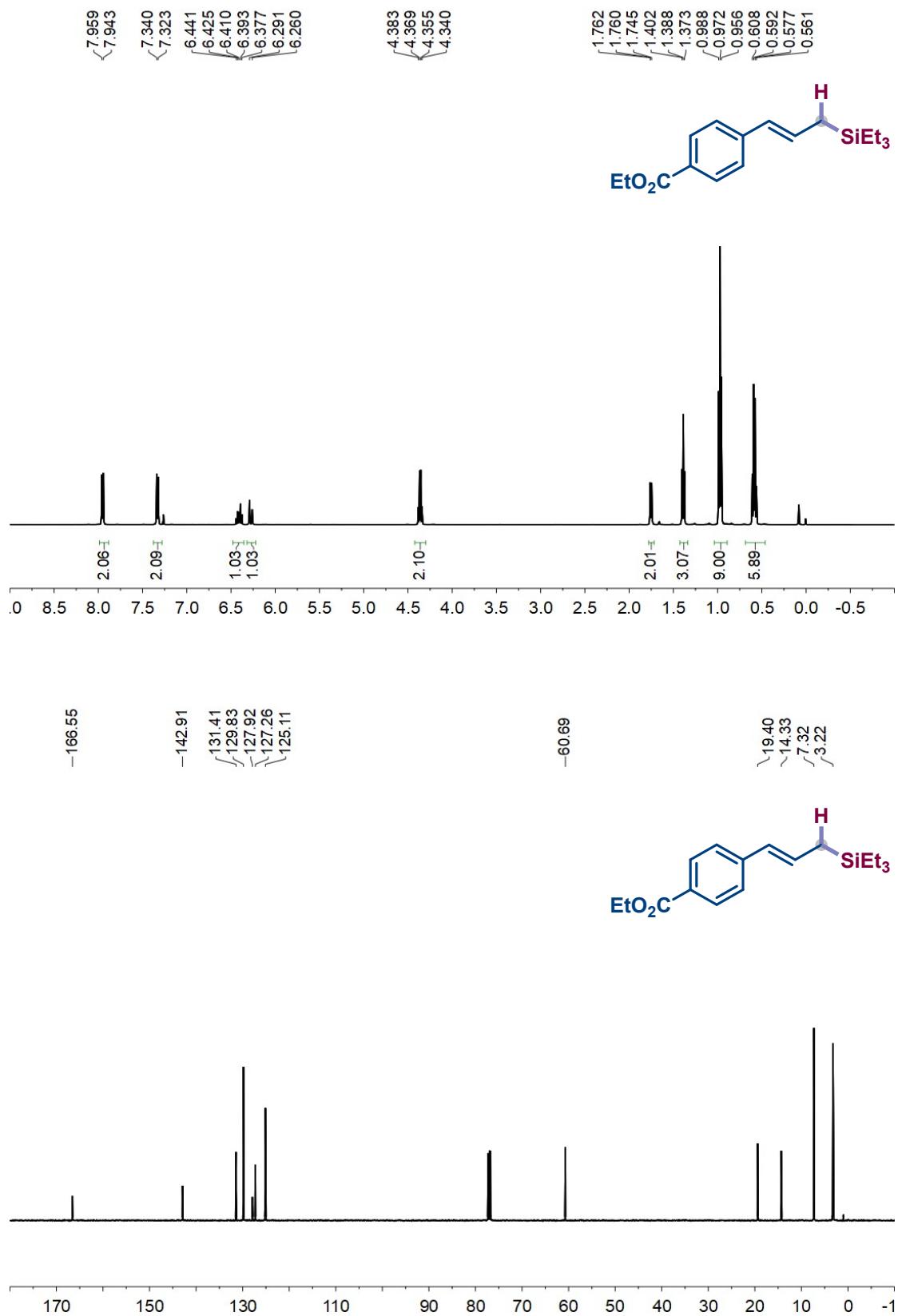


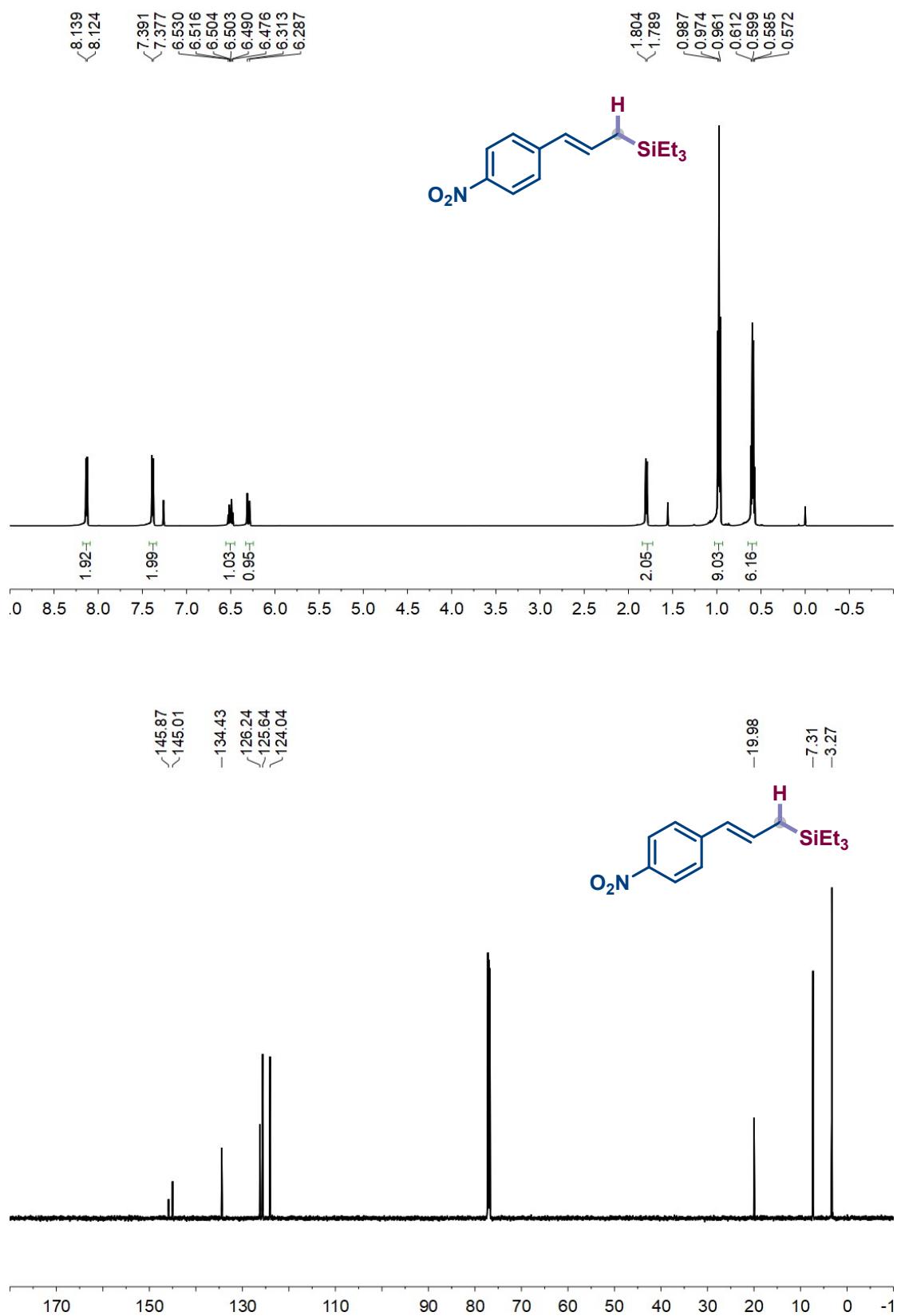


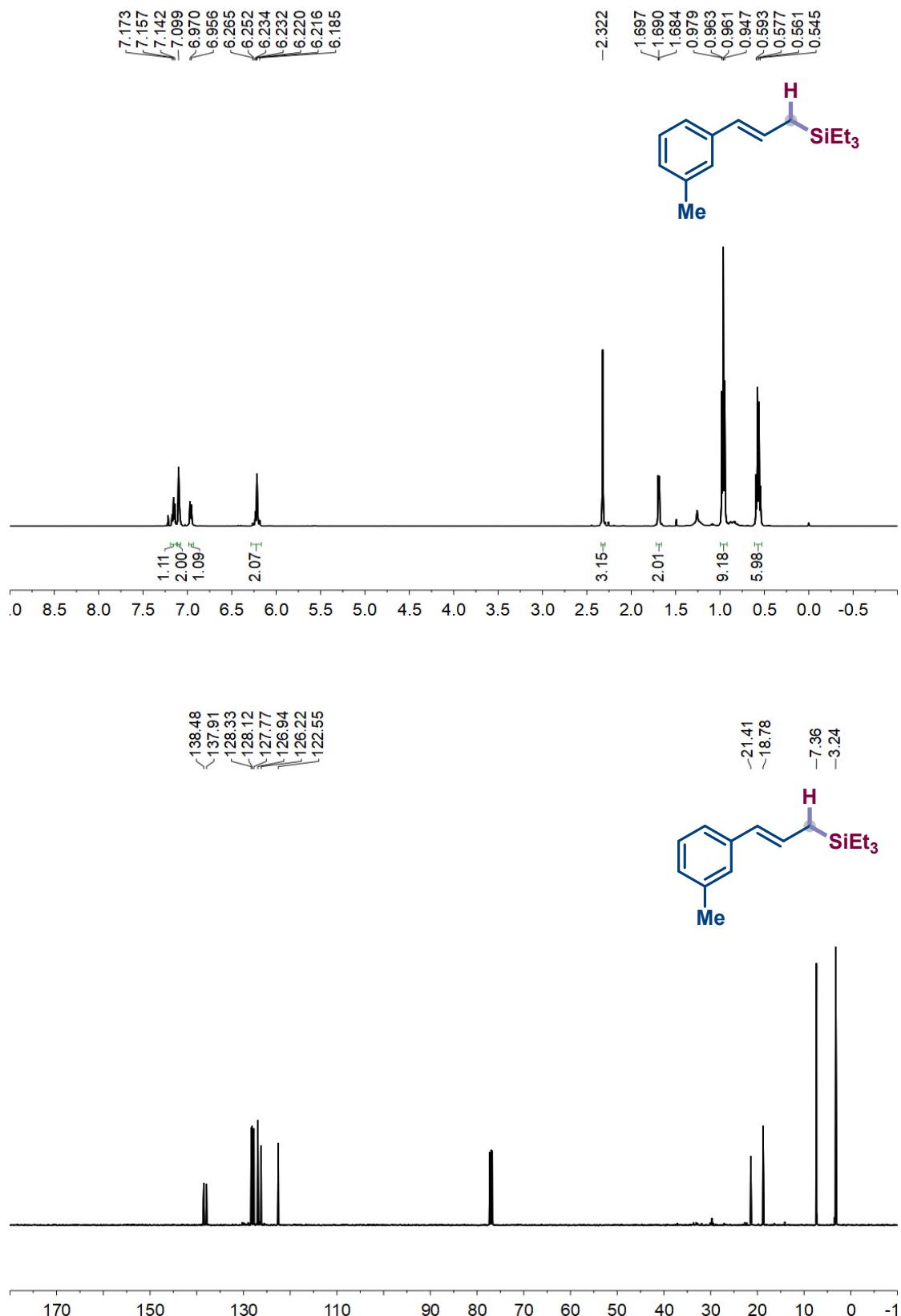


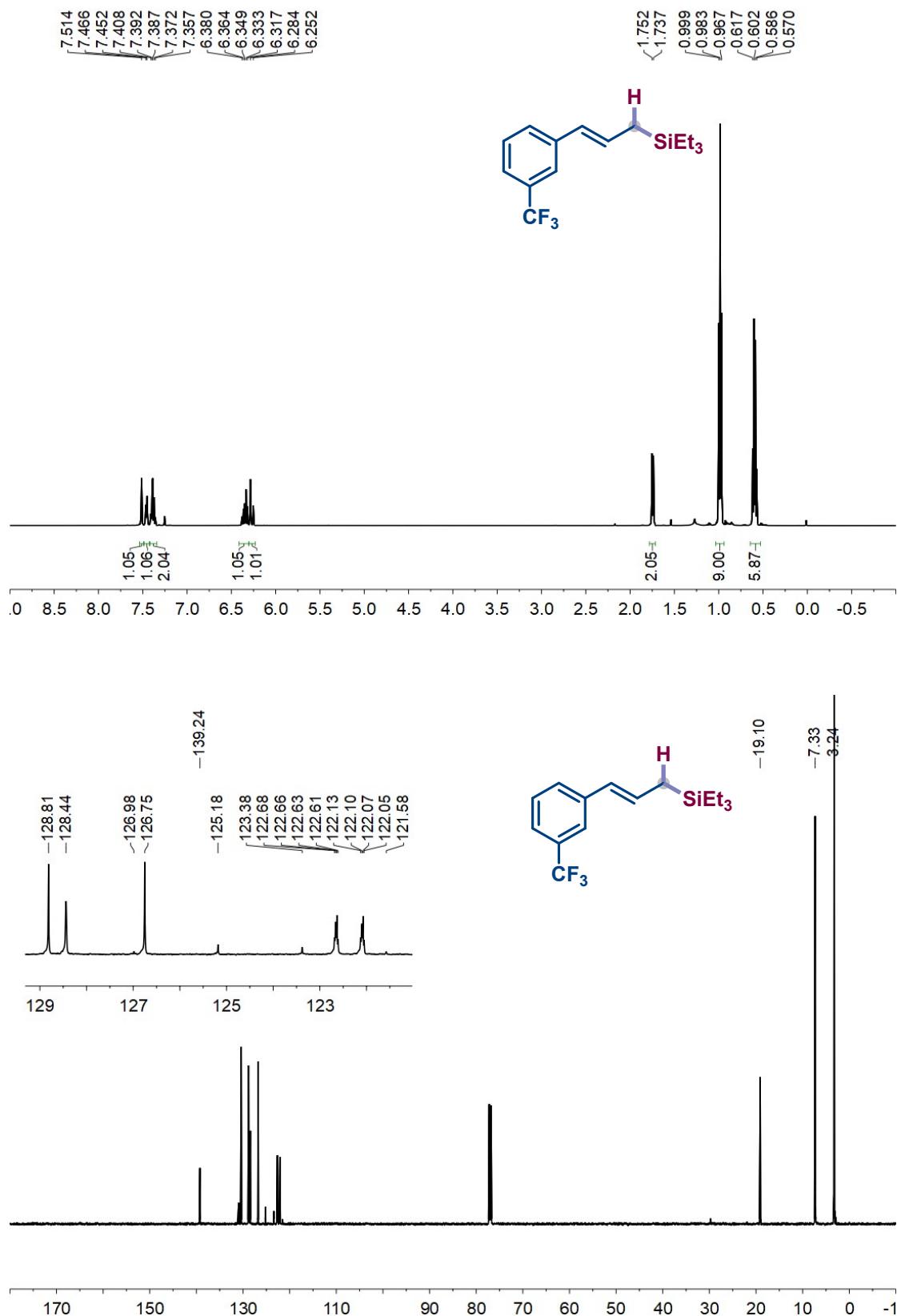


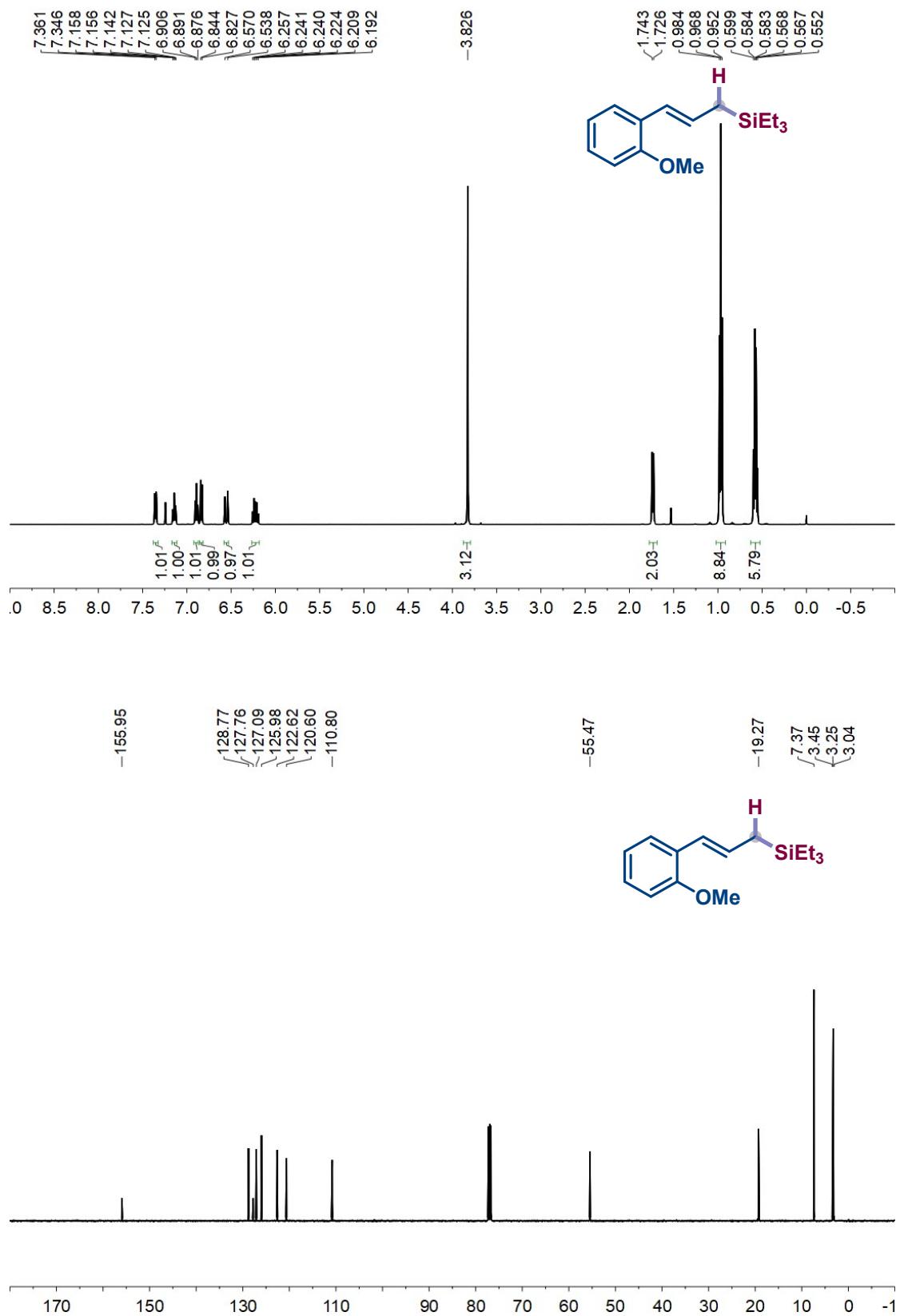


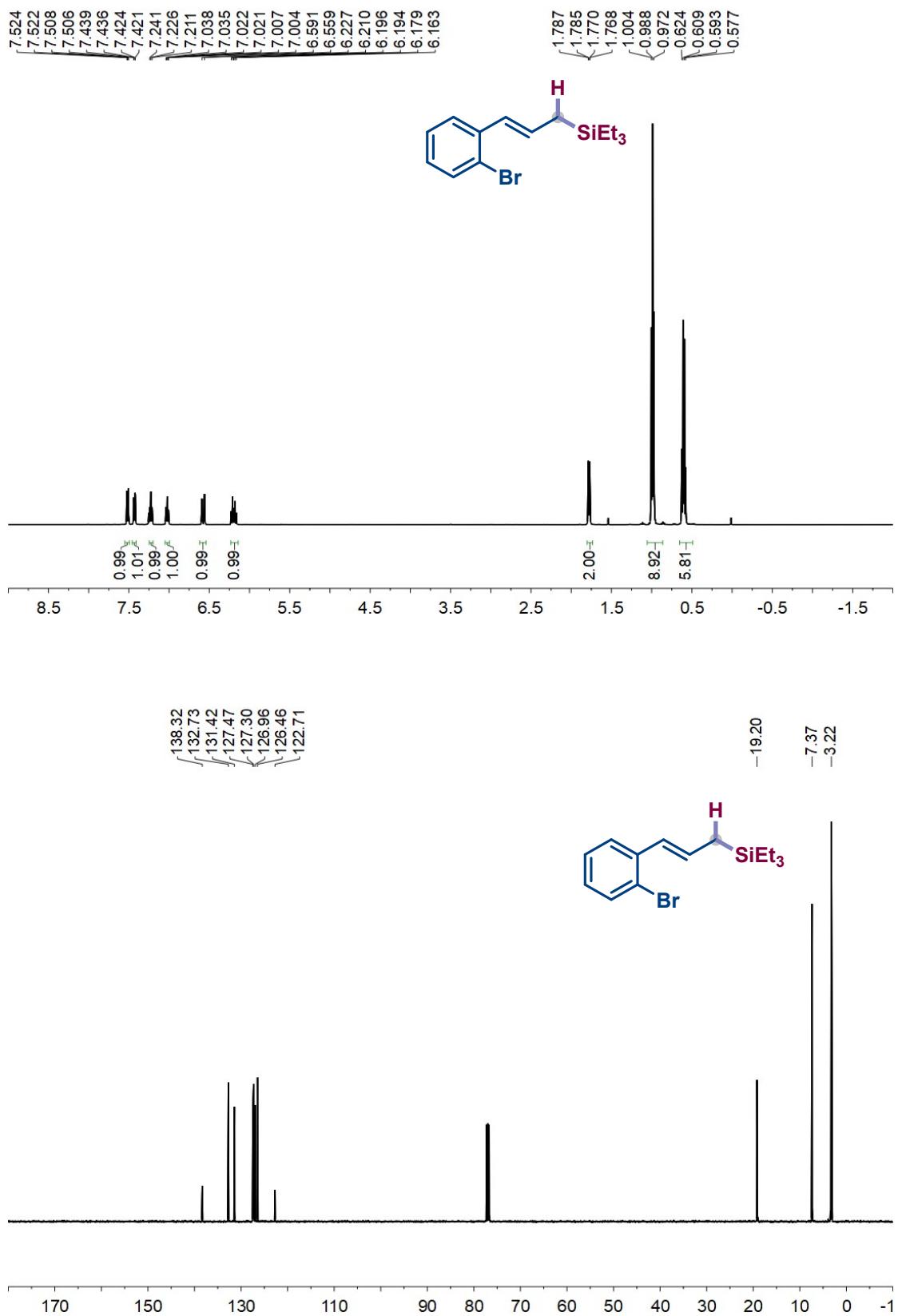


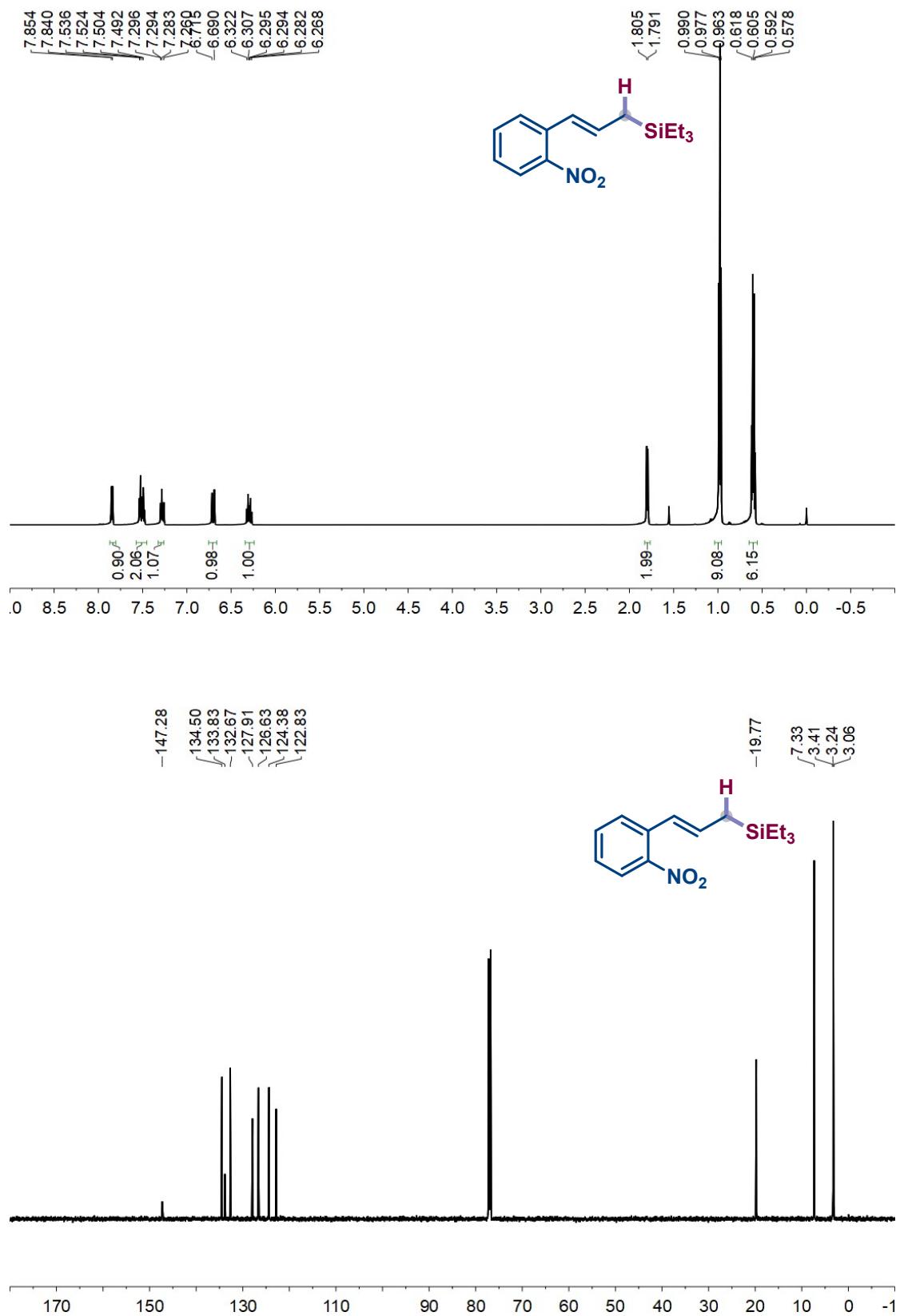


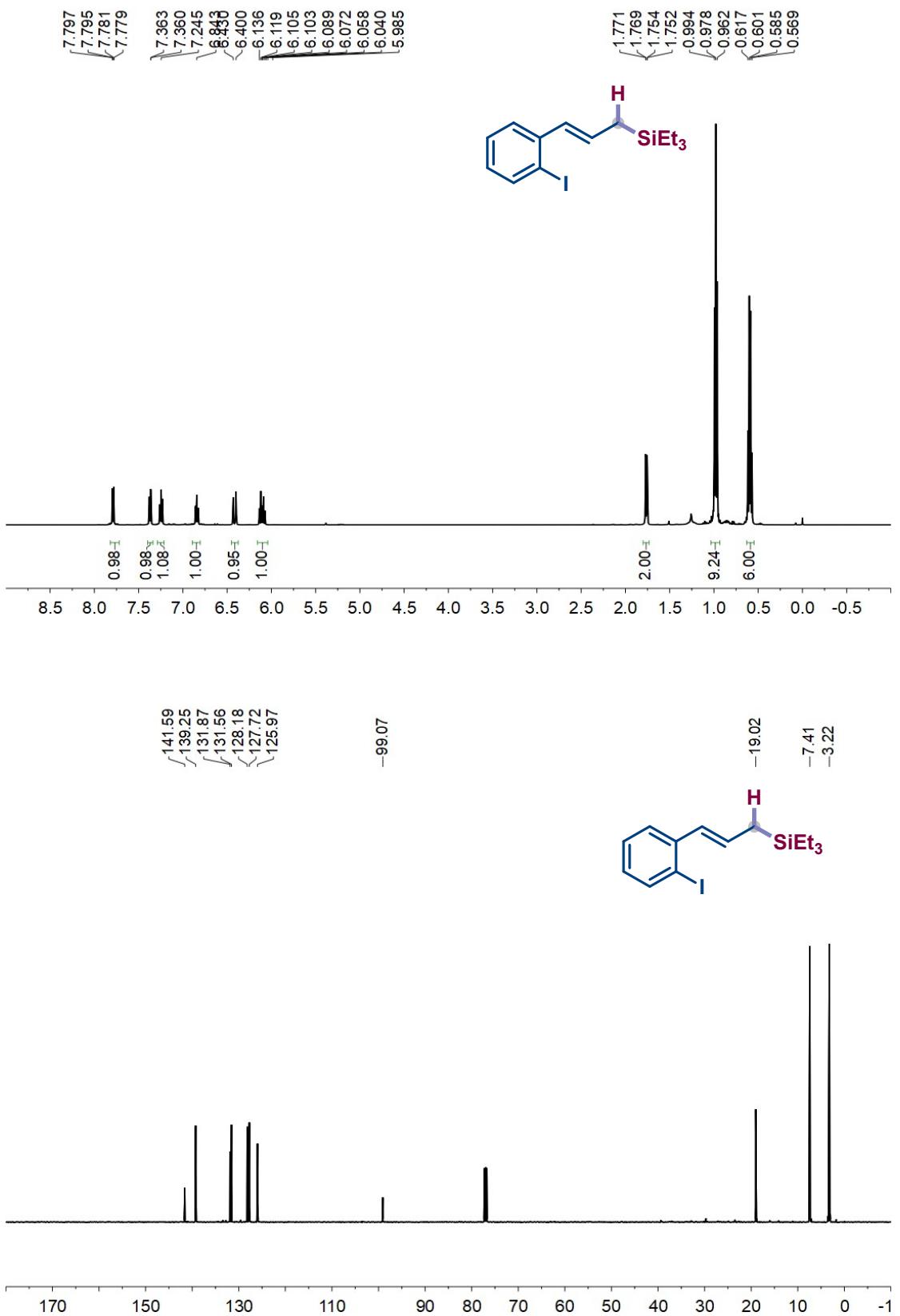


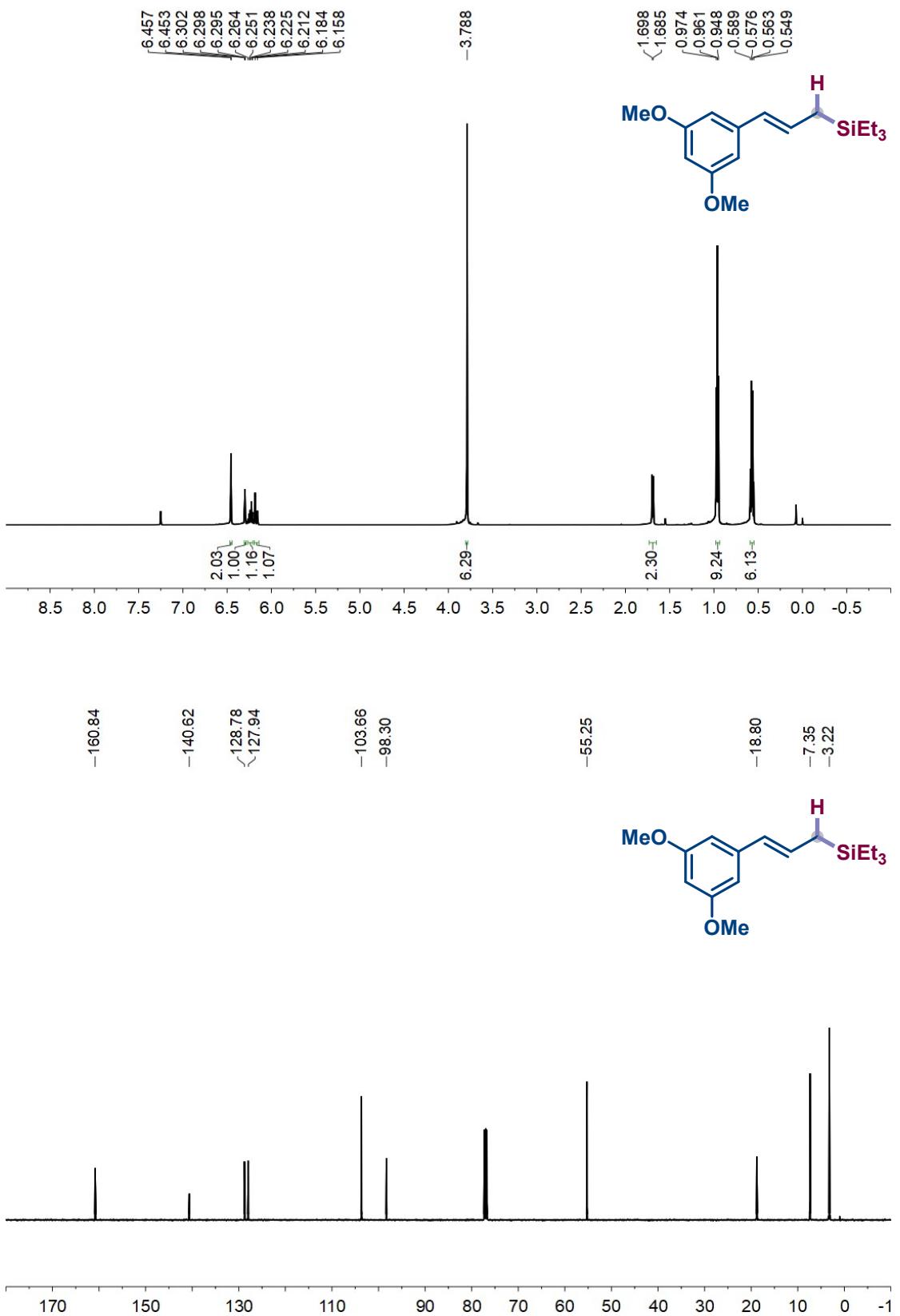


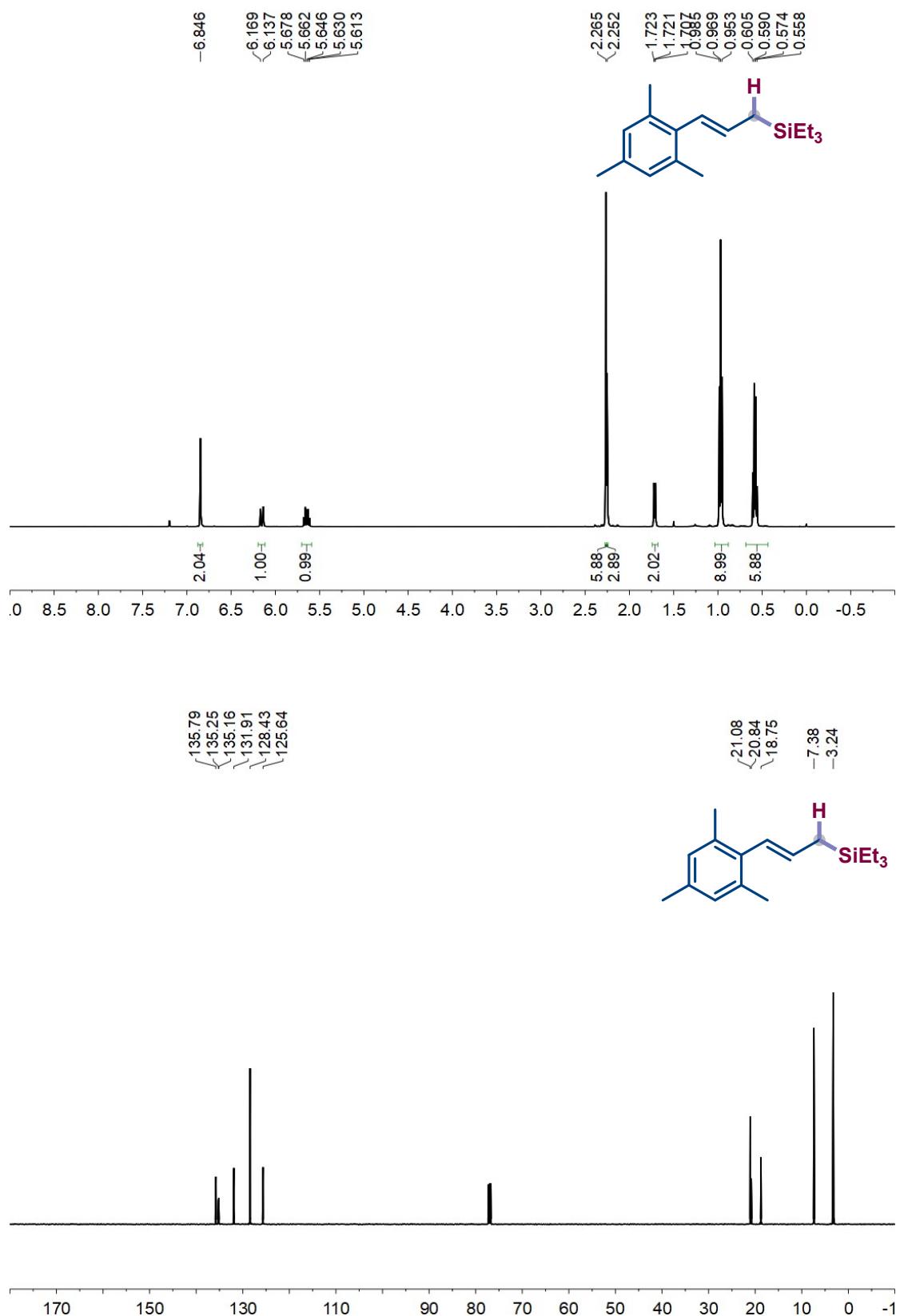


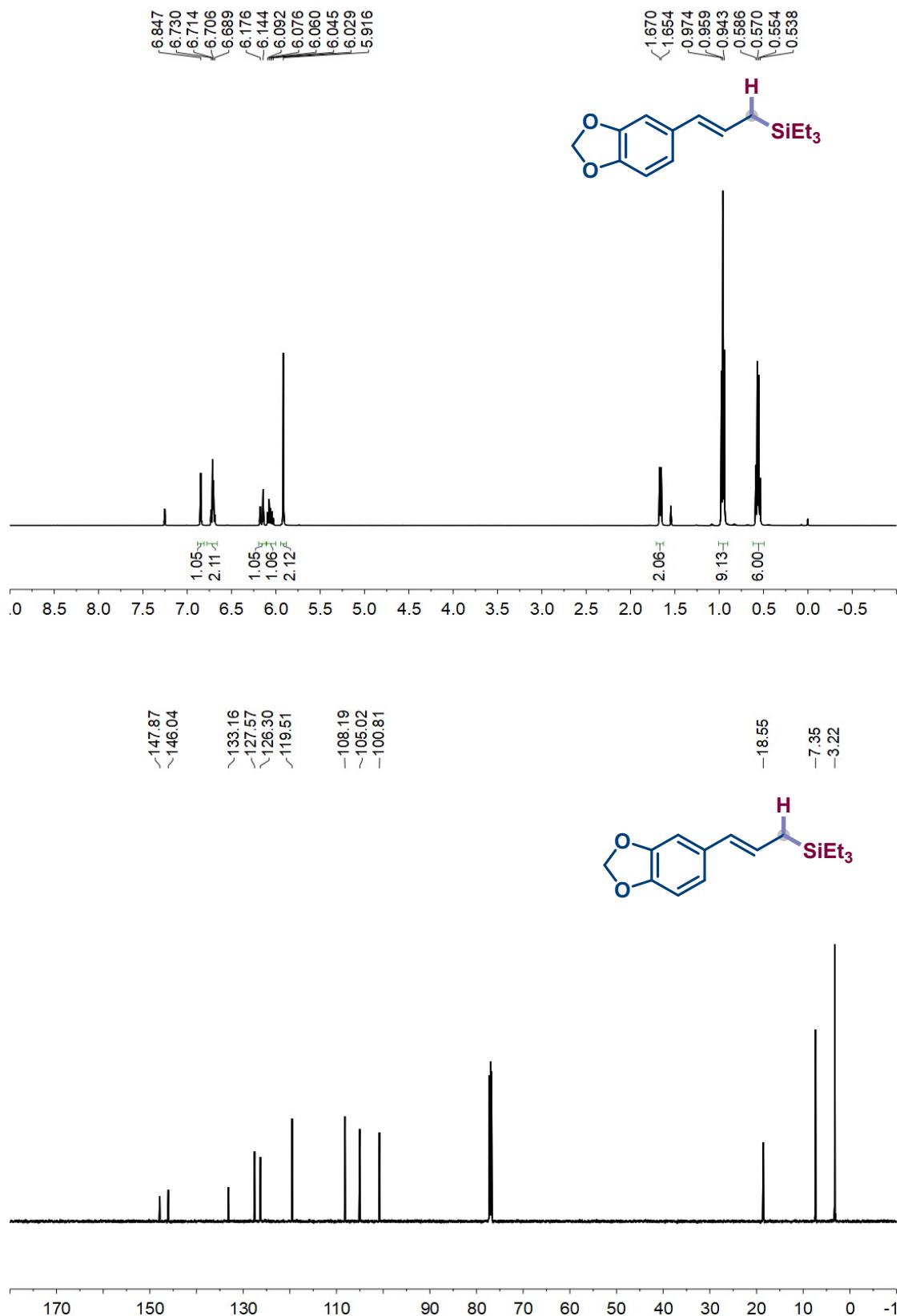


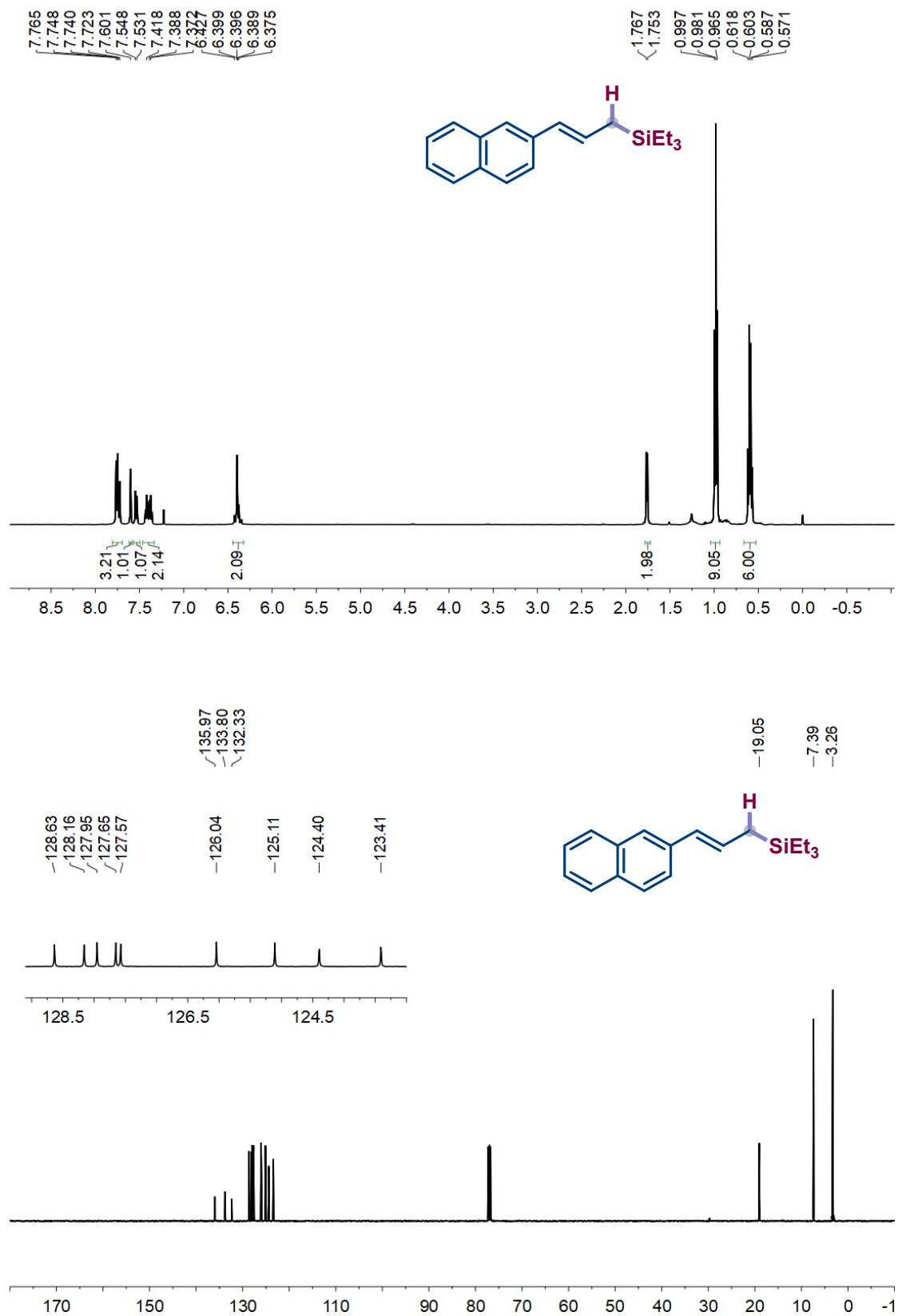


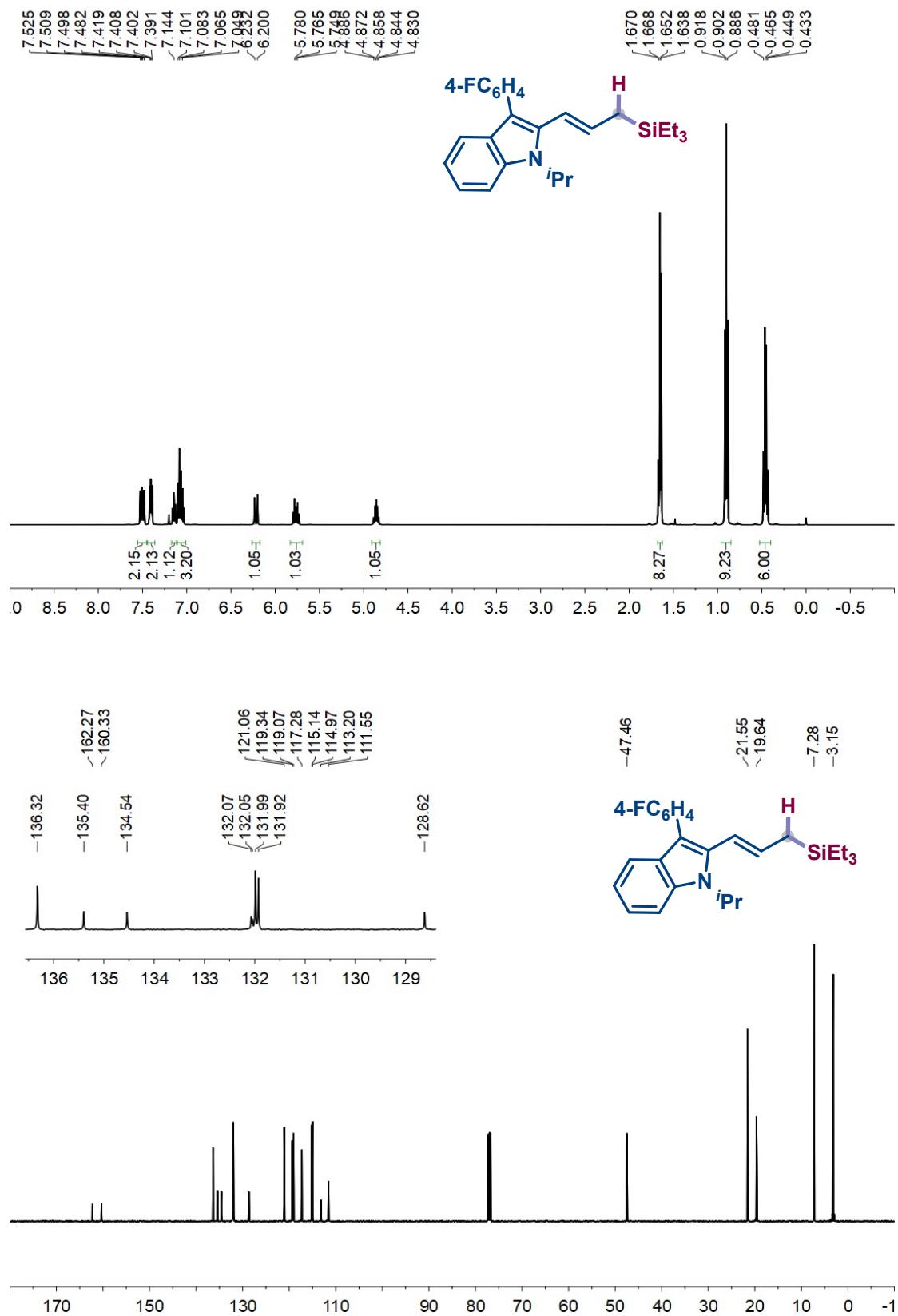


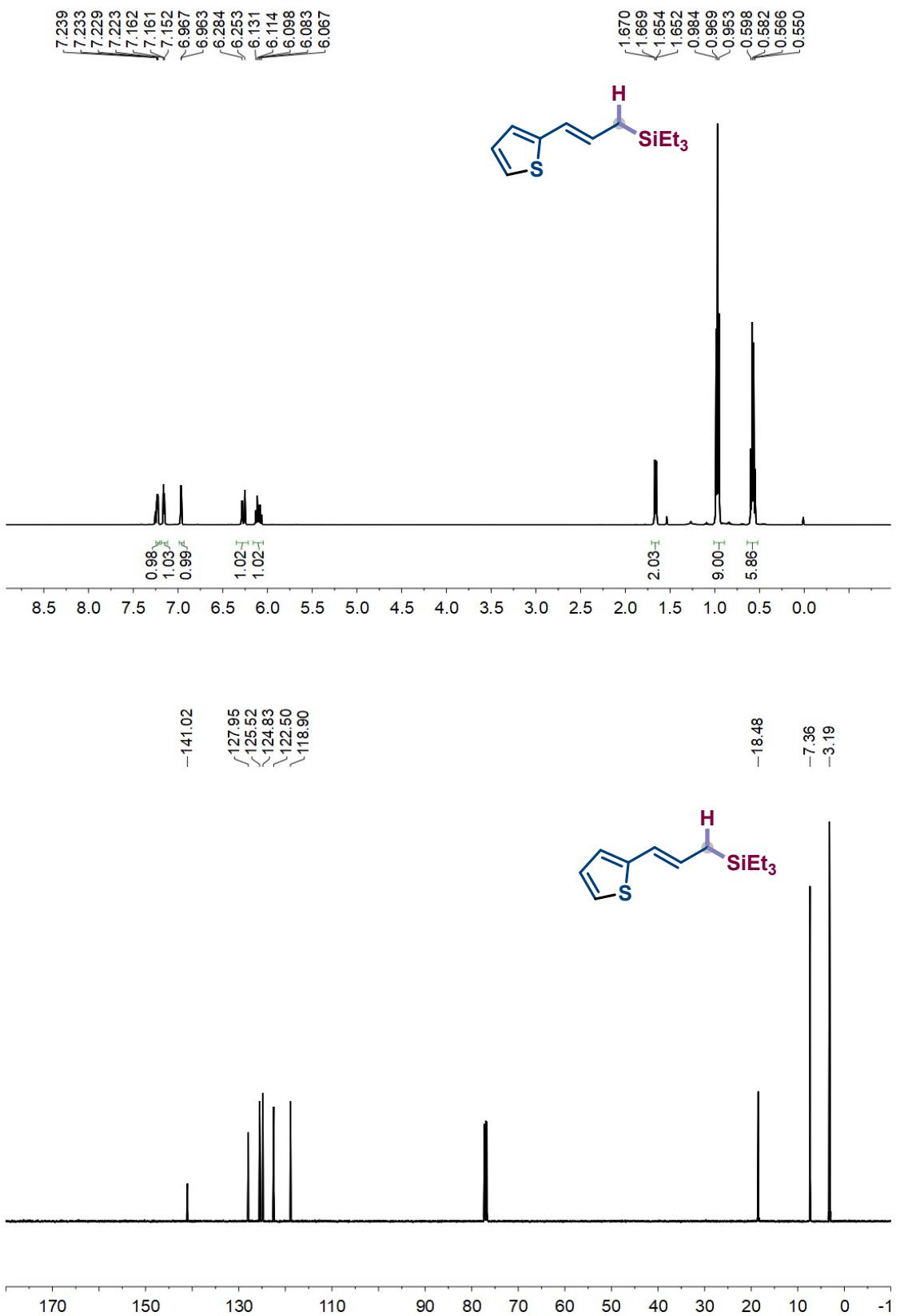


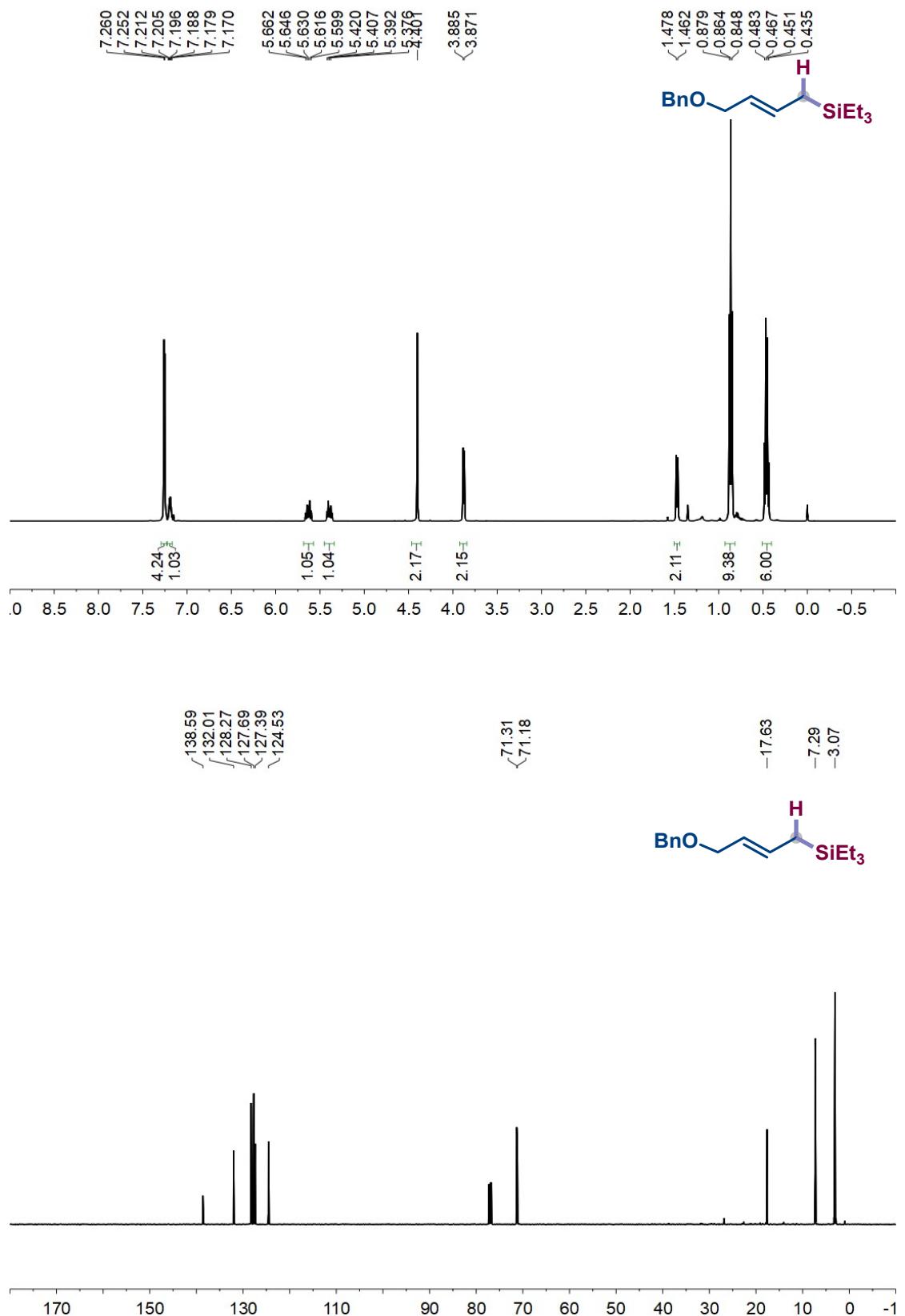


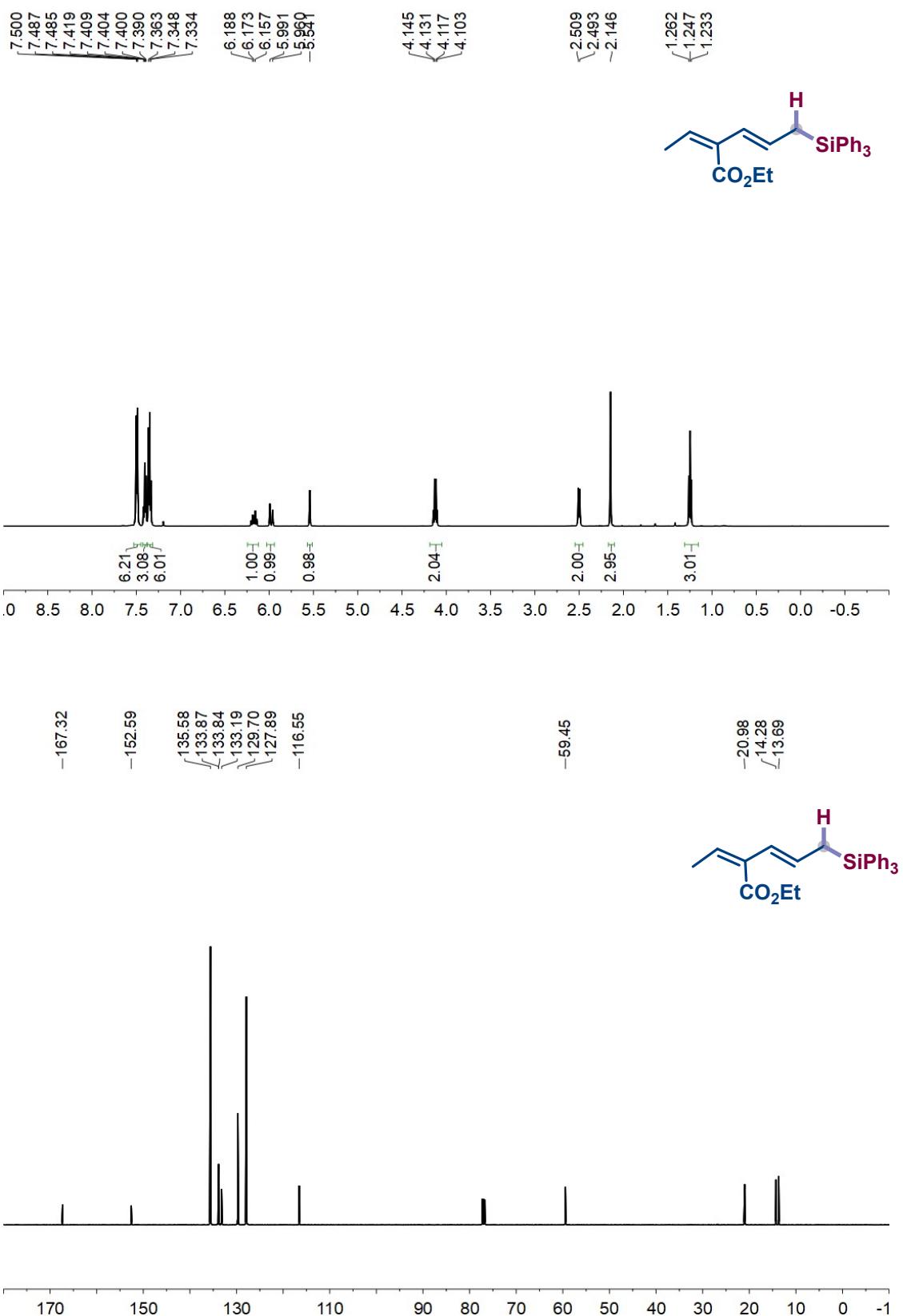


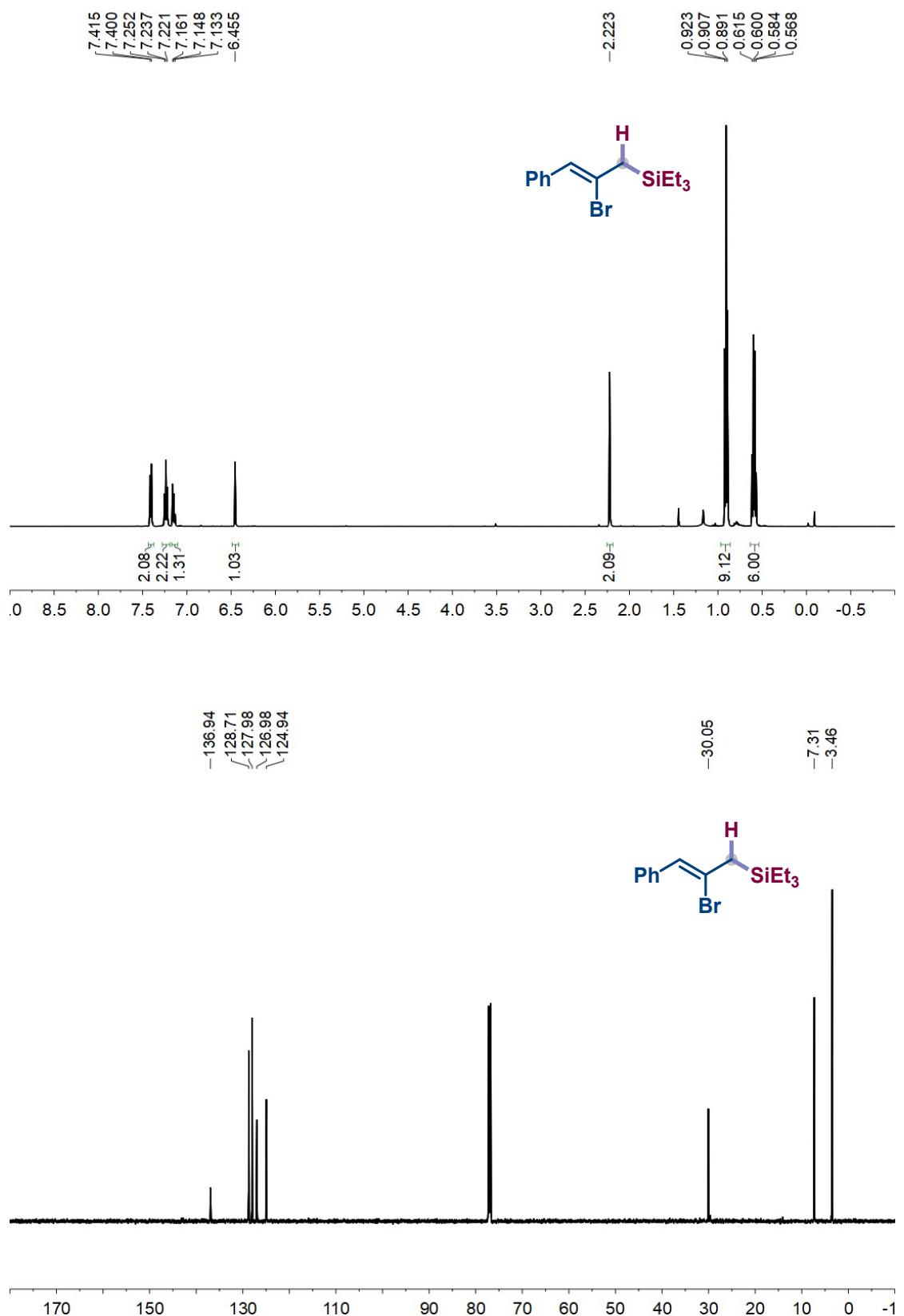


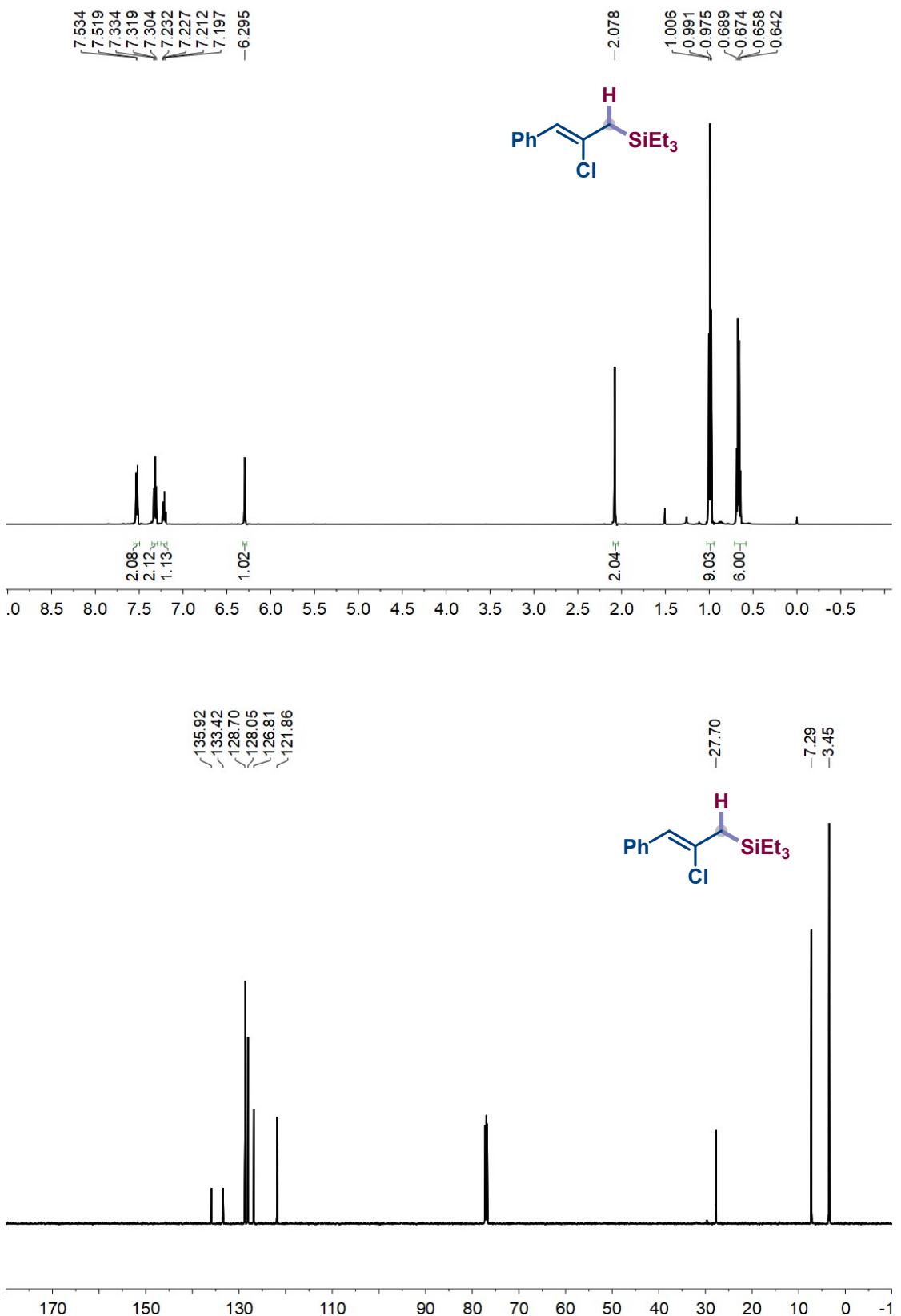


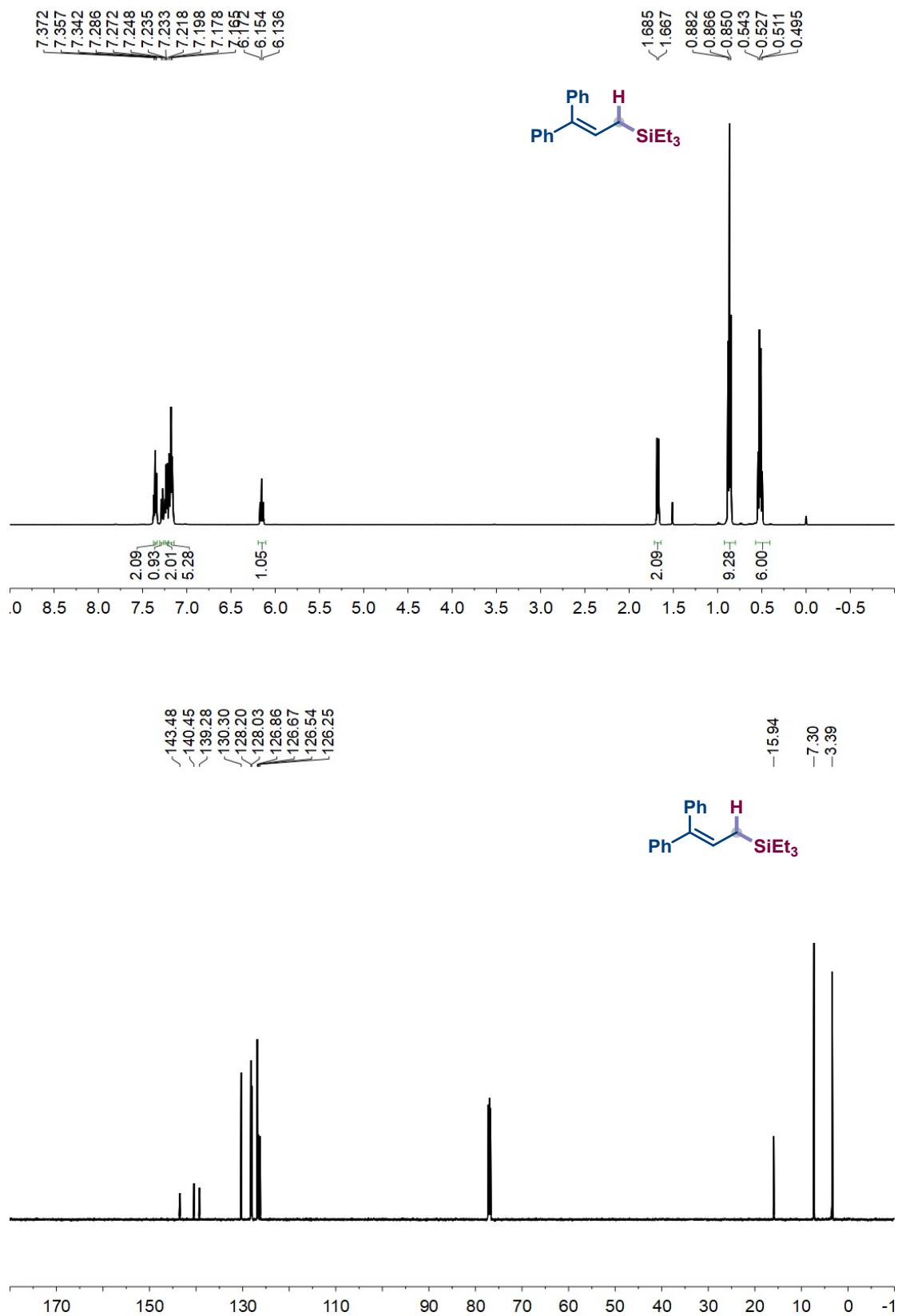


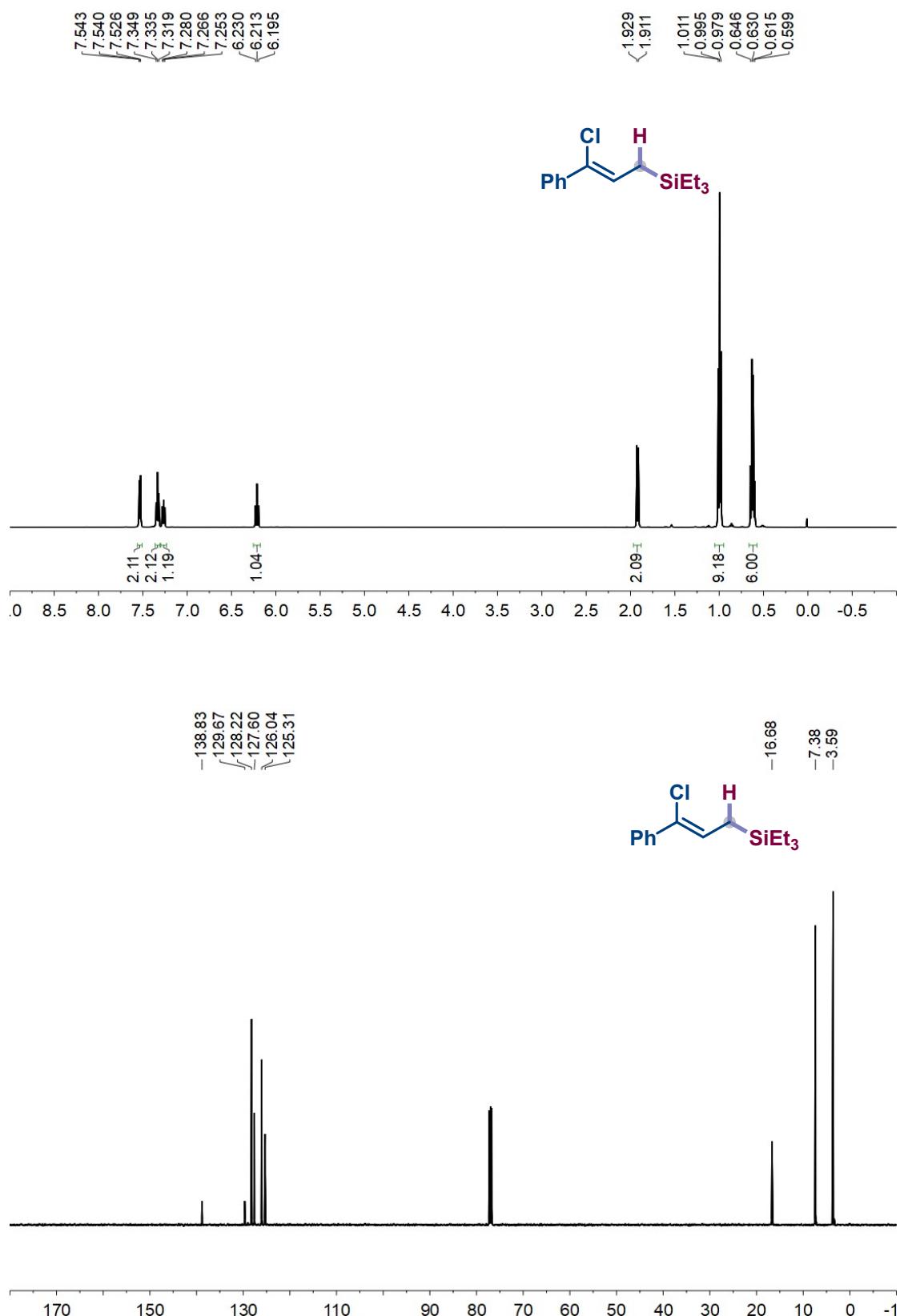


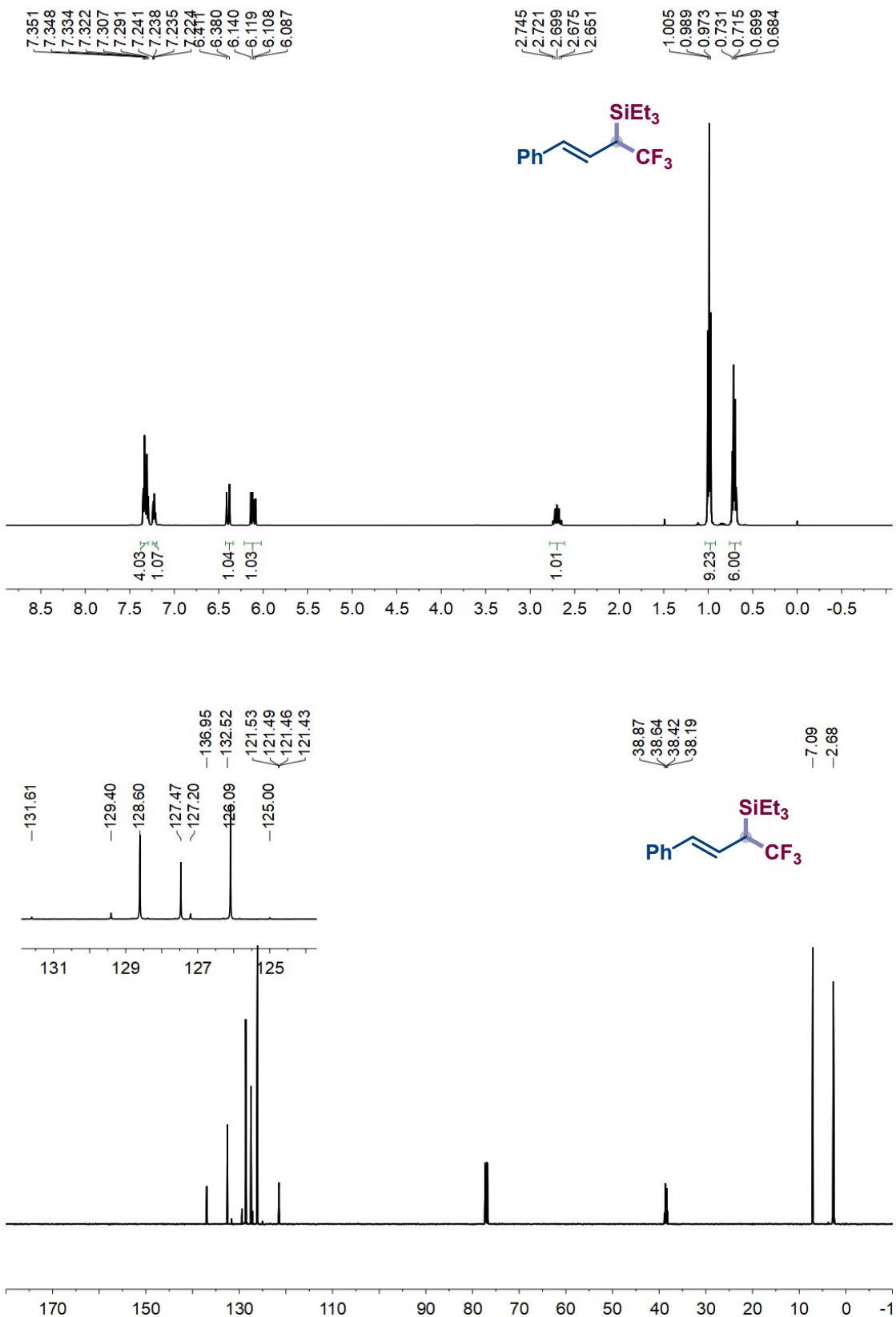


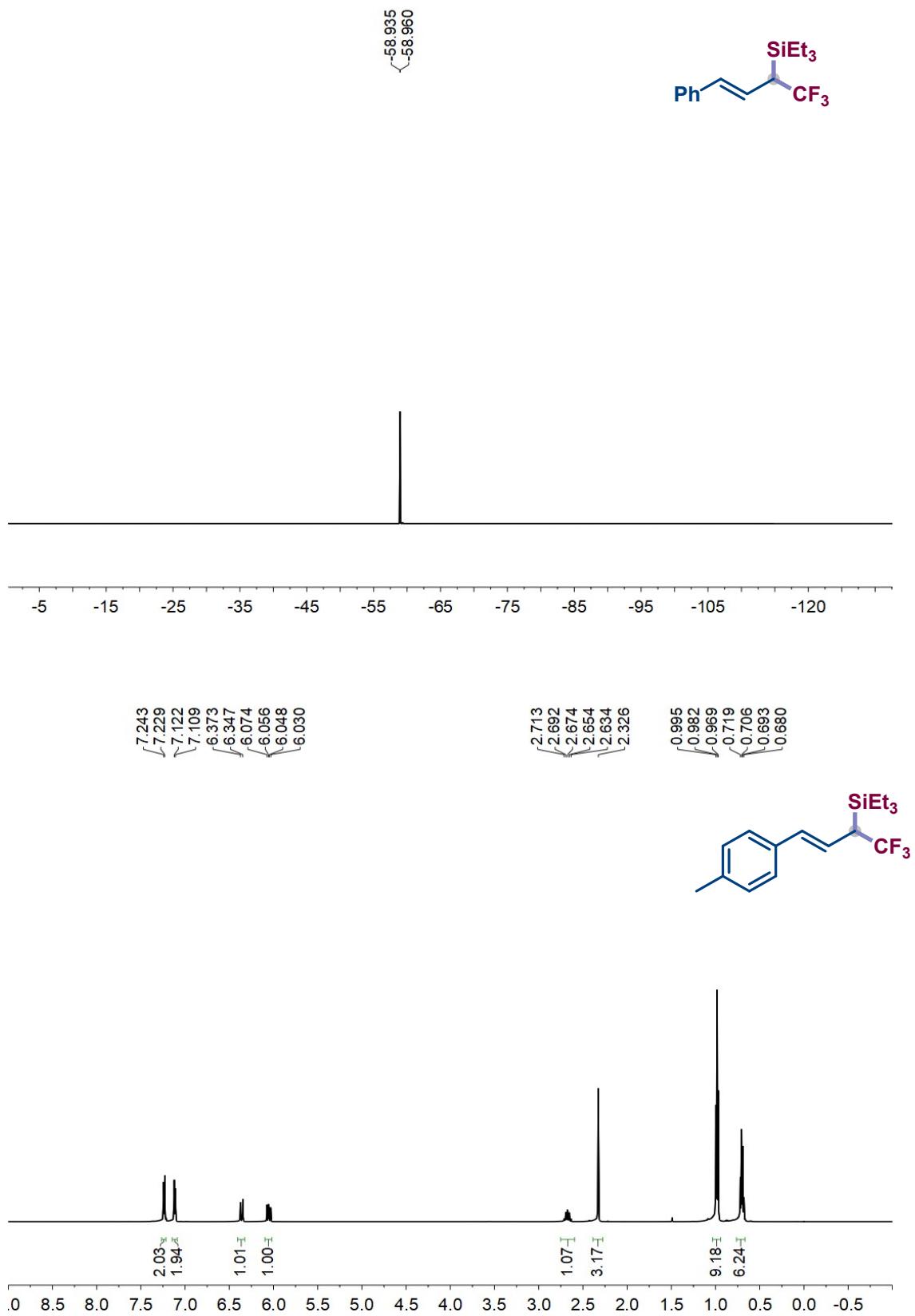


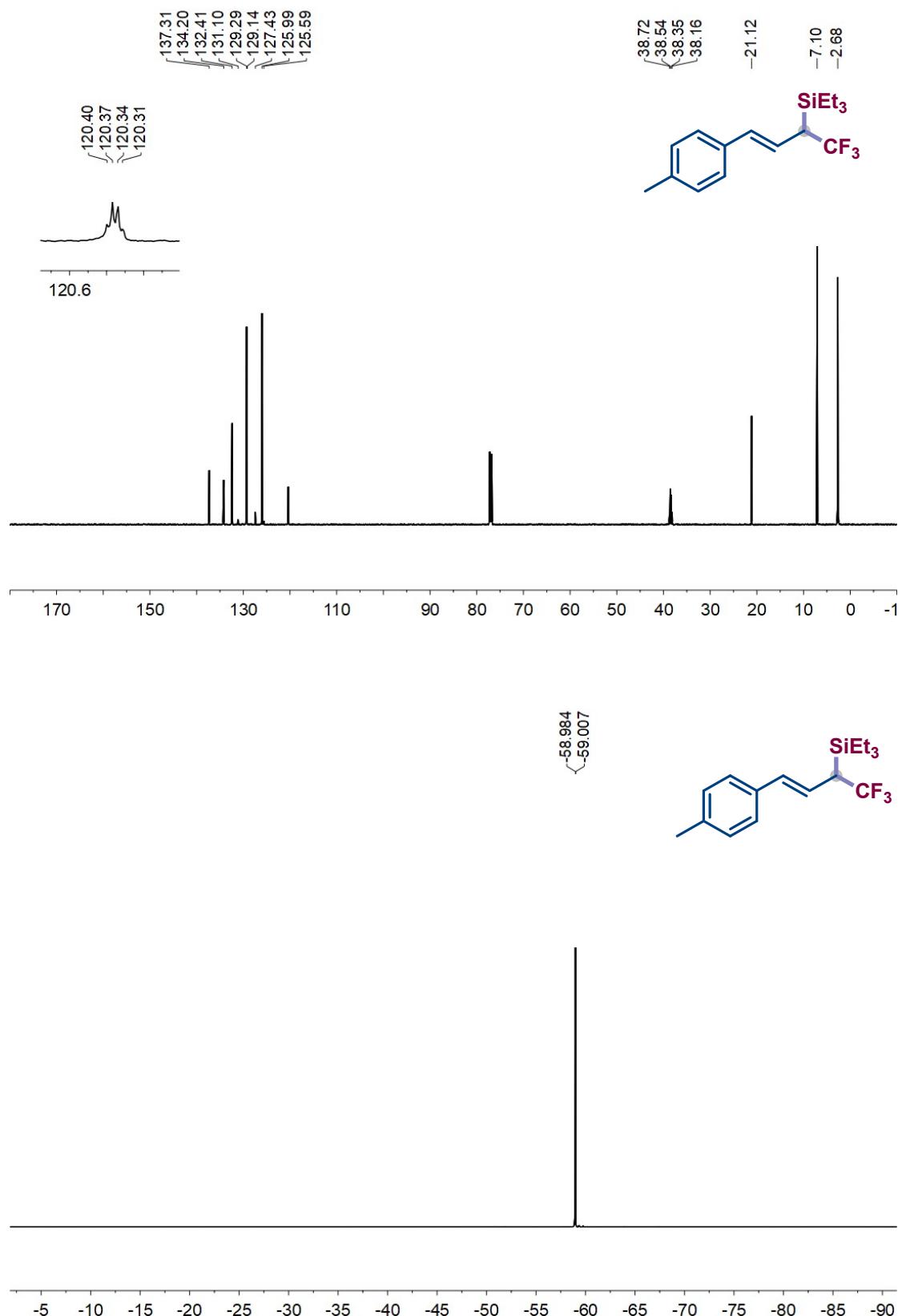


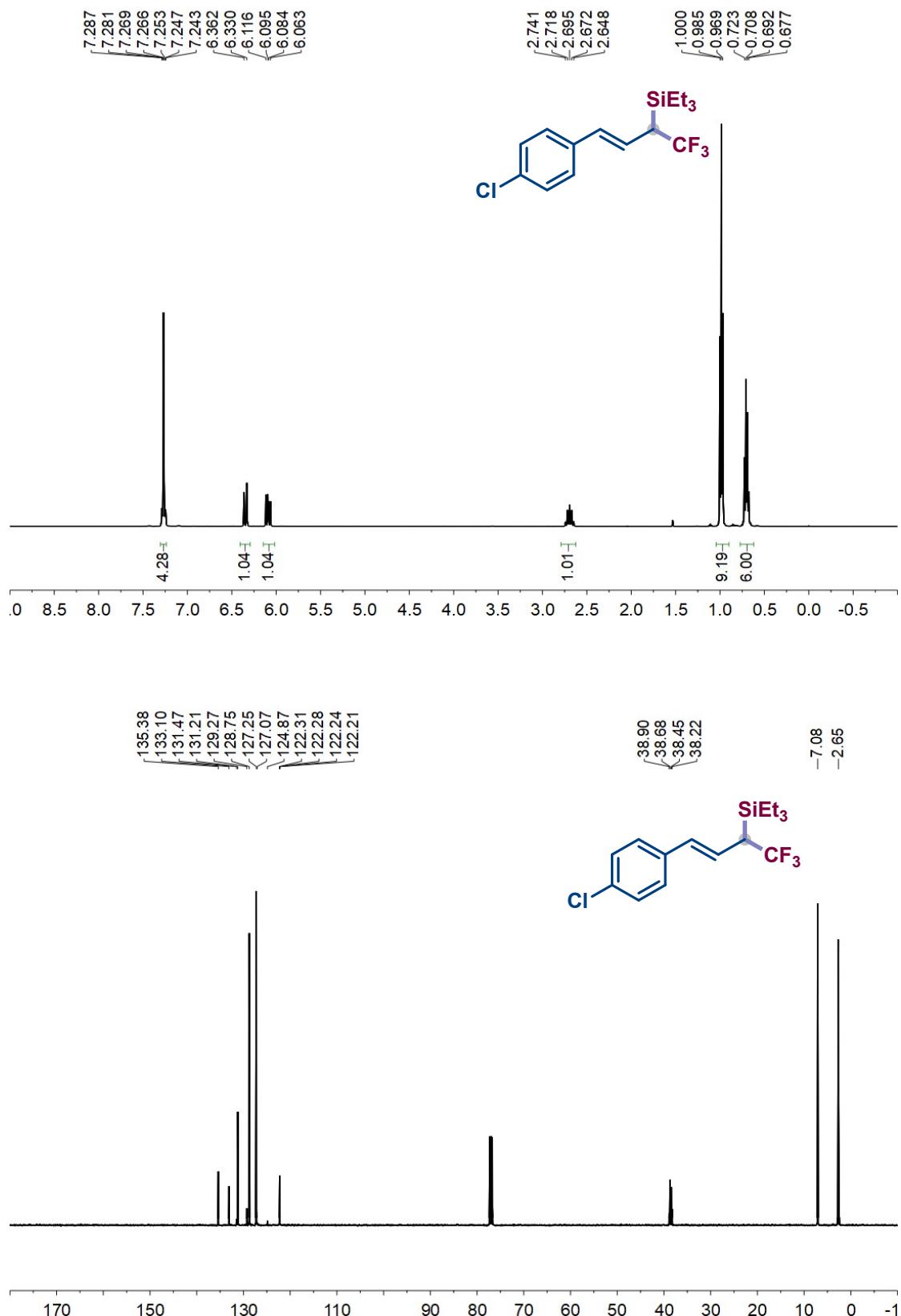


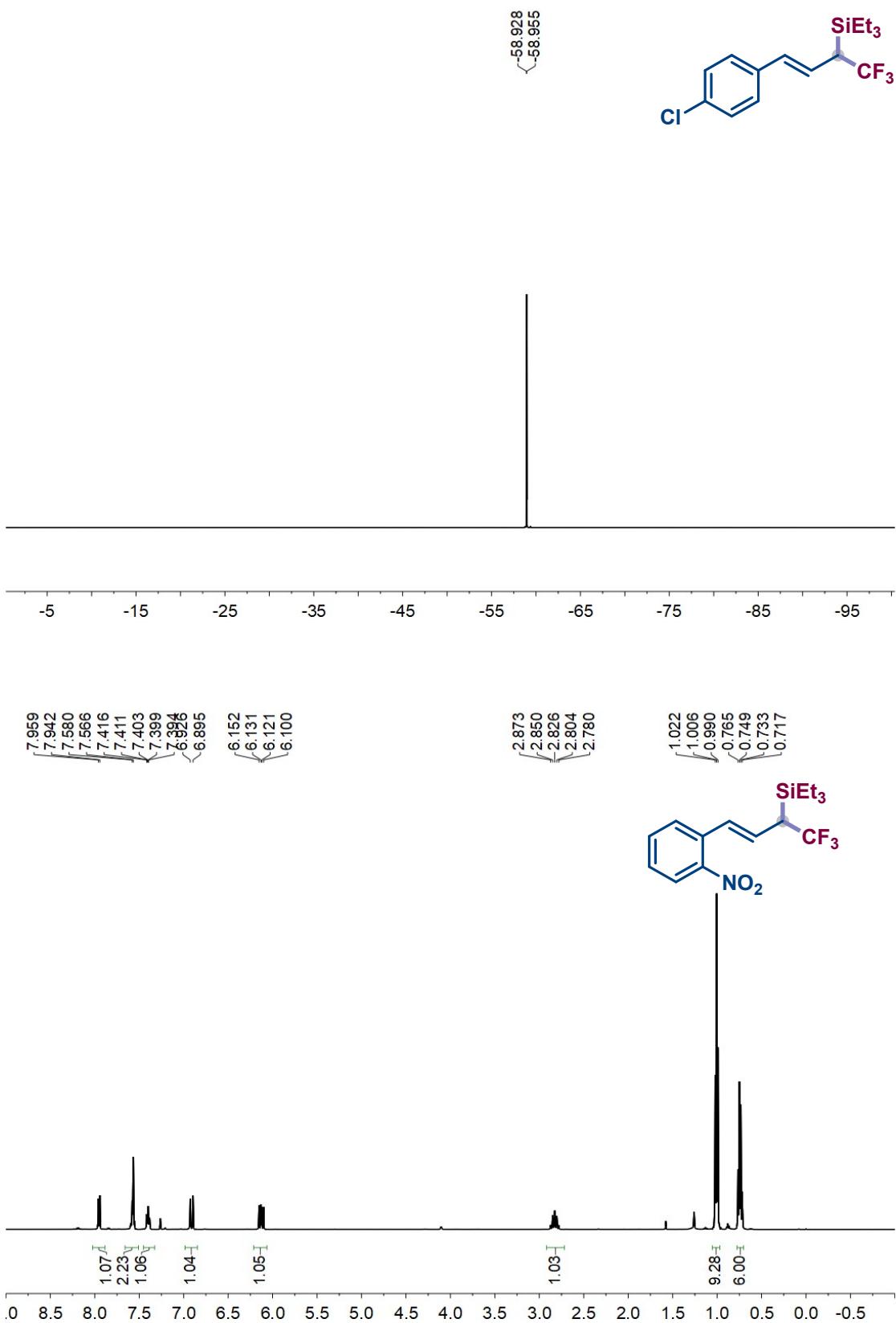


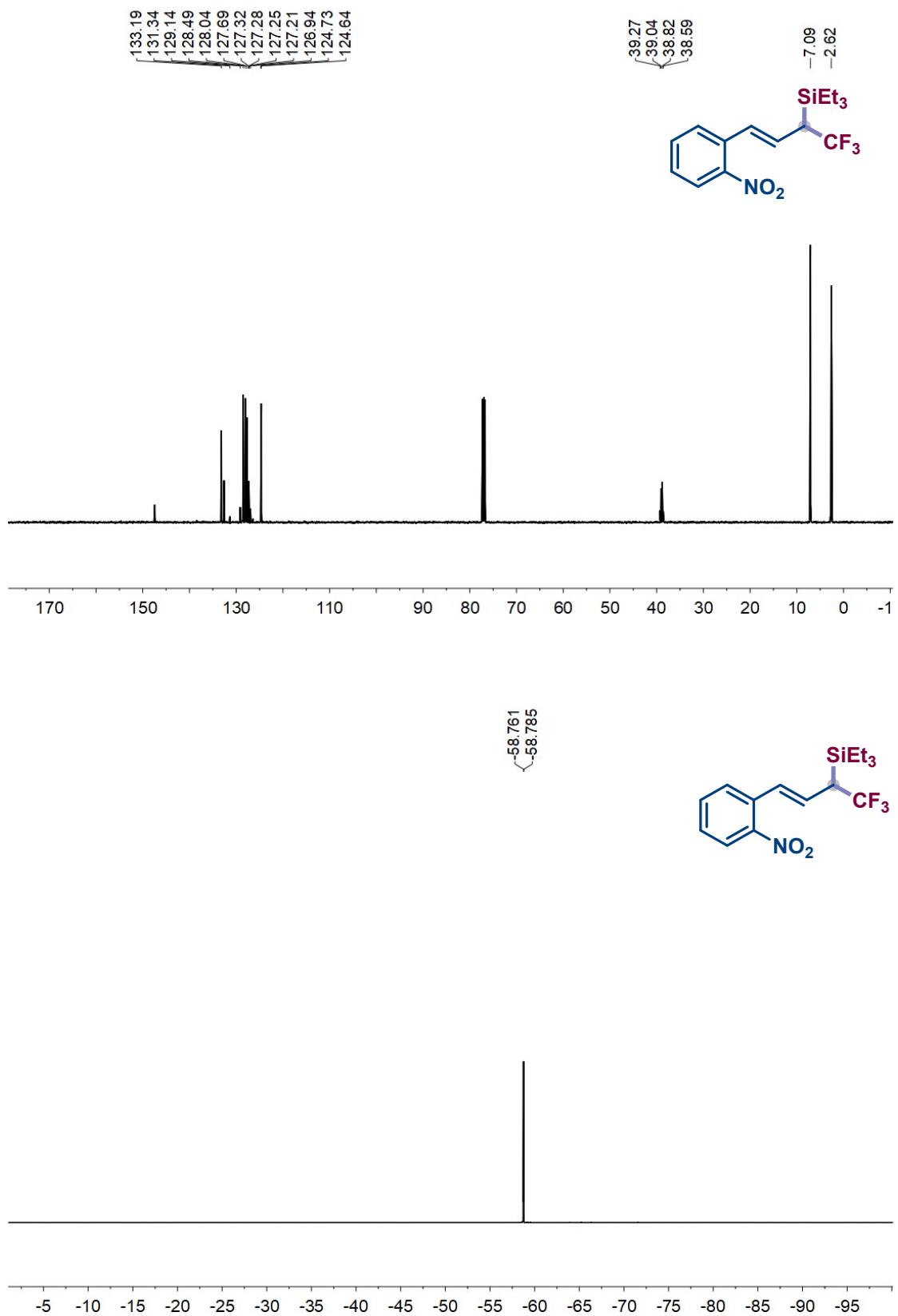


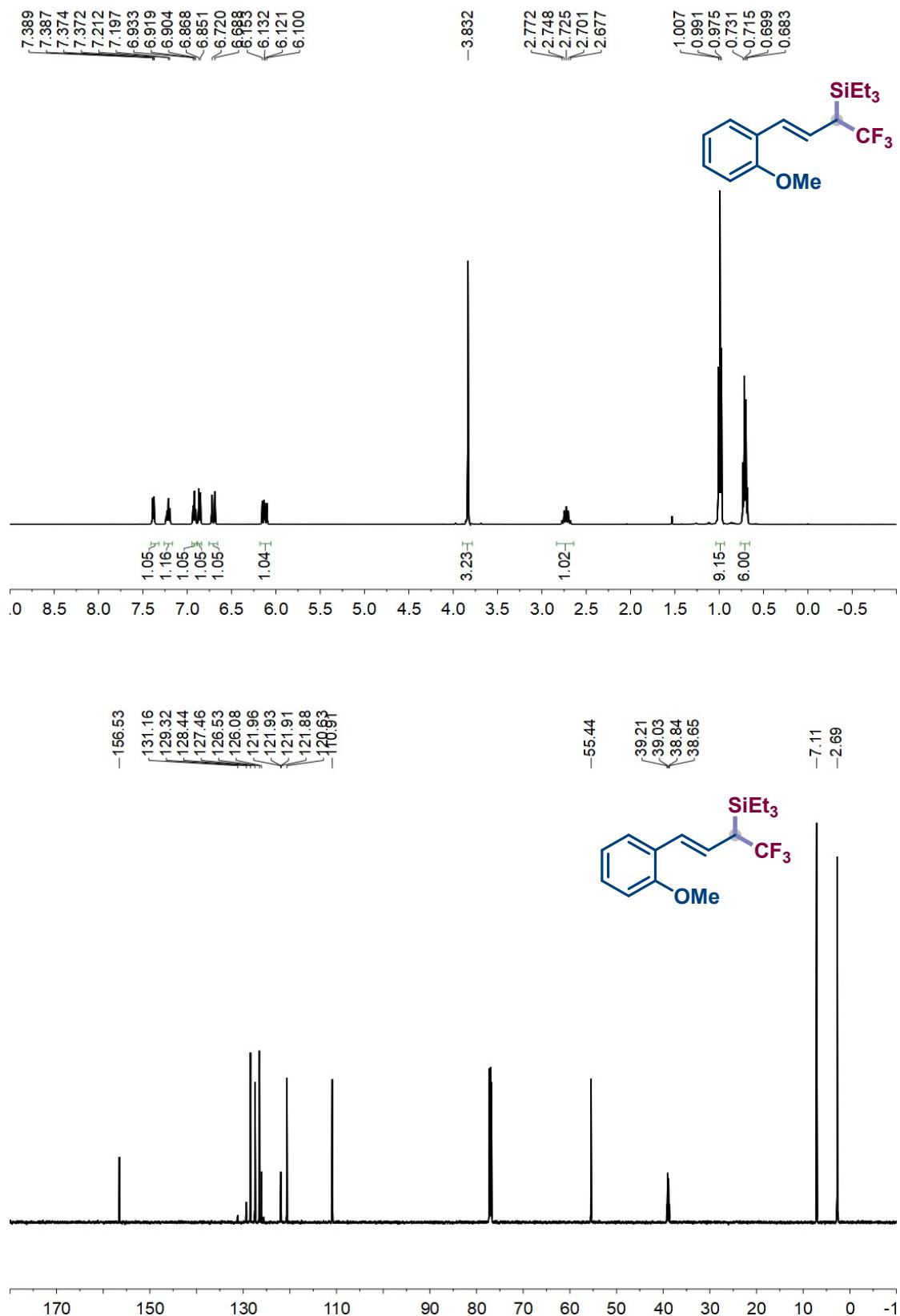


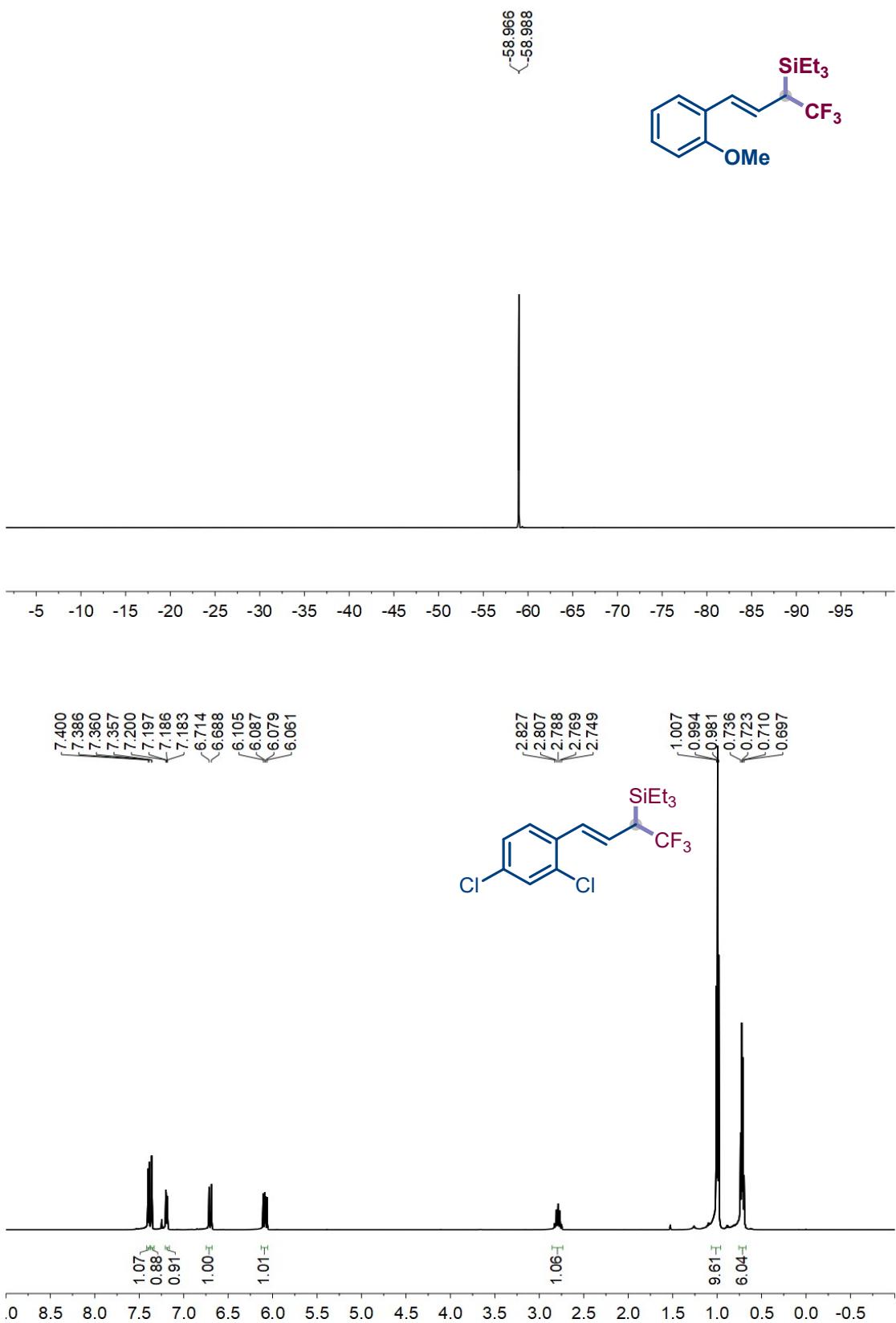


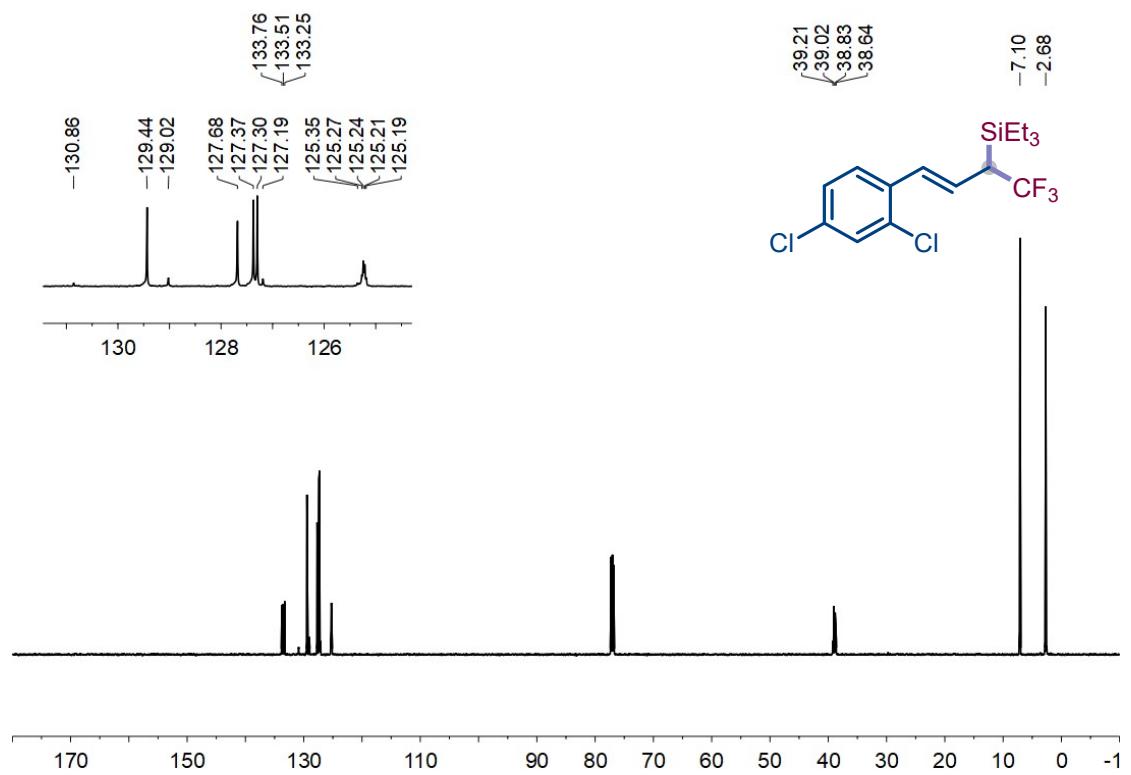


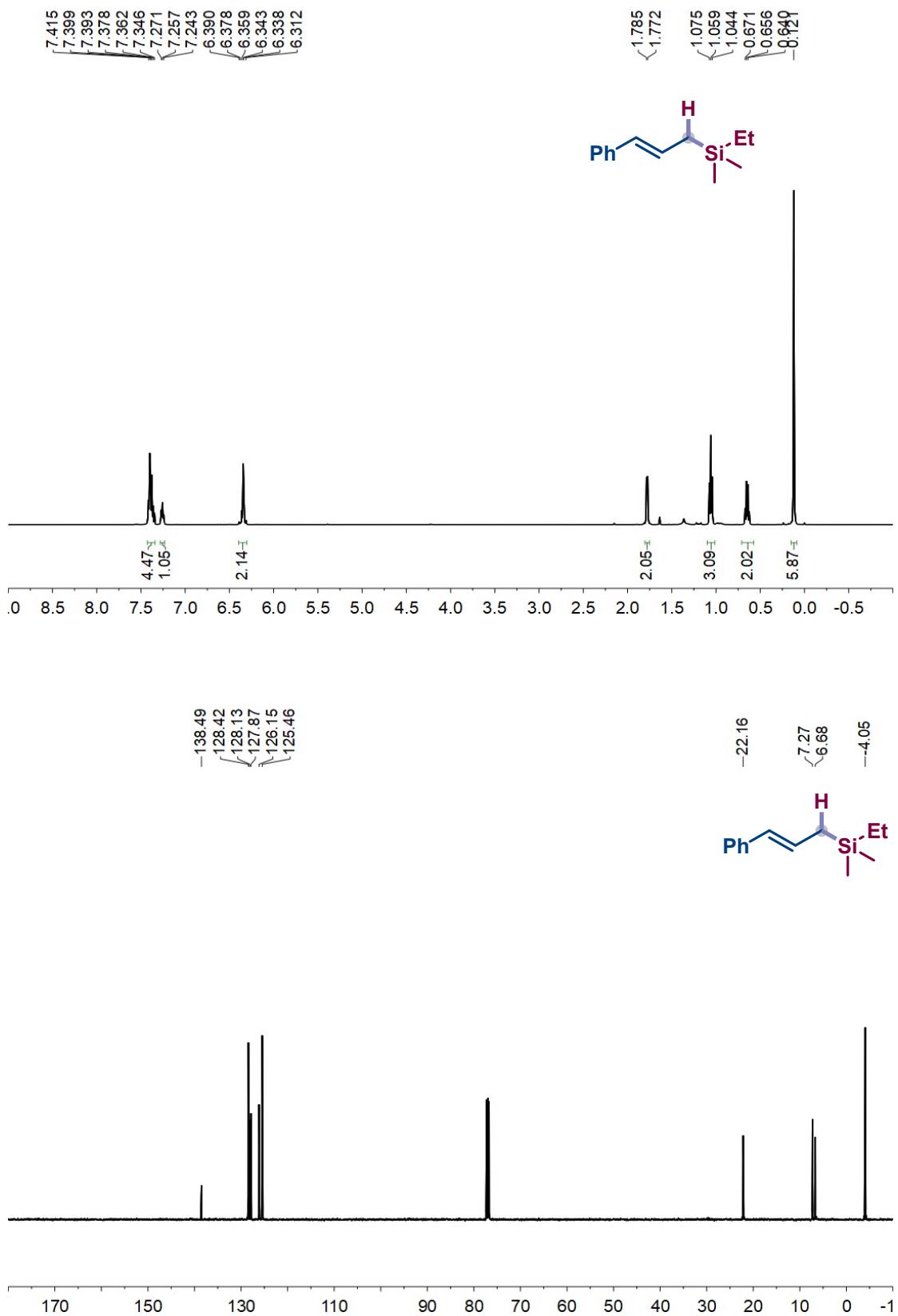


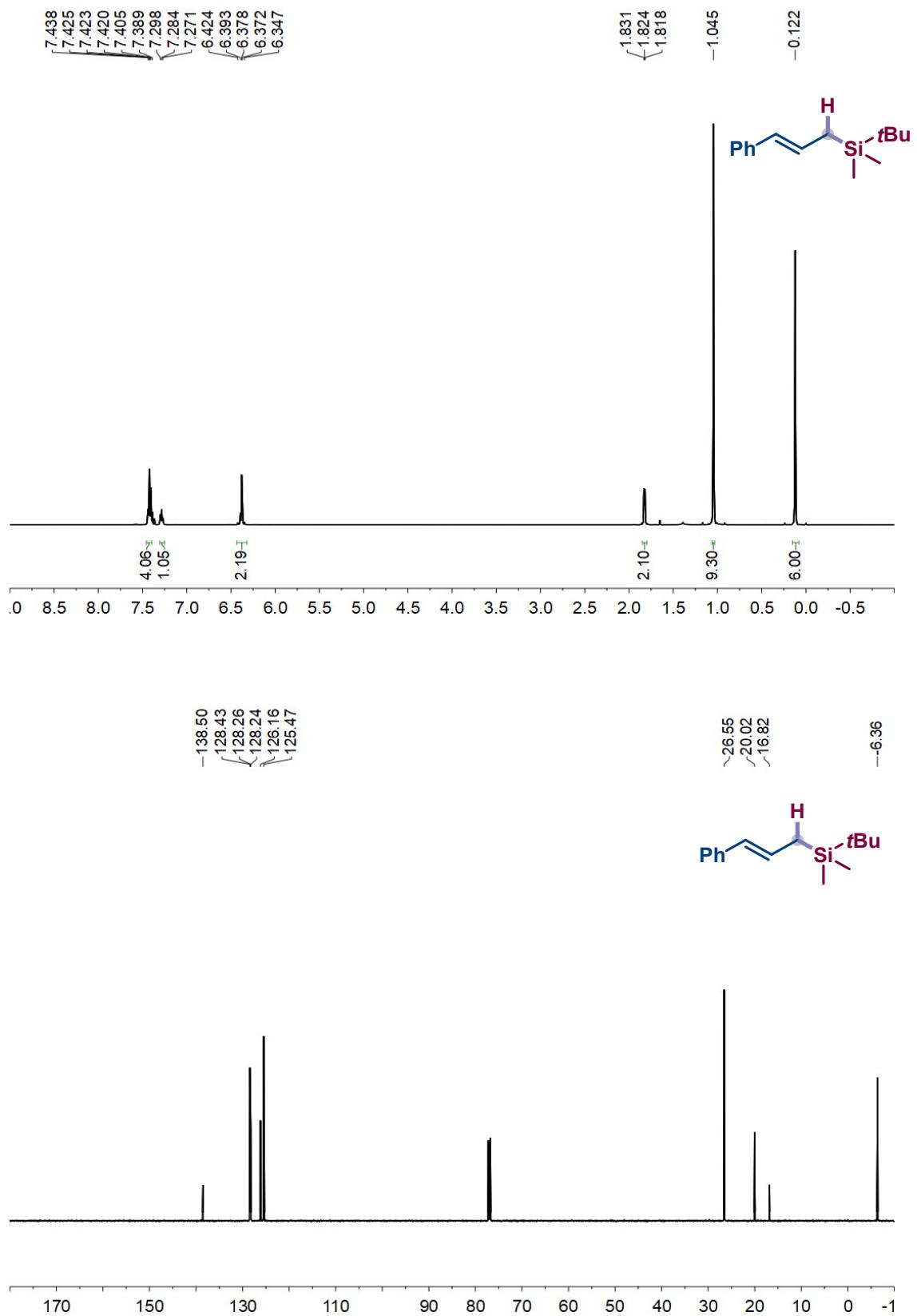


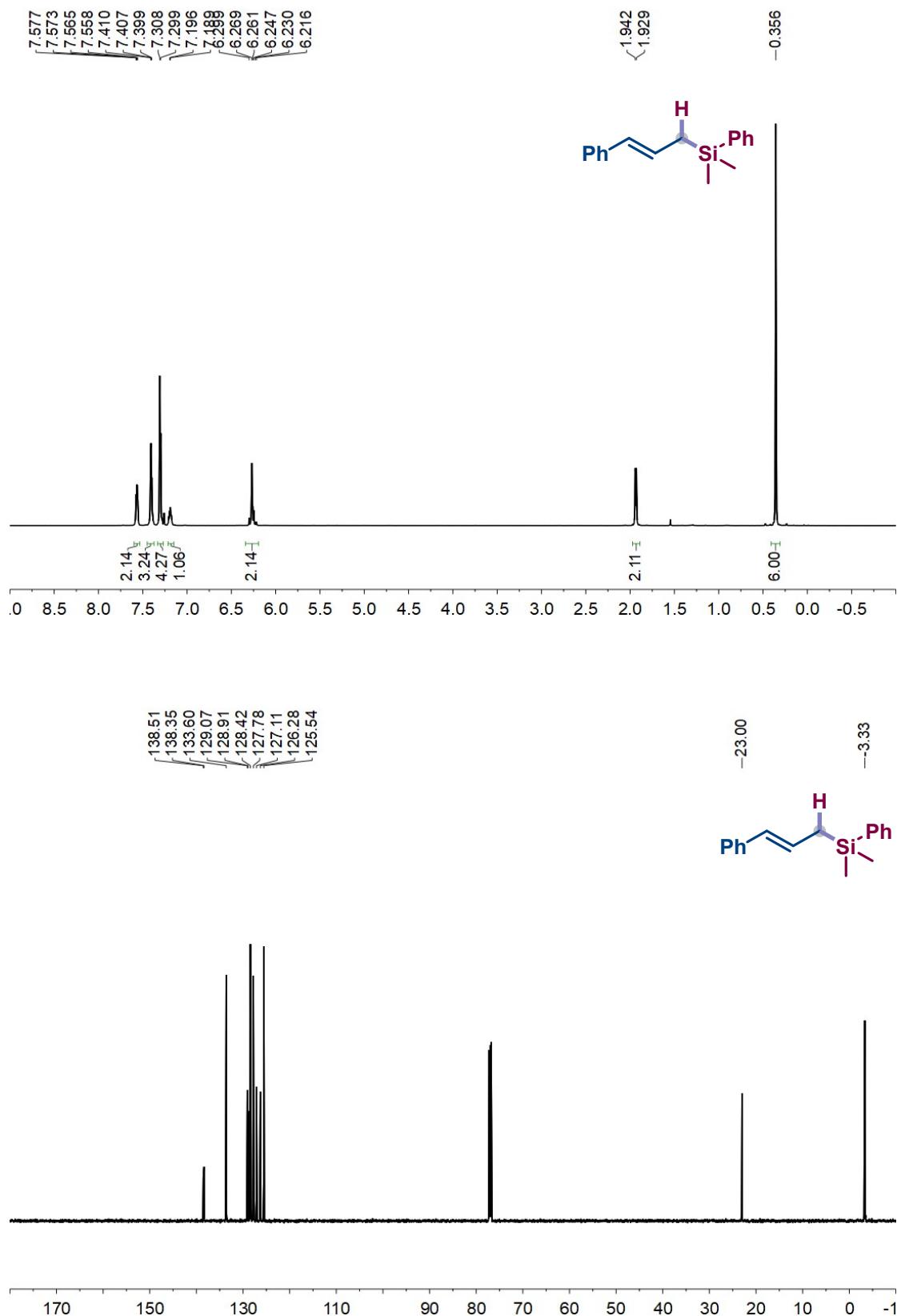


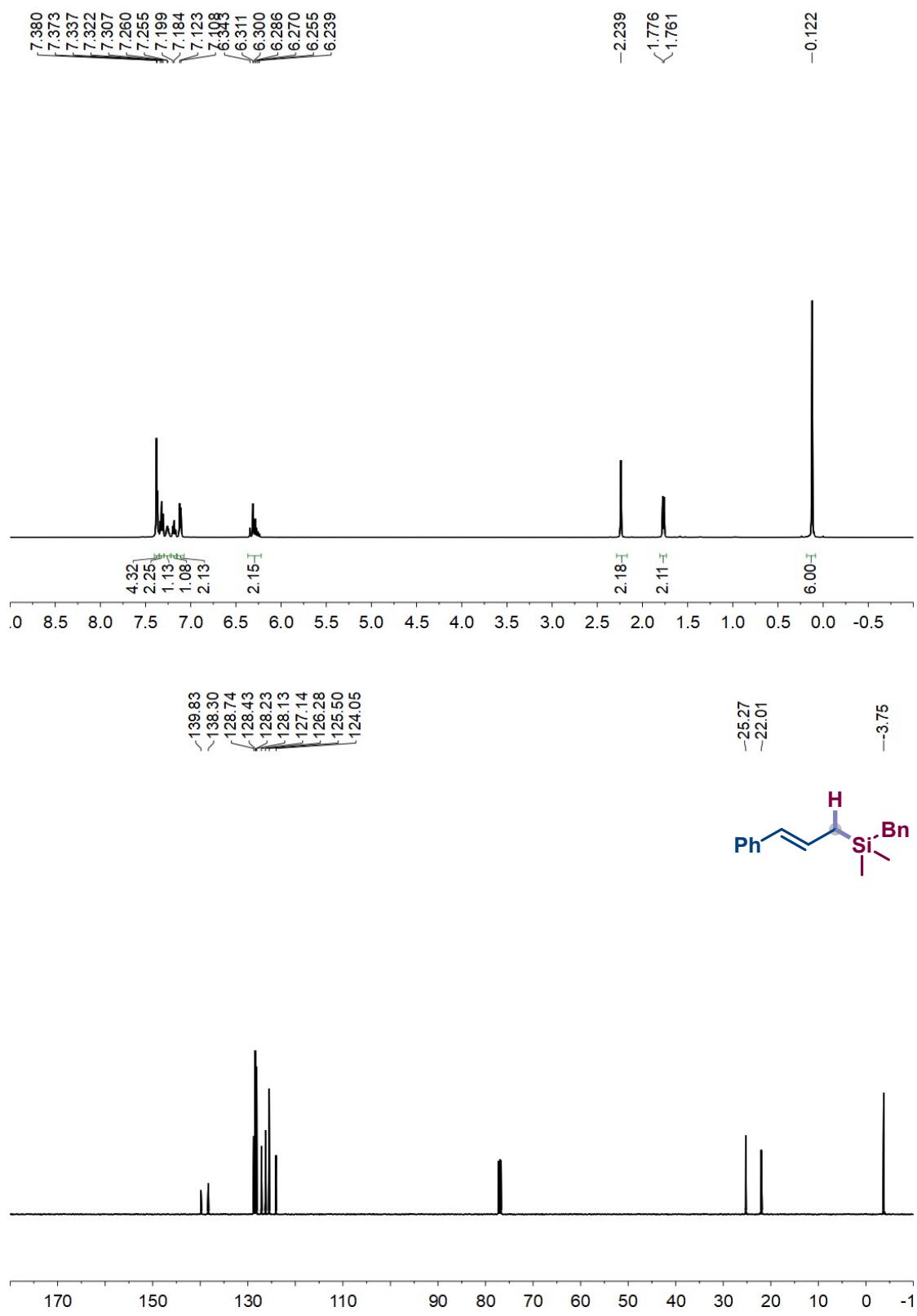


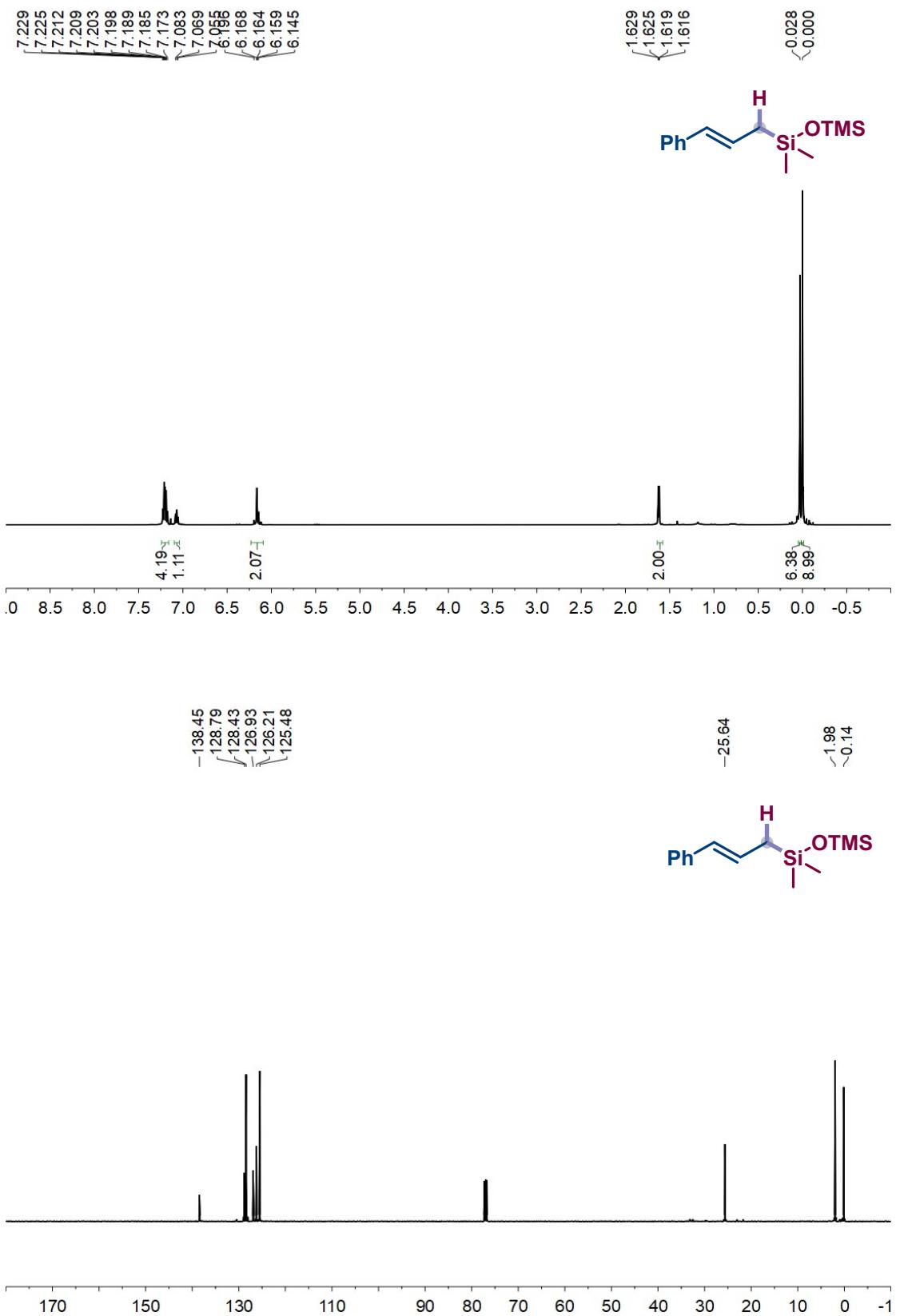


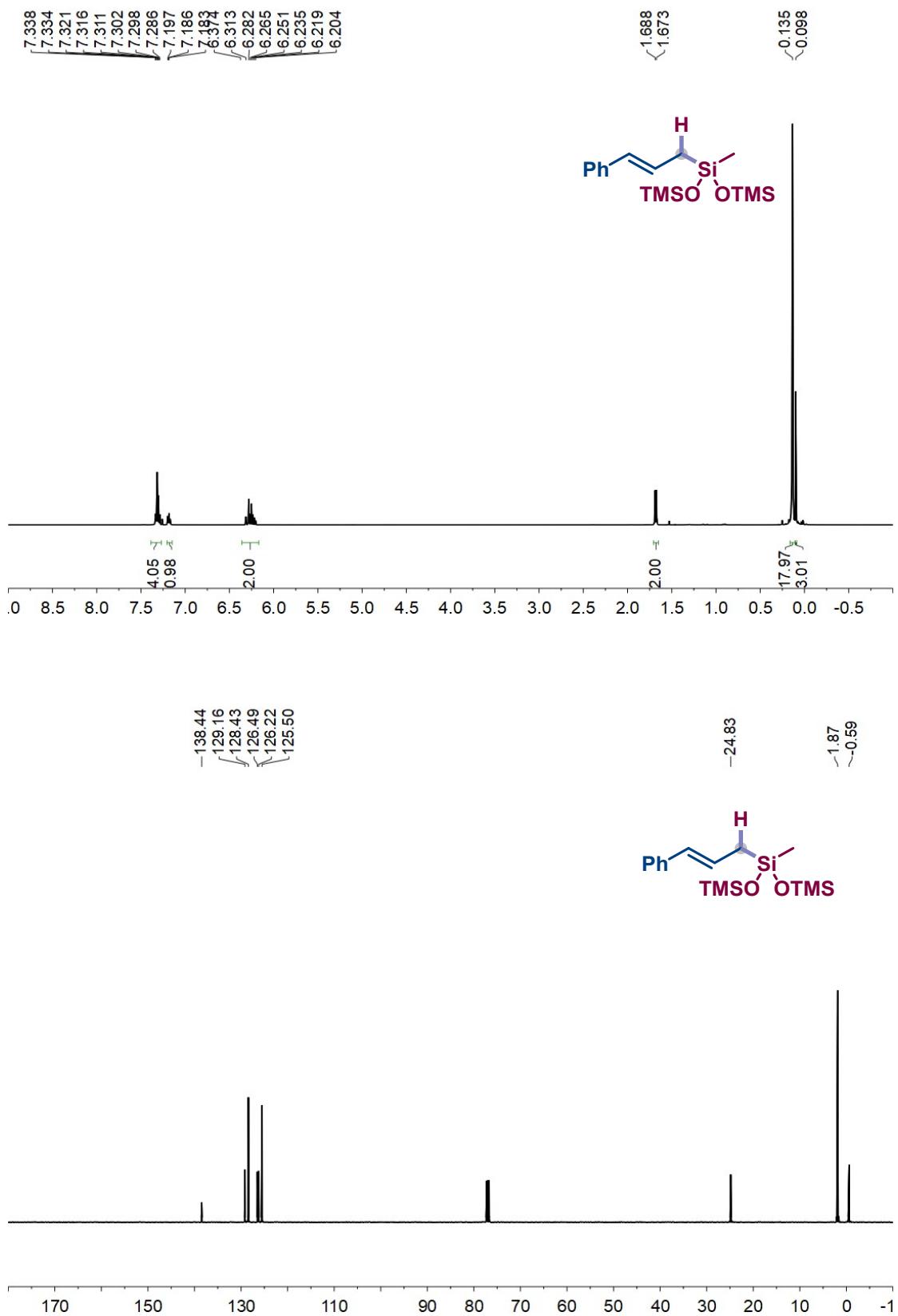


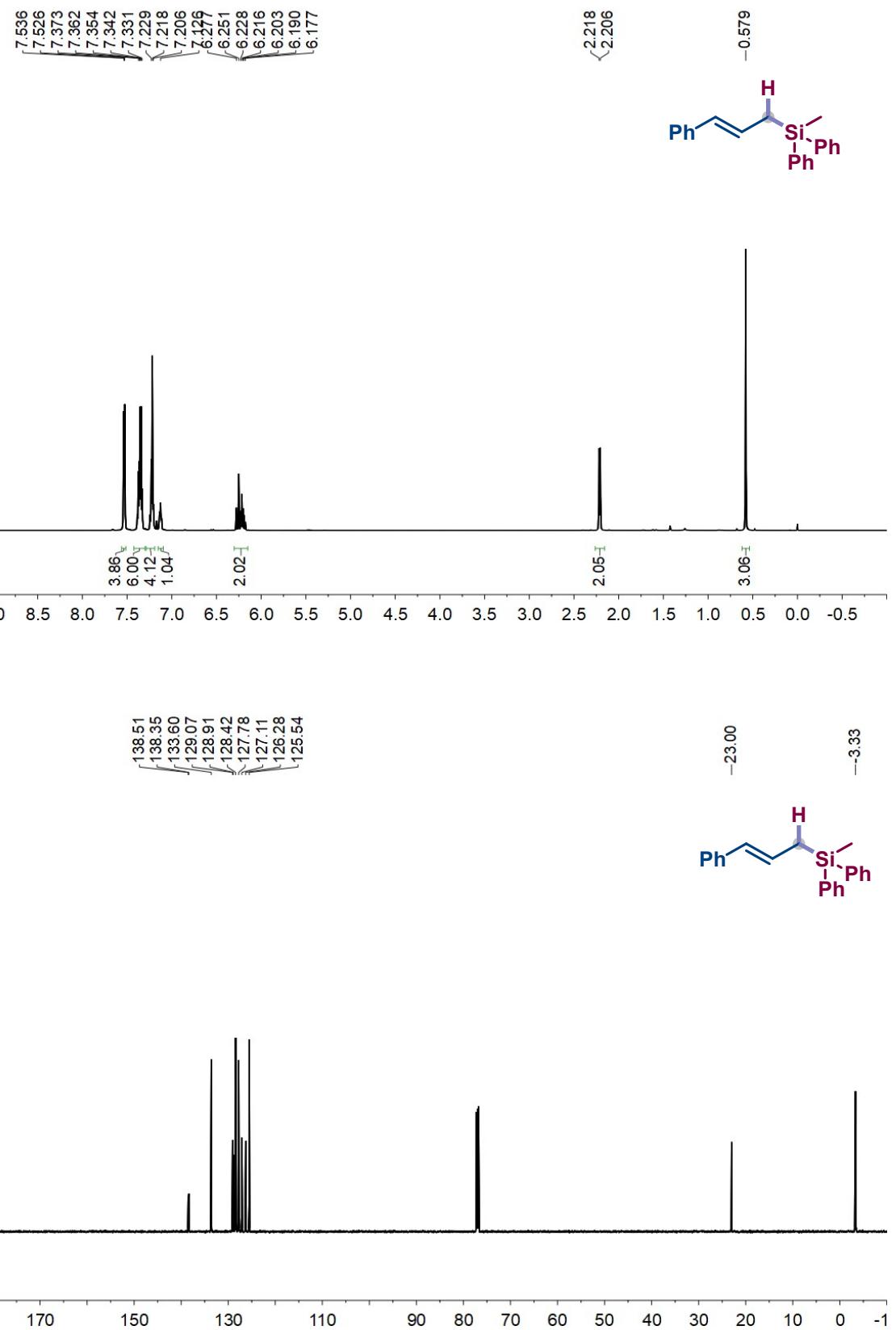


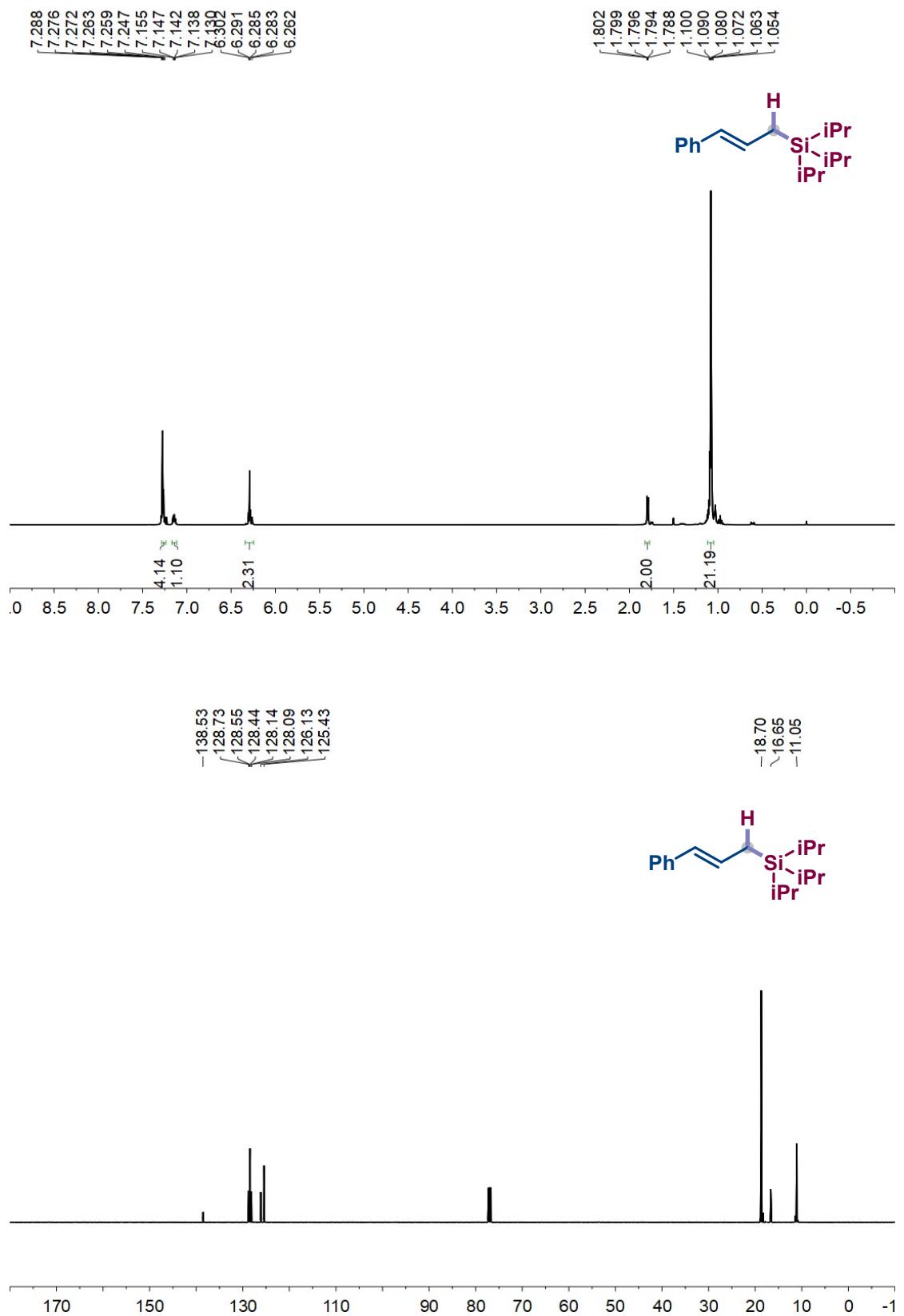




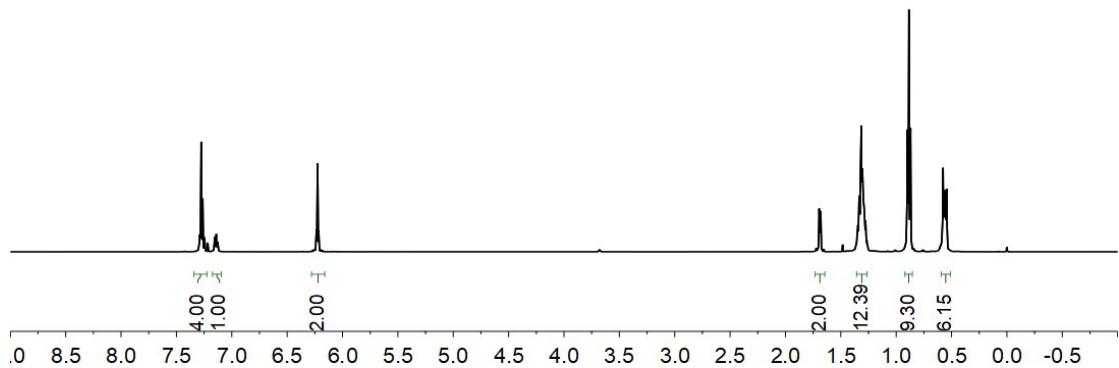
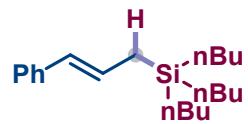






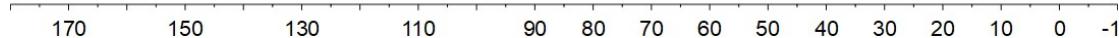
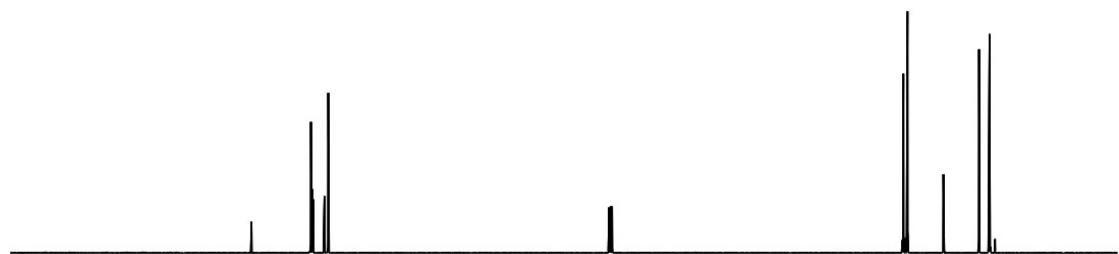
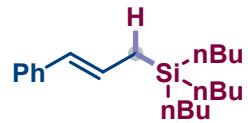


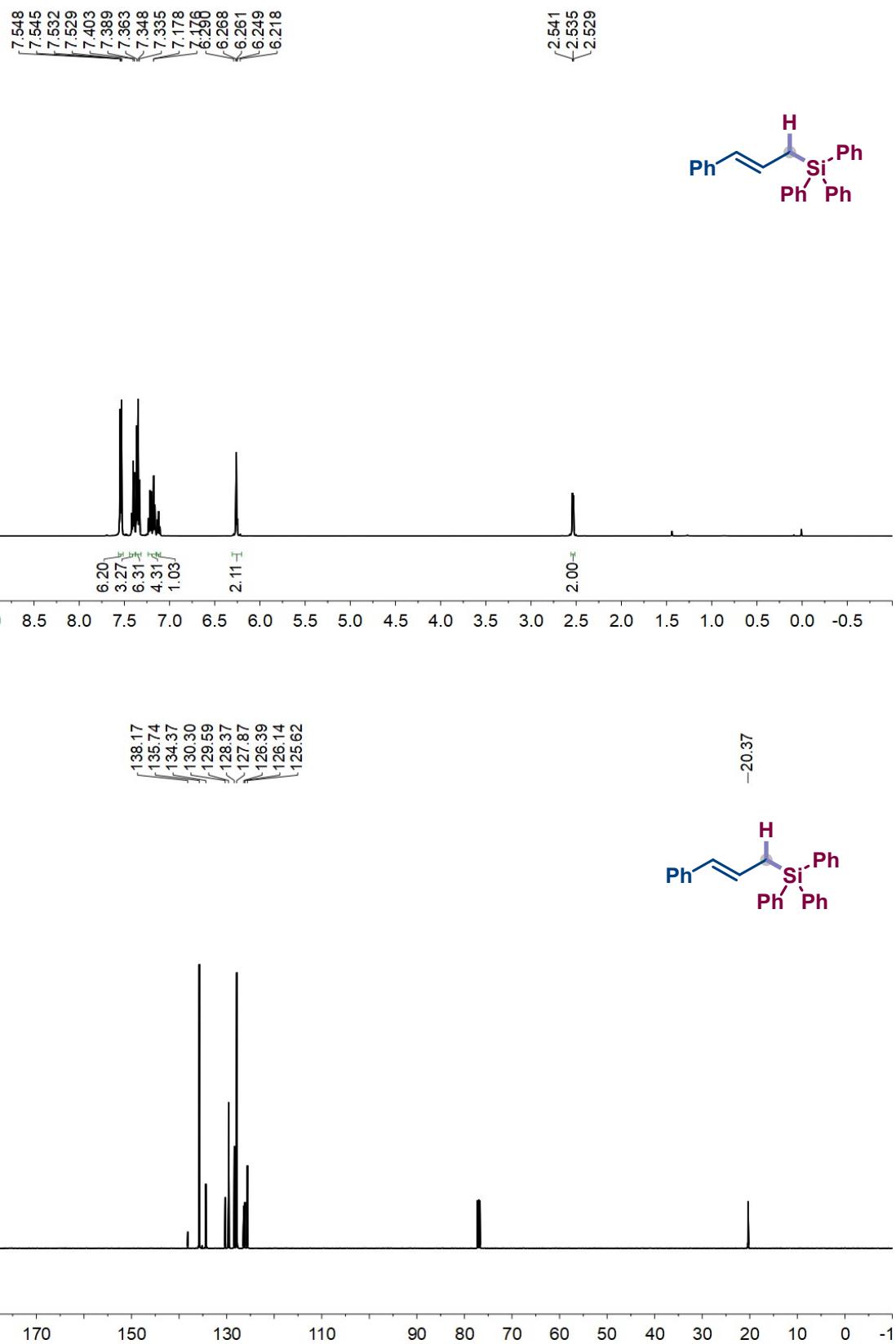
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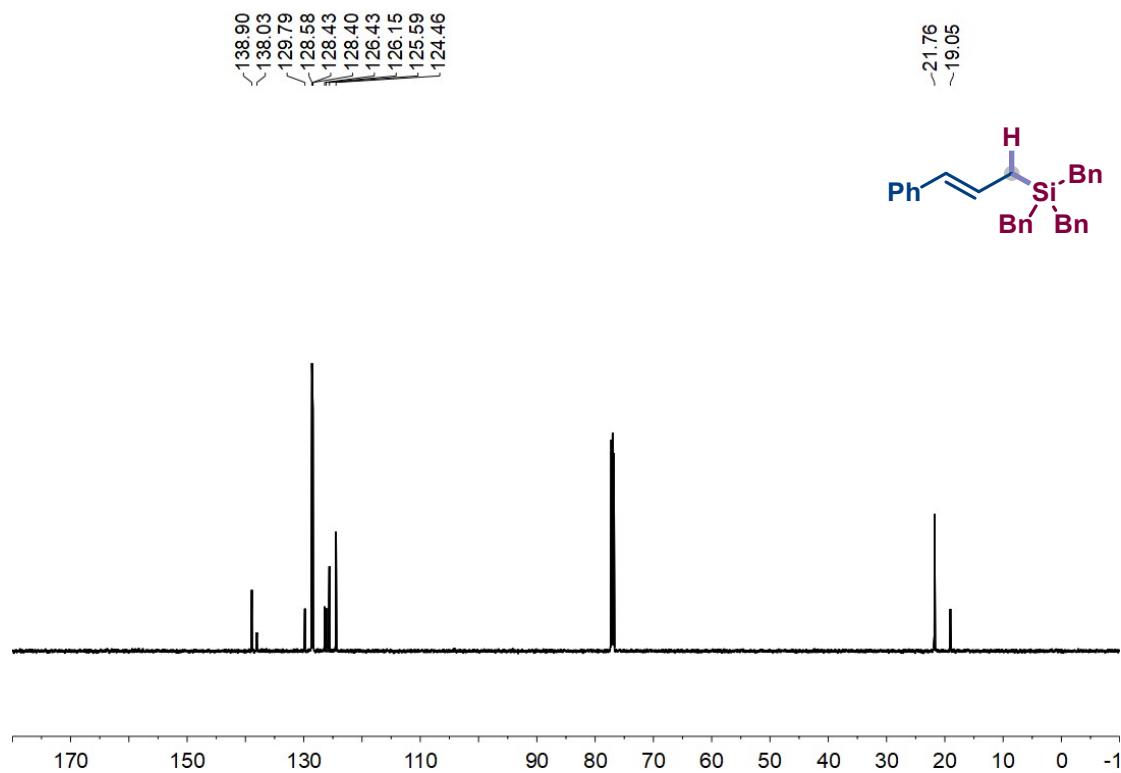
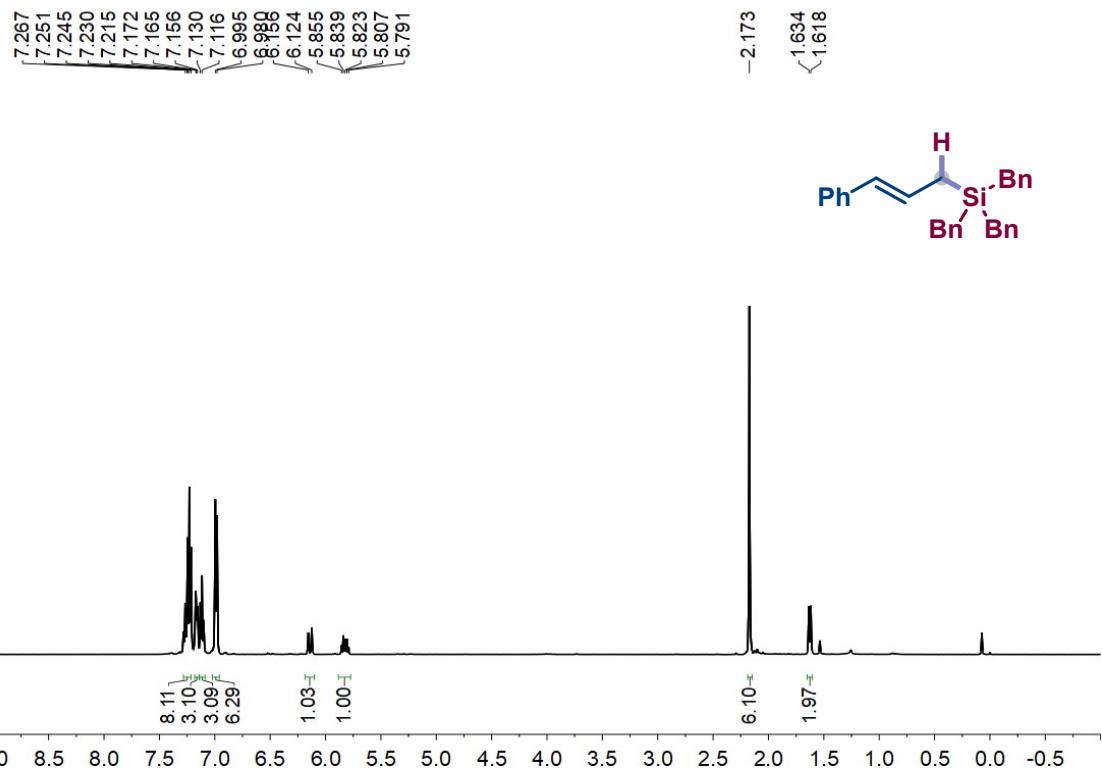


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 -125.44

-26.76
 -26.06
 -19.89
 -13.78
 -11.98







VII. Computational studies

1. Theoretical methodology:

The quantum chemical calculations described in this work were carried out with Gaussian16 package.^[1] Geometry optimizations were conducted in the framework of the density functional theory (DFT) at the M06^[2] level. The effective core potential SDD^[3] basis set was used to represent Ag and Br atoms, all the other atoms (C, H, O, N etc.) were described with 6-31G(d, p) basis set.^[4-6] The nature of the local minima was established with analytical frequencies calculations and The single-point energies were subsequently obtained at the same functional and basis set with SMD(CHCl₃) solvent model.^[7] Intrinsic reaction coordinate (IRC)^[8,9] calculations were carried out to ascertain the true nature of the transition states. 3D structures of optimized geometries were generated using CYLview visualization software.^[10]

- [1]. Gaussian 16 Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc. Wallingford CT, **2019**.
- [2]. Y. Zhao, D. G. Truhlar, Zhao, Y. and Truhlar, D. G. (2008). The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* 120, 215–241.
- [3]. M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, *86*, 866.
- [4]. J. Andzelm, S. Huzinaga, Gaussian Basis Sets for Molecular Calculations, Elsevier Science, New York, **1984**.
- [5]. W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257.

- [6]. J. D. Dill, J. A. Pople, *J. Chem. Phys.* **1975**, *62*, 2921.
- [7]. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378.
- [8]. K. Fukui, *J. Phys. Chem.* **1970**, *74*, 4161.
- [9]. K. Fukui, *Acc. Chem. Res.* **1981**, *14*, 363.
- [10]. C. Y. Legault, CYLview, 1.0b; Université de Sherbrooke: Canada, 2009. Available at: <http://www.cylview.org> (accessed September, 2014).

2、Cartesian coordinates of the computed structures

1a

Zero-point correction=	0.338308 (Hartree/Particle)
Thermal correction to Energy=	0.383646
Thermal correction to Enthalpy=	0.384590
Thermal correction to Gibbs Free Energy=	0.245608
Sum of electronic and zero-point Energies=	-1538.067034
Sum of electronic and thermal Energies=	-1538.021695
Sum of electronic and thermal Enthalpies=	-1538.020751
Sum of electronic and thermal Free Energies=	-1538.159734

N	1.39944100	3.29730600	-2.49219300
N	0.81499300	4.26830600	-2.51914500
C	2.04115600	2.13018400	-2.41612700
H	1.95841800	1.55863100	-3.34368900
C	3.26424400	2.06322200	-1.60587300
H	3.37956700	2.83035400	-0.84209800
C	4.17287200	1.08706100	-1.78781800
H	3.98094900	0.40282100	-2.61909700
C	5.38447700	0.82242400	-1.01301300
C	6.48209200	0.23944900	-1.69276600
C	5.48164100	1.04728500	0.37972000

C	7.64544100	-0.06504400	-0.99463400
C	6.66717500	0.71563100	1.03770100
C	7.76383600	0.17132400	0.37533700
H	8.48574900	-0.50418100	-1.53464100
H	6.72833800	0.88079000	2.11447800
Ag	0.74417500	0.84254900	-0.98575100
N	0.65598900	-1.26718800	0.11153400
N	-0.41335500	-1.50963000	0.92011700
N	-0.42906400	1.49283100	1.02337200
N	-1.52315600	0.75292200	1.34676400
N	-1.57192400	0.21428800	-1.55376400
N	-2.18460200	-0.61772300	-0.67010400
B	-1.72425300	-0.68866800	0.81194800
C	1.57096300	-2.17083900	0.41573400
C	1.13236800	-3.03095900	1.42659100
C	-0.13811800	-2.56765100	1.71318800
C	-0.62526200	2.69341600	1.53650700
C	-1.84599100	2.77940600	2.21166200
C	-2.38381900	1.51485900	2.05438300
C	-2.18743000	0.04908400	-2.70941600
C	-3.21773600	-0.89207100	-2.62252900
C	-3.17184800	-1.28955100	-1.29824300
H	-2.56572700	-1.22582100	1.45557500
Br	-4.40072800	-1.47585300	-3.97753700
Br	-2.58523000	4.25929000	3.12685700
Br	2.04936400	-4.48743000	2.20908400
Br	-1.33405800	-3.26682900	3.00473000
Br	3.24600300	-2.20366600	-0.47278000
Br	-4.06177300	0.90051200	2.68197000
Br	0.66435900	4.06644400	1.29517400
Br	-4.27380800	-2.57407900	-0.44776600

Br	-1.65066400	1.04364300	-4.23742600
C	4.35360900	1.58589300	1.21135500
H	4.28636200	2.68148100	1.16394100
H	3.37586000	1.19200600	0.90114100
H	4.50188100	1.32509100	2.26480200
C	9.03486300	-0.14092900	1.10321400
H	8.86034600	-0.28608200	2.17498200
H	9.51260300	-1.04507100	0.70858500
H	9.76170900	0.67597300	0.99981800
C	6.41904000	-0.04898600	-3.16471500
H	5.65625600	-0.80367500	-3.40463800
H	6.17337800	0.84566100	-3.75062400
H	7.37842500	-0.43260700	-3.52623500

TS1

Zero-point correction=	0.335951 (Hartree/Particle)
Thermal correction to Energy=	0.380576
Thermal correction to Enthalpy=	0.381521
Thermal correction to Gibbs Free Energy=	0.244737
Sum of electronic and zero-point Energies=	-1538.045406
Sum of electronic and thermal Energies=	-1538.000781
Sum of electronic and thermal Enthalpies=	-1537.999837
Sum of electronic and thermal Free Energies=	-1538.136621

N	2.09261200	0.72544700	-3.83014400
N	1.66814400	1.58129900	-4.40046800

C	2.51827900	-0.18567000	-2.36123300
H	2.67711300	-1.15120100	-2.85534100
C	3.72007700	0.42169000	-1.84700300
H	3.62838500	1.41342500	-1.40882900
C	4.82993800	-0.34862000	-1.68908100
H	4.76585100	-1.33170100	-2.16007400
C	6.03217600	-0.12898600	-0.90405700
C	6.77603700	-1.27843300	-0.52054300
C	6.50077500	1.15239000	-0.51592700
C	7.92266300	-1.12856600	0.25004300
C	7.66373500	1.24750000	0.24377900
C	8.38308700	0.12565400	0.65084800
H	8.47936700	-2.01812600	0.54671500
H	8.02357000	2.23770100	0.52577600
Ag	0.71481600	0.04732200	-1.20276900
N	0.22130400	-0.61526400	1.09539000
N	-0.99952800	-0.33082400	1.62227500
N	-0.87680500	1.69226600	-0.54651500
N	-2.04931900	1.33287600	0.03875700
N	-1.50412900	-1.06876100	-1.54230900
N	-2.24052600	-1.17042100	-0.40569500
B	-2.21293400	-0.06760700	0.68600900
C	1.05774200	-0.69910100	2.11395600
C	0.41201300	-0.47838000	3.33532400
C	-0.89966100	-0.24316800	2.96402300
C	-1.02654000	2.93210100	-0.96890700
C	-2.29757900	3.43098400	-0.66834200
C	-2.91058800	2.37115400	-0.02389500
C	-1.66242100	-2.20647900	-2.19275200
C	-2.49997700	-3.08969900	-1.50445900
C	-2.83540100	-2.38051400	-0.36425500

H	-3.22174900	-0.09912100	1.31762400
Br	-3.05707600	-4.82680100	-2.00472100
Br	-3.00834000	5.14345700	-1.03997300
Br	1.14657300	-0.50160700	5.07819400
Br	-2.36127600	0.16514500	4.09795300
Br	2.90148000	-1.05166800	1.82323500
Br	-4.66697500	2.33254300	0.68238300
Br	0.39639600	3.81307600	-1.86839500
Br	-3.91243800	-2.96255500	1.08171300
Br	-0.79058200	-2.48992800	-3.85914000
C	5.82339900	2.42863100	-0.91274900
H	5.52783100	2.43270700	-1.96841000
H	4.91760800	2.61141700	-0.31843300
H	6.49082400	3.28028000	-0.74687900
C	9.60504700	0.25882300	1.50333300
H	10.10279600	1.22212300	1.34820200
H	9.34594000	0.19583700	2.56870600
H	10.32598200	-0.54089900	1.30070000
C	6.35510100	-2.66701000	-0.90892400
H	5.34934400	-2.91612000	-0.54784700
H	6.34784300	-2.80695400	-1.99769600
H	7.04627700	-3.40573000	-0.49197500

Int1

Zero-point correction=	0.329178 (Hartree/Particle)
Thermal correction to Energy=	0.372442
Thermal correction to Enthalpy=	0.373386

Thermal correction to Gibbs Free Energy=	0.236970
Sum of electronic and zero-point Energies=	-1428.622582
Sum of electronic and thermal Energies=	-1428.579319
Sum of electronic and thermal Enthalpies=	-1428.578375
Sum of electronic and thermal Free Energies=	-1428.714790

C	3.00062500	-0.22889900	1.16989900
H	3.17236300	-0.69073900	2.15446600
C	4.19205500	0.07526500	0.52140800
H	4.14983900	0.53073100	-0.46235100
C	5.40991600	-0.20099200	1.14574600
H	5.27424600	-0.65769000	2.12740600
C	6.76823800	-0.00863500	0.77317200
C	7.75973500	-0.43147400	1.72189300
C	7.19885000	0.56399100	-0.46764700
C	9.10165000	-0.27719800	1.41985700
C	8.55745200	0.69001900	-0.71105500
C	9.52403100	0.28297100	0.21164400
H	9.85002300	-0.60249000	2.14165400
H	8.88350200	1.12112900	-1.65701700
Ag	1.06398500	0.08778000	0.44949700
N	-0.52808200	1.74569400	-0.08793400
N	-1.72360700	1.44650000	-0.66398000
N	-0.10816800	-0.81750900	-1.57510300
N	-1.45267900	-0.96445600	-1.44418300
N	-1.10138400	-0.93234800	1.40794800
N	-2.26878500	-0.48252000	0.87675100
B	-2.30581100	0.01099100	-0.59476000
C	-0.33479000	3.03940000	-0.26757000
C	-1.39748500	3.62946700	-0.95858300

C	-2.25785700	2.57126200	-1.18594400
C	0.31383400	-1.87369200	-2.24747500
C	-0.73223900	-2.74556000	-2.56530600
C	-1.83891500	-2.12058600	-2.02015800
C	-1.35929100	-1.22087600	2.66946700
C	-2.69524200	-0.97005300	3.00310200
C	-3.23133300	-0.49494800	1.82041800
H	-3.42552200	0.02489000	-1.00136200
Br	-3.57162000	-1.22912400	4.66054700
Br	-0.66452000	-4.37827500	-3.51878100
Br	-1.61599300	5.44149700	-1.45497800
Br	-3.93160000	2.64155800	-2.07036000
Br	1.23765500	3.88636700	0.37531500
Br	-3.62851700	-2.74533000	-2.00568400
Br	2.15486900	-2.07533000	-2.67615200
Br	-5.01052100	0.07763500	1.50662200
Br	0.00478800	-1.89753100	3.80803400
C	6.26249400	1.03770800	-1.53265800
H	5.61669800	0.23130200	-1.90126000
H	5.60967300	1.84366700	-1.17568800
H	6.82693600	1.42431400	-2.38607500
C	10.97569400	0.46614000	-0.07648000
H	11.17878300	0.44953700	-1.15219000
H	11.31699500	1.43871700	0.30338600
H	11.58378100	-0.30191000	0.41273600
C	7.40156600	-1.04602000	3.04244200
H	6.80461200	-0.36953100	3.66588200
H	6.82800000	-1.97325300	2.92398000
H	8.30791800	-1.29191100	3.60263500

Int2

Zero-point correction=	0.535697	(Hartree/Particle)
Thermal correction to Energy=	0.591441	
Thermal correction to Enthalpy=	0.592385	
Thermal correction to Gibbs Free Energy=	0.431776	
Sum of electronic and zero-point Energies=	-1956.001969	
Sum of electronic and thermal Energies=	-1955.946225	
Sum of electronic and thermal Enthalpies=	-1955.945281	
Sum of electronic and thermal Free Energies=	-1956.105891	

C	2.30893700	-2.32359400	-0.88329200
H	2.53658400	-2.89864700	-1.79425000
C	3.46353400	-2.00444700	-0.17539300
H	3.37598200	-1.43186200	0.74445700
C	4.71196200	-2.36412800	-0.68098200
H	4.64621600	-2.87055200	-1.64572000
C	6.03827500	-2.15880200	-0.20586600
C	7.10317900	-2.41003200	-1.13396300
C	6.36217100	-1.73200500	1.12041400
C	8.41185600	-2.19209800	-0.74162800
C	7.69493600	-1.54619500	1.45820100
C	8.73184200	-1.75739100	0.54826500
H	9.21677600	-2.36530200	-1.45554600
H	7.93913400	-1.22885700	2.47147800
Ag	0.36421300	-1.65116300	-0.51010600
N	-1.95505100	-2.01167000	-0.24440700
N	-2.85569100	-0.99499700	-0.14919500
N	-0.36410500	-0.09966400	1.41354500
N	-1.53427500	0.58547000	1.32957300

N	-0.70290800	0.19232400	-1.80407300
N	-1.61717300	0.98033100	-1.18177000
B	-2.41411900	0.47862300	0.05461900
C	-2.65165600	-3.12708000	-0.35249700
C	-4.02792600	-2.88177300	-0.32914800
C	-4.10533700	-1.50831600	-0.19615400
C	0.14104300	0.17493400	2.59910800
C	-0.67076400	1.05288600	3.32626800
C	-1.73162300	1.28283800	2.47015000
C	-0.18554300	0.91472800	-2.77968700
C	-0.73716200	2.20012400	-2.82251000
C	-1.64545000	2.19051900	-1.77928000
H	-3.37884800	1.15887900	0.19586500
Br	-0.35013300	3.61921200	-4.01363600
Br	-0.39109200	1.76073200	5.05842200
Br	-5.44563000	-4.12845300	-0.44585300
Br	-5.68959000	-0.47428500	-0.08211200
Br	-1.77775900	-4.80370300	-0.51261300
Br	-3.23848400	2.38334100	2.80133000
Br	1.77886400	-0.60911500	3.16318000
Br	-2.74844300	3.62405000	-1.21497600
Br	1.13184900	0.18255600	-3.93675000
C	5.34176600	-1.51170500	2.19194600
H	4.75987000	-0.59657900	2.01346100
H	4.63630100	-2.34806000	2.26442100
H	5.83399600	-1.39910700	3.16272100
C	10.15625000	-1.55675800	0.94366100
H	10.24441100	-0.99620600	1.87922600
H	10.65368500	-2.52543200	1.08550800
H	10.71319400	-1.02780000	0.16183500
C	6.85171800	-2.87547400	-2.53741700

H	6.33152300	-3.84116100	-2.56421100
H	6.24391500	-2.16219200	-3.10691000
H	7.79886900	-3.00031100	-3.06947100
Si	2.49336100	2.18153300	-0.36625700
H	2.08662700	0.81338900	-0.81728100
C	3.08548900	3.14600200	-1.88450500
C	3.12066900	4.66274400	-1.71583100
H	2.41449900	2.88549600	-2.71790600
H	4.07708000	2.76727000	-2.17714000
H	3.43070300	5.17020600	-2.63869400
H	2.13214400	5.06089700	-1.44999100
H	3.81560100	4.97531100	-0.92557100
C	3.91208700	1.94059400	0.86724800
C	4.76501300	3.16994600	1.16718700
H	4.54905700	1.14207700	0.45084900
H	3.49180800	1.53052800	1.79911600
H	5.56560000	2.94853900	1.88490500
H	5.24593400	3.55546600	0.25867800
H	4.16964100	3.98861400	1.59180800
C	0.97217600	3.02460000	0.39320500
C	1.20571900	3.88866900	1.62847600
H	0.24920900	2.23169500	0.63070400
H	0.49814900	3.62356200	-0.40104400
H	0.26321200	4.29549100	2.02169900
H	1.67170200	3.31457100	2.44191700
H	1.86308400	4.74312600	1.41826700

TS2

Zero-point correction=	0.533544	(Hartree/Particle)
Thermal correction to Energy=	0.588709	
Thermal correction to Enthalpy=	0.589653	
Thermal correction to Gibbs Free Energy=	0.430353	
Sum of electronic and zero-point Energies=	-1955.995235	
Sum of electronic and thermal Energies=	-1955.940070	
Sum of electronic and thermal Enthalpies=	-1955.939126	
Sum of electronic and thermal Free Energies=	-1956.098426	

C	-2.57137300	0.61331600	-0.83147300
H	-2.91773100	0.17863900	-1.78085300
C	-3.63951500	1.14324500	-0.05615800
H	-3.40127000	1.59510300	0.90320300
C	-4.90493500	1.20822400	-0.58182900
H	-4.99853800	0.73585800	-1.56282900
C	-6.10787500	1.84727500	-0.10184400
C	-7.12601200	2.11900700	-1.06144500
C	-6.34109200	2.17827500	1.26124300
C	-8.30384400	2.73073500	-0.65650600
C	-7.54785700	2.77463400	1.61351100
C	-8.53539100	3.07347100	0.67665000
H	-9.07059100	2.94733600	-1.40076900
H	-7.72676700	3.01056600	2.66278100
Ag	-0.50805200	0.98048800	-0.55142900
N	1.57802000	1.87651900	-0.51977400
N	2.70975300	1.11937000	-0.54550500
N	0.63241800	-0.42541100	1.36342700
N	1.98786300	-0.45470300	1.28806000
N	1.12205800	-0.62463000	-2.08282700
N	1.86591100	-1.20489000	-1.10752300
B	2.68663800	-0.36564400	-0.09351400

C	1.92839900	3.09810500	-0.88422700
C	3.29619400	3.18080400	-1.15491400
C	3.74736100	1.89371100	-0.92460800
C	0.33970300	-0.41071500	2.64992800
C	1.48521800	-0.43390000	3.45316900
C	2.51396700	-0.45589600	2.52947200
C	0.54693800	-1.61629600	-2.73757500
C	0.88888000	-2.86810500	-2.21199000
C	1.73321900	-2.54478300	-1.16405900
H	3.80523200	-0.77545200	-0.00835400
Br	0.37690600	-4.58896400	-2.81476700
Br	1.60625000	-0.44616000	5.34153300
Br	4.29457000	4.69030900	-1.70076000
Br	5.52612000	1.27167300	-1.10266700
Br	0.63886300	4.48243200	-0.99726100
Br	4.37624100	-0.47091700	2.87705100
Br	-1.47178000	-0.36179200	3.22806900
Br	2.59302600	-3.71494700	0.05474800
Br	-0.58050100	-1.25160500	-4.22710000
C	-5.37136700	1.87788300	2.36327800
H	-4.97876900	0.85530800	2.30187700
H	-4.51067700	2.55958000	2.35299100
H	-5.85851900	1.99195200	3.33675500
C	-9.80355900	3.75358900	1.08107700
H	-10.00923900	3.62536400	2.14891200
H	-9.74340100	4.83273900	0.88648300
H	-10.66086700	3.37481200	0.51329000
C	-6.96029000	1.78728500	-2.51602000
H	-6.08443400	2.27872700	-2.95657000
H	-6.84456700	0.70859600	-2.68476100
H	-7.83947700	2.10959000	-3.08179200

Si	-2.85116100	-2.34205200	-0.01107900
H	-2.28711500	-0.90861500	-0.19065600
C	-3.38024400	-2.91178300	-1.72814300
C	-3.54811600	-4.42554700	-1.85409500
H	-2.61493500	-2.56505000	-2.44094400
H	-4.30952900	-2.39106700	-2.00804600
H	-3.78790300	-4.72180500	-2.88292800
H	-2.62639000	-4.95301600	-1.57427500
H	-4.34951900	-4.80799100	-1.20942500
C	-4.32009800	-2.16232100	1.15666600
C	-5.29479400	-3.33972900	1.15355800
H	-4.85415400	-1.24437700	0.86125800
H	-3.94589300	-1.97847300	2.17443200
H	-6.12682200	-3.17271900	1.84868500
H	-5.73254800	-3.49673400	0.15949000
H	-4.80916600	-4.27823900	1.44974500
C	-1.41241600	-3.35869000	0.66212700
C	-1.80106400	-4.50205400	1.59574400
H	-0.72176000	-2.67037100	1.17026100
H	-0.85509800	-3.74447400	-0.20533300
H	-0.91590200	-5.05274300	1.93938300
H	-2.31996400	-4.13366400	2.49064200
H	-2.46382600	-5.22858100	1.10733400

Pr

Zero-point correction=	0.429389 (Hartree/Particle)
Thermal correction to Energy=	0.453256
Thermal correction to Enthalpy=	0.454200
Thermal correction to Gibbs Free Energy=	0.375749
Sum of electronic and zero-point Energies=	-992.533027

Sum of electronic and thermal Energies=	-992.509160
Sum of electronic and thermal Enthalpies=	-992.508216
Sum of electronic and thermal Free Energies=	-992.586667

C	-1.43657500	1.37533800	-1.10619300
H	-1.42005000	2.35667600	-0.60755300
C	-0.09617100	0.73461000	-1.06904200
H	0.05600100	-0.09586800	-1.76203000
C	0.90188400	1.07953100	-0.24138100
H	0.73487100	1.95270100	0.39736700
C	2.22451900	0.44766600	-0.12364000
C	3.34394900	1.28909000	0.08228400
C	2.42393500	-0.94859900	-0.16473300
C	4.61396300	0.73850800	0.21050800
C	3.71786200	-1.45772000	-0.02361300
C	4.82710800	-0.63913300	0.15555900
H	5.46616700	1.40410400	0.35863300
H	3.85690200	-2.53995100	-0.04585900
C	1.30241700	-1.93547000	-0.32135700
H	0.39095200	-1.61174300	0.19618000
H	1.03128900	-2.09469500	-1.37366600
H	1.59615800	-2.91164000	0.08029000
C	6.20806900	-1.20742800	0.27899200
H	6.18474200	-2.28672100	0.46472500
H	6.79035400	-1.04485300	-0.63771300
H	6.76627900	-0.73460400	1.09602100
C	3.18318700	2.77980600	0.14788200
H	2.66725500	3.17453700	-0.73626700
H	2.59341300	3.09221000	1.02055900

H	4.15745900	3.27455800	0.21870900
Si	-2.75730100	0.31278900	-0.23409100
H	-1.76990300	1.53873600	-2.14217100
C	-2.20051200	0.08563400	1.55980200
C	-3.28688300	-0.29994500	2.55998600
H	-1.73967500	1.03816400	1.86755600
H	-1.38165000	-0.64952500	1.58533600
H	-2.88852100	-0.39815600	3.57791000
H	-4.08382200	0.45405000	2.59986800
H	-3.76031900	-1.25737300	2.30709300
C	-2.89471800	-1.33279100	-1.16160500
C	-3.42304800	-2.51451200	-0.35343400
H	-1.89717400	-1.57828000	-1.55718600
H	-3.52512800	-1.16510500	-2.04901300
H	-3.48842200	-3.42862900	-0.95728800
H	-2.76796600	-2.73950400	0.49870700
H	-4.42590400	-2.32354800	0.05049700
C	-4.38413100	1.27574300	-0.32933000
C	-5.65772100	0.46328900	-0.11233100
H	-4.41601600	1.75116300	-1.32229700
H	-4.33314100	2.10749100	0.39068000
H	-6.55966300	1.08266100	-0.19902500
H	-5.75089000	-0.34215100	-0.85261800
H	-5.68419000	-0.00545100	0.87970500