Supporting Information

Boradigermaallyl : inhibition of CH bond activation by borane CO adduct formation followed by CO Insertion

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Content

Experimental

General procedures: All manipulations were carried out under argon atmosphere using standard Schlenk techniques and gloveboxes. Benzene was dried with activated aluminium oxide, *n*-pentane and *n*-hexane were obtained from a MBraun solvent purification systems (SPS). All other solvents (Et_2O, THF, toluene, benzene-d_6, cyclohexane-d_{12}) were distilled from a sodium-potassium alloy and like the previous mentioned solvents subsequently degassed by three freeze–pump–thaw cycles. Starting material boradigermaallyl (**1**) was prepared according to a literature procedure.[1] For the reaction with ^{13}C-labeled carbon monoxide, ^{13}CO from Sigma-Aldrich with an isotopic distribution of 99.0 % ^{13}C and 12 % ^{18}O was commercially purchased. Further chemicals were purchased commercially and used as received.

Elemental analysis: Elemental analysis was performed at the Institute of Inorganic Chemistry, University of Tübingen using an *elementar* vario MICRO Cube.

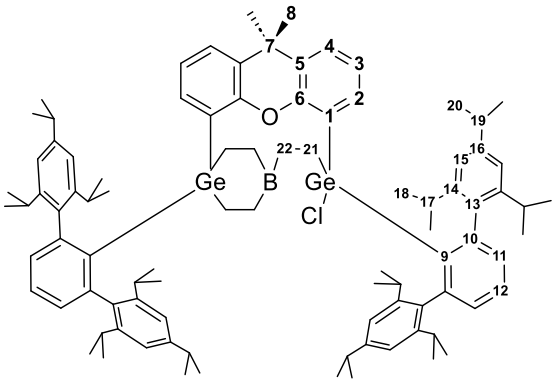
NMR spectroscopy: NMR spectra were recorded with either a Bruker Avance III HD 300 NanoBay spectrometer equipped with a 5 mm BBFO probe head and operating at 300.13 (^{1}H) and 96.29 (^{11}B) MHz, a Bruker AVII+400 NMR spectrometer equipped with Brukers 5 mm QNP (quad nucleus probe) or a 5 mm BBFO probe head operating at 400.11 (^{1}H), 100.61 (^{13}C) and 128.37 (^{11}B) MHz, a Bruker Avance III HDX 600 spectrometer with a 5 mm Prodigy BBO cryo probe head operating at 600.13 (^{1}H) and 150.90 (^{13}C) or a Bruker Avance III HDX 700 NMR spectrometer equipped with a 5 mm TXI probe head operating at 700.29 (^{1}H) and 176.9 (^{13}C) MHz. Chemical shifts are reported in δ values in ppm relative to external $SiMe_4$ (^{1}H, ^{13}C) or $BF_3 \cdot OEt_2$ (^{11}B) referenced in most cases on the solvent ^{2}H resonance frequency as follows: Ξ = 25.145020 % for ^{13}C, Ξ = 32.083 974 % for ^{11}B. The multiplicity of the signals is indicated as s = singlet, d = doublet, t = triplet, sept = septet, m = multiplet or br = broad/unresolved. For the assignment of proton and carbon signals detailed analysis of ^{1}H, ^{13}C{^{1}H}, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC and ^{13}C{^{1}H} DEPT 135 spectra was done.

Powdered sample of **9** was packed into 4 mm o.d. zirconia rotors under the inert atmosphere of a glove box. Solid-state NMR spectra were obtained on a Bruker Avance III HD 300 wide-bore NMR spectrometer (B_0 = 7.05 T) operating at 300.13 (^{1}H) and 96.29 (^{11}B) MHz. Spectra were acquired under high-power proton decoupling (hpdec) using a background suppression sequence (zgbsig) to eliminate the contributionof the stator material, employing a selective “90°” pulse on the central transition (half of solution 90° pulse). . Referencing against Ξ = 32.083974 % (^{11}B)[2] was achieved by the substitution method: an external sample of $CHCl_3$ in acetone in a zirconia rotor was spun at 1.5 kHz and the external magnetic field was adjusted such that the ^{1}H chemical shift of $CHCl_3$ matched a predetermined chemical shift wrt. external 1% TMS in $CHCl_3$. The 4 mm double-bearing-double resonance probe head produced a strong ^{11}B background signal (Fig. SI26) that was eliminated by acquiring and subtracting the spectrum of an empty rotor. Simulation of spectra was achieved using the sola module of Bruker TopSpin 4.1.4.

Crystallography: X-ray data were collected with a Bruker Smart APEX II diffractometer with graphite-monochromated Mo-K_α radiation. The programs used were Bruker’s APEX2 v2011.8-0, including SAINT for data reduction, SADABS for absorption correction, and SHELXS for structure solution, as well as the WinGX suite of programs version 1.70.01 or the GUI ShelXle, including SHELXL for structure refinement.[3-9]

UV/Vis Spectroscopy: Visible UV/Vis absorption spectra were recorded on PerkinElmer Lambda 35 spectrophotometer in gas tight 1 cm quartz cuvettes sealed with Teflon stoppers or Teflon lined screw caps.

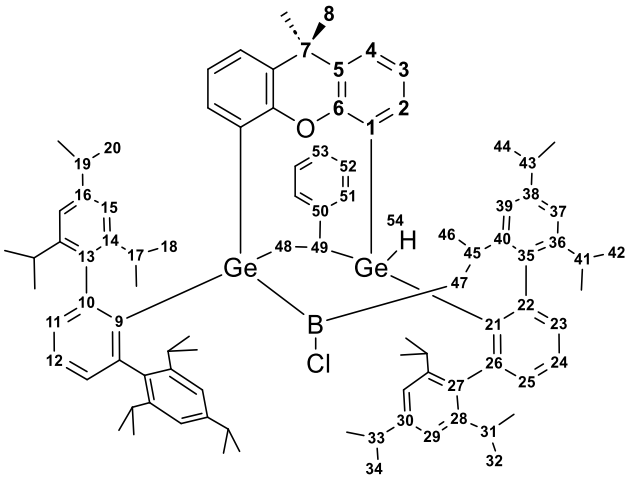
IR spectroscopy. The IR spectra were recorded as potassium bromide pellets, which were prepared in an MBraun glovebox and measured with a Bruker VERTEX 70 IR spectrometer. In addition, IR spectra were measured with an ATR unit on the same device.



Synthesis of compound 2: A turquoise solution of boradigermaallyl **1** (80.0 mg, 58.7 µmol, 1.00 equiv.) in *n*-pentane (5.00 ml) was transferred to a Schlenk tube with a volume of approximately 50 ml and subsequently degassed with one "freeze-pump-thaw" cycle. The argon atmosphere was exchanged for 1 bar ethylene and the solution was then stirred for 2 days at room temperature. A decolorization of the reaction solution already occurred after 60 minutes, however, a complete turnover was not achieved until after 2 days. In the next step, small, suspended solids in the colorless to mint-green solution were filtered off and the solvent was removed under reduced pressure. The residue was dissolved in Et_2O and the solution was concentrated by partial evaporation of the solvent under reduced pressure. Crystallization over a period of one week at −38 °C led to colorless crystals of the product **2** suitable for X-ray diffraction (37.3 mg, 25.8 µmol, 44 %).

^{1}H-NMR (700.21 MHz, tol-d_8, 255 K): δ [ppm] = −0.06 (d, 1H, $^2J_{HH}$ = 11.0 Hz, H-21), 0.39 – 0.46 (m, 2H, H-21 (1H) + H-22 (1H)), 0.53 (d, 3H, $^3J_{HH}$ = 6.5 Hz, H-18), 0.71 – 0.83 (m, 2H, H-22), 0.85 – 0.91 (m, 2H, H-21 (1H) + H-22 (1H)), 0.92 – 0.96 (m, 4H, H-18 (3H) + H-22 (1H)), 0.97 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.00 – 1.04 (m, 1H, H-22) 1.07 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.10 – 1.13 (m, 6H, H-18), 1.16 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.18 – 1.25 (m, 21H, H-18 (6H) + H-20 (15H)), 1.25 – 1.28 (m, 4H, H-18 (3H) + H-21 (1H)), 1.29 – 1.31 (m, 6H, H-8 (3H) + H-20 (3H)), 1.33 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-20), 1.34 – 1.37 (m, 6H, H-18 (3H) + H-20 (3H)), 1.37 – 1.41 (m, 6H, H-18), 1.44 – 1.47 (m, 6H, H-8 (3H) + H-18 (3H)), 1.58 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-18), 1.65 – 1.70 (m, 1H, H-21), 1.73 (d, 3H, $^3J_{HH}$ = 6.6 Hz, H-18), 1.80 – 1.84 (m, 1H, H-21), 2.49 – 2.59 (m, 1H, H-17), 2.73 – 2.84 (m, 4H, H-17 (1H) + H-19 (3H)), 2.92 – 3.00 (m, 2H, H-17 (1H) + H-19 (1H)), 3.09 (sept, 1H, $^3J_{HH}$ = 6.7 Hz, H-17), 3.20 – 3.30 (m, 2H, H-17), 3.30 – 3.38 (m, 1H, H-17), 3.43 (sept, 1H, $^3J_{HH}$ = 6.7 Hz, H-17), 6.38 (t, 1H, $^3J_{HH}$ = 7.4 Hz, H-3), 6.69 (t, 1H, $^3J_{HH}$ = 7.4 Hz, H-3), 6.72 – 6.77 (m, 2H, H-2 (1H) + H-15 (1H)), 6.89 (dd, 1H, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.2 Hz, H-4), 6.95 (s, br, 1H, H-15), 6.96 – 6.98 (m, 2H, H-11 (1H) + H-12 (1H), overlapped by solvent signal), 7.02 (dd, 1H, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.3 Hz, H-4, overlapped by solvent signal), 7.06 – 7.09 (m, 3H, H-15), 7.09 – 7.11 (m, 1H, H-2, overlapped by solvent signal), 7.13 (s, br, 1H, H-15), 7.16 – 7.19 (m, 2H, H-11 (1H) + H-12 (1H)), 7.20 (s, br, 1H, H-15), 7.23– 7.26 (m, 2H, H-11), 7.31 (s, br, 1H, H-15). **^{13}C{^{1}H}-NMR** (176.07 MHz, tol-d_8, 255 K): δ [ppm] = 7.3 (br, C-21), 11.7 (br, C-21), 18.0 (br, C-22), 18.3 (br, C-21), 21.6 (C-18), 22.5 (C-18), 22.7 (C-18), 22.8 (C-18), 23.0 (C-18), 23.1 (C-22), 23.6 (C-18), 23.8 (C-20), 23.9 (C-22), 24.2 (C-18), 24.5 (C-20), 24.5 (C-20), 24.5 (C-20), 24.6 (C-20), 24.6 (C-20), 24.7 (C-20), 24.7 (C-18), 25.1

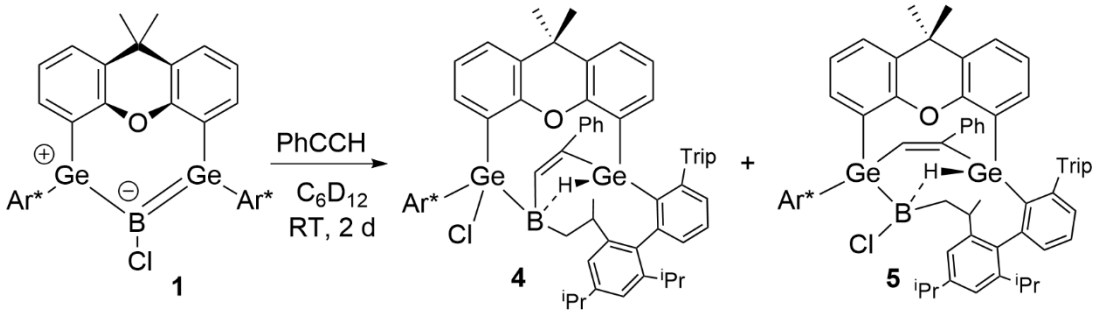
(C-18), 25.2 (C-20), 25.5 (C-18), 26.5 (C-18), 26.6 (C-18), 26.7 (C-18), 26.9 (C-18), 27.0 (C-18), 27.4 (C-18), 31.0 (C-17), 31.1 (C-17), 31.2 (C-17), 31.3 (2 x C-17), 31.4 (C-17), 31.5 (C-17), 32.2 (C-17), 33.9 (C-8), 34.1 (C-8), 34.5 (C-7), 34.7 (C-19), 34.8 (2x C-19), 34.9 (C-19), 120.3 (C-15), 120.4 (C-15), 120.7 (2x C-15), 120.8 (C-15), 121.4 (C-15), 121.8 (C-3 + 2x C-15), 122.4 (C-1), 123.0 (C-3), 126.8 (C-4), 127.4 (C-12), 127.8 (C-4, overlapped by solvent signal), 128.0 (C-12, overlapped by solvent signal), 128.9 (C-1, overlapped by solvent signal), 129.3 (2x C-5), 130.4 (C-11), 131.2 (C-11), 131.4 (C-11), 132.4 (C-11), 133.8 (C-2), 136.9 (C-2), 138.1 (C-13), 138.8 (C-13), 138.9 (C-13), 139.7 (C-9), 139.7 (C-13), 141.4 (C-9), 146.1 (C-14), 146.3 (3x C-14), 146.7 (C-10), 146.9 (C-10), 147.2 (C-14), 147.3 (C-14), 147.5 (C-14 + C-16), 147.6 (C-14), 148.1 (C-10), 148.1 (C-10), 148.3 (C-16), 148.3 (C-16), 149.5 (C-16), 153.8 (C-6), 154.7 (C-6). **^{11}B{^{1}H}-NMR**: No boron NMR signal could be observed in solution. **Elemental analysis calcd (%)** for $C_{93}H_{122}BClGe_2O$ + Et_2O: C 76.57, H 8.74; found: C 76.62, H 8.54.



Synthesis of compound 3: Boradigermaallyl **1** (60.0 mg, 44.0 µmol, 1.00 equiv.) was dissolved in pentane (2.00 ml) and styrene (30.0 µl, 261 µmol, 5.92 equiv.) was added while stirring at room temperature. A color change from turquoise to brown-red was already visible within half an hour, however, the complete conversion of the reactants required one day of stirring at room temperature and resulted in a salmon-colored suspension. Volatile components were removed under reduced pressure and the colorless-pink residue was dissolved in Et_2O (2.00 ml). By partially evaporating the solvent under reduced pressure, the concentration of the product in solution was increased and colorless crystals of product **3** suitable for X-ray structure analysis were obtained after three days of crystallization at room temperature (12.9 mg, 8.79 µmol, 20 %, 95 % purity). Due to the C-H bond activation, this compound was not the intended target of this work, and therefore no reaction optimization was carried out to increase yield or purity.

^{1}H-NMR (700.29 MHz, C_6D_6): δ [ppm] = −0.16 (d, 1H, $^{2}J_{HH}$ = 15.2 Hz, H-47), 0.28 (d, 3H, H-18), 0.46 – 0.51 (m, 1H, H-48), 0.82 – 0.85 (m, 6H, H-18 (3H) + H-32 (3H)), 0.89 – 0.92 (m, 6H, H-32 (3H) + H-20 (3H)), 0.92 – 0.95 (m, 9H, H-18 (3H) + H-42 (6H)), 0.97 (d, 3H, $^{3}J_{HH}$ = 7.0 Hz, H-20), 1.05 (d, 3H,

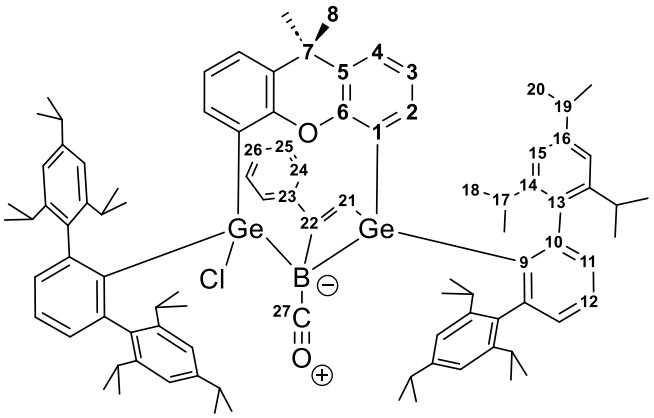
$^{3}J_{HH}$ = 6.8 Hz, H-18), 1.11 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-44), 1.15 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-44), 1.18 – 1.20 (m, 6H, H-8 (3H)) + H-18 (3H)), 1.22 – 1.24 (m, 1H, H-48), 1.31 (d, 3H, $^{3}J_{HH}$ = 7.0 Hz, H-46), 1.36 – 1.41 (m, 15H, H-18 (3H) + H-20 (3H) + H-32 (3H) + H-34 (6H)), 1.43 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.45 (s, 3H, H-8), 1.64 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-18), 1.67 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 1.72 – 1.76 (m, 1H, H-47), 1.78 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-18), 2.36 (sept, 1H, $^{3}J_{HH}$ = 6.7 Hz, H-41), 2.45 (sept, 1H, $^{3}J_{HH}$ = 7.0 Hz, H-19), 2.64 (sept, 1H, $^{3}J_{HH}$ = 6.9 Hz, H-43), 2.95 (sept, 1H, $^{3}J_{HH}$ = 7.0 Hz, H-33), 2.99 – 3.06 (m, 2 H, H-19, H-17), 3.10 (sept, 1H, $^{3}J_{HH}$ = 6.8 Hz, H-17), 3.18 (sept, 1H, $^{3}J_{HH}$ = 6.8 Hz, H-31), 3.27 (s, 1H, H-54), 3.29 – 3.40 (m, 4H, H-17 (2H) + H-45 (1H) + H-49 (1H)), 3.61 (sept, 1H, $^{3}J_{HH}$ = 6.7 Hz, H-31), 5.46 – 5.49 (m, 2H, H-51), 6.47 (dd, 1H, $^{3}J_{HH}$ = 7.2 Hz, $^{4}J_{HH}$ = 1.1 Hz, H-2), 6.52 – 6.55 (m, 2H, H-52), 6.55 – 6.58 (m, 2H, H-3 (1H) + H-37 (1H)), 6.62 (d, 1H, $^{4}J_{HH}$ = 1.6 Hz, H-15), 6.63 – 6.66 (m, 1H, H-53), 6.72 (t, 1H, $^{3}J_{HH}$ = 7.4 Hz, H-3), 6.81 (dd, 1H, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 1.1 Hz, H-2), 6.93 – 6.97 (m, 4H, H-4 (2H) + H-15 (1H) + H-29 (1H)), 6.97 – 7.00 (m, 2H, H-23 (1H) + H-24 (1H)), 7.01 – 7.03 (m, 1H, H-25), 7.08 – 7.11 (m, 1H, H-12), 7.13 (d, 1H, $^{4}J_{HH}$ = 1.5 Hz , H-39), 7.14 – 7.15 (m, 1H, H-11, overlapped by solvent signal), 7.22 (dd, 1H, $^{3}J_{HH}$ = 7.4 Hz, $^{4}J_{HH}$ = 1.5 Hz, H-11), 7.30 (d, 1H, $^{4}J_{HH}$ = 1.6 Hz , H-15), 7.35 (d, 1H, $^{4}J_{HH}$ = 1.6 Hz, H-15), 7.43 (d, 1H, $^{4}J_{HH}$ = 1.6 Hz, H-29). **^{13}C-NMR** (176.10 MHz, C_6D_6): δ [ppm] = 21.9 (C-32), 22.5 (C-18), 23.0 (C-42), 23.0 (C-44), 23.3 (C-18), 23.3 (C-18), 23.7 (C-20), 24.1 (C-34), 24.2 (C-20), 24.4 (C-20), 24.5 (C-34), 24.6 (C-20), 24.6 (C-18), 24.7 (C-44), 25.1 (C-32), 25.5 (C-8 + C-18), 25.7 (C-18), 26.3 (C-32), 26.4 (C-18), 26.8 (C-18), 27.0 (C-42), 27.2 (C-48), 27.2 (C-32), 28.2 (C-46), 30.6 (C-31 + C-41 + C-17), 31.0 (C-17), 31.3 (C-31), 31.3 (C-17), 31.5 (C-17), 33.3 (C-8), 33.5 (C-43), 34.0 (C-19), 34.1 (C-19), 34.2 (C-45), 34.5 (C-33), 35.3 (C-7), 36.2 (C-49), 36.7 (C-47), 120.1 (C-37), 120.5 (C-15), 120.8 (C-15), 121.1 (C-15), 121.8 (C-39), 122.0 (C-29), 122.1 (C-15 + C-29), 123.0 (C-3), 123.4 (C-3), 124.2 (C-53), 124.7 (C-4), 125.7 (C-4), 126.2 (C-1), 126.7 (C-12), 127.3 (2x C-52), 128.1 (C-24, overlapped by solvent signal), 128.2 (2x C-51, overlapped by solvent signal), 130.1 (C-11), 130.5 (C-5), 130.7 (C-5), 131.7 (C-25), 132.5 (C-11 + C-23), 132.8 (C-2), 134.0 (C-1), 135.3 (C-2), 137.7 (C-21), 138.0 (C-35), 139.5 (C-13), 139.9 (C-27), 141.6 (C-13), 142.9 (C-9), 144.0 (C-50), 145.6 (C 14), 146.4 (C-28), 146.6 (C-36), 147.4 (C-14), 147.4 (C-40), 147.7 (C-26), 147.9 (C-28), 148.1 (C-10), 148.1 (C-38), 148.2 (C-16), 148.2 (C-14), 148.3 (C-14), 148.5 (C-16), 148.8 (C-22), 148.9 (C-30), 149.3 (C-10), 153.8 (C-6), 154.1 (C-6). **^{11}B{^{1}H}-NMR**: No boron NMR signal could be observed in solution. **An elemental analysis was not carried out due to insufficient purity.**



Scheme S1. Phenylalkyne reaction with **1**.

Synthesis of a mixture of compounds 4 and 5:Boradigermaallyl **1** (60.0 mg, 44.0 µmol, 1.00 equiv.) was dissolved in *n*-pentane (2.00 ml) and phenylacetylene (4.83 µl, 44.0 µmol, 1.00 equiv.)) was added while stirring at room temperature Over a period of three days, a color change from turquoise to pale yellow and a complete conversion of the reactants was observed. The solvent was then removed under reduced pressure and the residue was dissolved in Et_2O (8.00 ml). The concentration was increased by partial evaporation of the solvent under reduced pressure and the products **4** and **5** were isolated over a period of three days using fractional crystallization at room temperature.

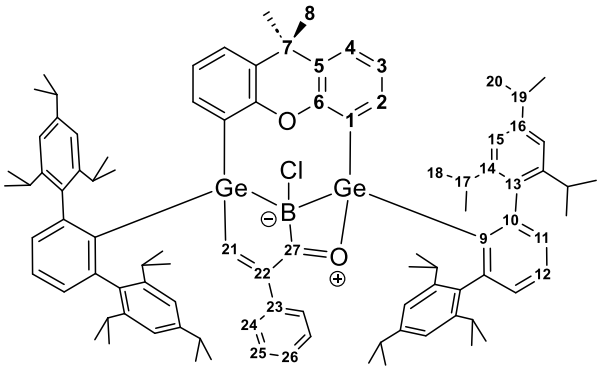
In the crystallization process, two types of colorless crystals, both suitable for X-ray structure analysis, were obtained in two fractions in different ratios. Due to the C-H bond activation, the compounds were not the intended targets of this work and therefore no reaction optimization was carried out. In addition, it was not possible to separate the two compounds, for which reason the yield and purity were not reported. Due to the extremely complex NMR spectra and the inability to separate the compounds from each other, no NMR characterization is provided.



Synthesis of compound 6: Boradigermaallyl **1** (100 mg, 73.4 µmol, 1.00 equiv.) was dissolved in cyclohexane (2.00 ml) and then frozen at −38 °C inside a Schlenk tube with a volume of approximately 50 ml. Afterwards, phenylacetylene (8.06 µl, 73.4 µmol, 1.00 equiv.) that was already dissolved in cyclohexane (0.20 ml) was added to the Schlenk tube in such a way that the solution froze on the cold glass wall, while avoiding contact with the frozen turquoise solid of the boradigermaallyl. Subsequently, the argon atmosphere of the Schlenk tube was removed under reduced pressure and replaced with carbon monoxide. The entire frozen Schlenk tube was then brought to room temperature and the resulting turquoise solution was stirred for 4 h, resulting in a color change from turquoise to green to light yellow. The solvent was then removed under reduced pressure and the yellow residue was suspended in pentane. The resulting suspension had an orange-brown color from which product **6** precipitates at −38 °C as a colorless solid (76.1 mg, 51.0 µmol, 70 %). Colorless crystals suitable for X-ray diffraction were obtained from a concentrated Et_2O solution of **6** at −38 °C after three days of crystallization. The compound continues to react at room temperature over the course of a few hours and should be stored at −38 °C.

^{1}H-NMR (700.29 MHz, C_6D_6, 283 K): δ [ppm] = − 0.21 (d, 3H, $^3J_{HH}$ = 6.8 Hz, H-18), 0.36 (d, 3H, $^3J_{HH}$ = 6.6 Hz, H-18), 0.86 – 0.89 (m, 3H, H-18), 0.92 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 0.93 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-18), 0.97 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.01 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.02 – 1.05 (m, 6H, H-18 (3H), H-20 (3H)), 1.09 – 1.11 (m, 6H, H-18 (3H), H-20 (3H)), 1.15 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-18), 1.21 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-18), 1.30 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-20), 1.32 (d, 3H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.33 – 1.36 (m, 6H, H-18 (3H), H-20 (3H)), 1.37 (s, 3H, H-8), 1.40 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-20), 1.44 – 1.47 (m, 9H, H-8 (3H), H-18 (3H), H-20 (3H)), 1.49 – 1.51 (m, 6H, H-18 (3H), H-20 (3H)), 1.59 (d, 3H, $^3J_{HH}$ = 6.9 Hz, H-20), 1.76 (d, 3H, $^3J_{HH}$ = 6.8 Hz, H-18), 2.31 (sept., 1H, $^3J_{HH}$ = 6.7 Hz, H-17), 2.45 – 2.58 (m, 4H, H-17 (3H), H-19 (1H)), 2.87 (sept., 1H, $^3J_{HH}$ = 6.9 Hz, H-19), 2.97 (sept., 1H, $^3J_{HH}$ = 6.9 Hz, H-19), 3.10 (sept., 1H, $^3J_{HH}$ = 6.9 Hz, H-19), 3.46 (sept., 1H, $^3J_{HH}$ = 6.9 Hz, H-17), 3.66 (sept., 1H, $^3J_{HH}$ = 6.8 Hz, H-17), 3.71 (sept., 1H, $^3J_{HH}$ = 6.7 Hz, H-17), 3.93 (sept., 1H, $^3J_{HH}$ = 6.8 Hz, H-17), 5.81 (s, 1H, H-21), 6.49 (d, 1H, $^4J_{HH}$ = 1.5 Hz, H-15), 6.54 – 6.56 (m, 1H, H-2), 6.57 – 6.60 (m, 1H, H-3), 6.69 – 6.71 (m, 2H, H-3, H-15), 6.76 – 6.78 (m, 1H, H-4), 6.80 (d, 1H, $^4J_{HH}$ = 1.5 Hz , H-15), 6.95 – 6.97 (m, 1H, H-11), 7.00 – 7.04 (m, 7H, H-4 (1H), H-12 (2H), H-15 (1H), H-25 (2H), H-26(1H)), 7.13 – 7.15 (m, 3H, H-11 (1H), H-24 (2H)), 7.19 (d, 1H, $^4J_{HH}$ = 1.5 Hz, H-15), 7.22 (dd, 1H,

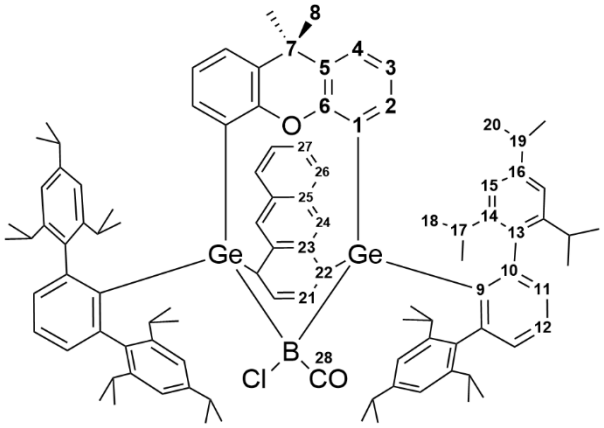
$^{3}J_{HH}$ = 7.6 Hz, $^{4}J_{HH}$ = 1.3 Hz, H-11), 7.24 (d, 1H, $^{4}J_{HH}$ = 1.5 Hz, H-15), 7.30 (d, 1H, $^{4}J_{HH}$ = 1.5 Hz, H-15), 7.32 (d, 1H, $^{4}J_{HH}$ = 1.5 Hz, H-15), 7.43 (dd, 1H, $^{3}J_{HH}$ = 7.8 Hz, $^{4}J_{HH}$ = 1.4 Hz, H-11), 7.47 (dd, 1H, $^{3}J_{HH}$ = 7.5 Hz, $^{4}J_{HH}$ = 1.2 Hz, H-2). **^{13}C-NMR** (176.10 MHz, C_6D_6, 283 K): δ [ppm] = 20.7 (C-18), 21.5 (C-18), 21.9 (C-18), 22.0 (C-18), 22.2 (C-18), 22.3 (C-20), 22.6 (C-18), 23.4 (C-8), 23.5 (C-20), 24.3 (C-20), 24.4 (C-18), 24.5 (C-20), 24.7 (C-20), 24.8 (C-18), 24.9 (2 x C-18), 25.0 (C-20) , 25.7 (C-20), 25.8 (C-20), 25.9 (C-18), 26.0 (C-18), 26.2 (C-18), 27.4 (C-18), 27.7 (C-18), 28.5 (C-18), 30.2 (C-8), 30.5 (C-17), 30.6 (C-17), 30.7 (C-17), 30.9 (C-17), 31.3 (C-17), 31.9 (C-17), 32.0 (C-17), 32.1 (C-17), 34.4 (C-19), 34.7 (C-19), 34.9 (C-19), 34.9 (C-19), 36.8 (C-7), 120.2 (C-15), 120.6 (C-15), 120.7 (C-15), 120.9 (C-15), 121.1 (C-15), 121.2 (C-15), 121.6 (C-15), 122.6 (C-15), 123.1 (C-3), 123.7 (C-3), 124.1 (C-4), 125.1 (C-4), 127.0 (C-12), 127.3 (2 x C-24), 127.5 (C-12), 127.5 (C-26), 127.9 (2 x C-25, overlapped by solvent signal), 130.1 (C-1), 130.5 (C-11), 131.5 (C-5), 132.6 (C-11), 133.9 (C-1), 134.2 (C-11), 134.3 (C-2), 135.0 (C-11), 135.3 (C-2), 135.3 (C-5), 137.7 (C-13), 138.1 (C-13), 138.9 (C-13), 139.1 (C-13), 139.9 (C-23), 141.5 (C-9), 141.6 (C-9), 145.1 (C-14), 145.5 (C-14), 146.1 (C-14), 146.9 (C-16), 147.0 (C-14), 147.1 (C-10), 147.5 (C-14 + C-10), 147.8 (C-10), 147.9 (C-14), 148.3 (C-10), 148.4 (C-16), 148.4 (C-16), 148.5 (C-16), 148.7 (C-14), 149.1 (C-14), 151.3 (C-22, br), 154.8 (C-21), 156.0 (C-6), 158.7 (C-6), 181.6 (C-27, br). **^{11}B-NMR** (128.37 MHz, C_6D_6): δ [ppm] = −23.2. **IR** (KBr, cm^{-1}): 2077 ($\nu_{C\text{-}O}$). **Elemental analysis cacld (%) for** $C_{96}H_{116}BClGe_2O_2$: C 77.21, H 7.83; found: C 77.57, H 7.95.



Synthesis of compound 7: A solution of boradigermaallyl **1** (100 mg, 73.4 µmol, 1.00 equiv.) in cyclohexane (3.00 ml) was frozen in a Schlenk tube with a volume of approximately 50 ml at −38 °C. A standard solution of phenylacetylene in cyclohexane (200 µl, 0.37 M in cyclohexane, 73.4 µmol, 1.00 equiv.) was added to the Schlenk tube in such a way that the solution froze on the cold glass wall while avoiding contact with the frozen turquoise solid of the boradigermaallyl. Subsequently, the argon atmosphere was removed under reduced pressure and replaced with one bar of carbon monoxide. In the next step, the Schlenk tube was warmed to room temperature and then heated to 50 °C for 44 hours, whereby a color change from turquoise to yellow and finally orange was visible. Following this, the solvent was removed under reduced pressure and the product was extracted using *n*-pentane (10 ml). Fine suspended particles were filtered off and the filtrate was concentrated by partial evaporation of the solvent under reduced pressure.

Crystallization overnight at room temperature led to yellow crystals of the product **7** suitable for X-ray diffraction (75.2 mg, 50.4 µmol, 69 %).

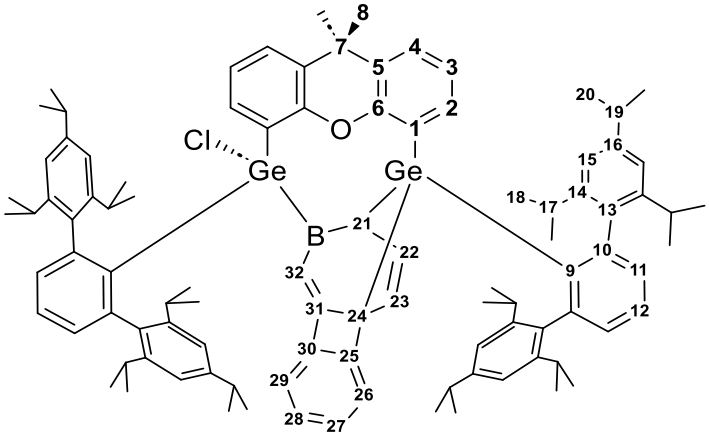
^{1}H-NMR (700.21 MHz, C_6D_6): δ [ppm] = 0.51 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 0.56 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 0.78 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 0.90 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 0.96 (d, 6H, $^{3}J_{HH}$ = 6.8 Hz, H-18 (3H) + H-20 (3H)), 0.99 – 1.01 (m, 6H, H-8 (3H) + H-18 (3H)), 1.01 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.05 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.18 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.19 – 1.21 (m, 6H, H-18), 1.23 – 1.29 (m, 12H, H-8 (3H) + H-18 (3H) + H-20 (6H)), 1.31 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.33 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 1.36 – 1.39 (m, 6H, H-18 (3H) + H-20 (3H), 1.42 – 1.45 (m, 6H, H-18), 1.46 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 1.57 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 1.63 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 2.50 (sept, 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 2.56 (sept, 1H, $^{3}J_{HH}$ = 6.9 Hz, H-19), 2.60 (sept, 1H, $^{3}J_{HH}$ = 6.9 Hz, H-19), 2.84 – 2.91 (m, 2H, H-19), 3.11 (sept, 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 3.42 (sept, 1H, $^{3}J_{HH}$ = 6.9 Hz, H-17), 3.54 – 3.64 (m, 3H, H-17), 3.68 (sept, 1H, $^{3}J_{HH}$ = 6.9 Hz, H-17), 3.84 (sept, 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 6.36 (t, 1H, $^{3}J_{HH}$ = 7.6 Hz, H-3), 6.70 – 6.73 (m, 4H, H-3 (1H) + H-15 (1H) + H-24 (2H)), 6.82 (dd, 1H, $^{3}J_{HH}$ = 7.8 Hz, $^{4}J_{HH}$ = 1.3 Hz, H-4), 6.90 (d, 1H, $^{4}J_{HH}$ = 1.5 Hz, H-15), 6.97 – 7.02 (m, 7H, H-2 (1H) + H-4 (1H) + H-11 (1H) + H-15 (1H) + H-25 (2H) + H-26 (1H)), 7.03 – 7.05 (m, 2H, H-12 (1H) + H-15 (1H)), 7.12 (d, 1H, $^{4}J_{HH}$ = 1.6 Hz, H-15), 7.13 – 7.15 (m, 2H, H-11 (1H) + H-21 (1H)), 7.16 – 7.20 (m, 3H, H-2 (1H) + H-11 (1H) + H-12 (1H), overlapped by solvent signal), 7.21 (s, br, 2H, H-15), 7.27 (d, 1H, $^{4}J_{HH}$ = 1.7 Hz, H-15), 7.32 (dd, 1H, $^{3}J_{HH}$ = 7.0 Hz, $^{4}J_{HH}$ = 1.8 Hz, H-11). **^{13}C{^{1}H}-NMR** (176.07 MHz, C_6D_6): δ [ppm] = 21.5 (C-18), 22.2 (C-20), 22.9 (C-18), 23.0 (C-18), 23.4 (C-18), 23.4 (C-20), 23.6 (C-18), 23.8 (C-18 + C-20), 23.9 (C-18), 24.1 (C-20), 24.3 (C-20), 24.6 (C-20), 24.9 (C-20), 25.1 (C-18), 25.5 (C-18), 25.6 (C-18), 25.7 (C-18), 25.8 (C-20), 26.2 (C-18), 26.2 (C-18), 26.4 (C-18), 27.4 (C-18), 27.9 (C-18), 30.0 (C-8), 30.4 (C-17), 30.5 (C-17), 30.9 (2x C-17), 30.9 (C-8), 31.0 (C-17), 31.3 (C-17), 31.8 (C-17), 31.8 (C-17), 33.9 (C-19), 34.3 (C-19), 34.4 (2x C-19), 34.8 (C-7), 119.1 (C-15), 119.5 (C-15), 120.1 (C-15), 120.8 (C-15), 122.4 (C-15), 122.6 (C-15), 122.8 (C-15), 122.9 (C-3 + C-15), 123.0 (C-3), 125.1 (C-4), 125.4 (C-22), 127.1 (C-12), 127.5 (C-26), 127.7 (2x C-24), 127.8 (2x C-25), 127.9 (C-12, overlapped by solvent signal), 128.5 (C-4), 128.6 (C-1), 128.8 (C-1), 128.9 (C-5), 130.6 (C-5), 130.9 (C-11), 131.7 (C-11), 132.7 (C-11), 132.8 (C-11), 134.5 (C-2), 135.1 (C-23), 135.9 (C-2), 138.4 (C-13), 138.8 (C-13), 138.9 (C-9), 138.9 (C-13), 139.7 (C-13), 143.8 (C-9), 145.4 (C-14), 145.8 (C-10), 146.6 (C-14), 147.2 (C-14), 147.3 (C-14), 147.3 (C-14), 147.6 (C-14), 147.8 (C-14 + C-16), 147.9 (C-16), 148.1 (2x C-10), 148.3 (C-10), 148.5 (C-16), 149.4 (C-14), 149.4 (C-16), 151.8 (C-27), 152.3 (C-6), 155.6 (C-6), 181.9 (C-21). **^{11}B{^{1}H}-NMR** (128.37 MHz, C_6D_6): δ [ppm] = 10.1 (s). **IR** (ATR, cm^{-1}): 1401 (ν_{C-O}). **Elemental analysis calcd (%)** for $C_{96}H_{116}BClGe_2O_2$: C 77.21, H 7.83; found: C 77.16, H 7.85.



Synthesis of compound 8: A turquoise solution of boradigermaallyl **1** (100 mg, 73.4 µmol, 1.00 equiv.) in cyclohexane (2.00 ml) was frozen at −38 °C in a Schlenk tube with a volume of approximately 20 ml. To avoid premature contact with the next reactant, the frozen solution was covered with cyclohexane (1.00 ml) and the latter was then frozen at −38 °C as well. In the next step, a suspension of anthracene (13.1 mg, 73.4 µmol, 1.00 equiv.) in cyclohexane (5.00 ml) was added, frozen and the argon atmosphere of the Schlenk tube replaced by 1 bar carbon monoxide. The Schlenk tube was then brought to room temperature, and the entire turquoise reaction mixture was stirred for two hours at room temperature, during which a color change to pale green was observed. Volatile components were then removed under reduced pressure, the residue dissolved in *n*-pentane (10.0 ml) and the volume of the resulting green solution reduced under reduced pressure until crystals were formed. After crystallization overnight at room temperature, colorless crystals of the product **8** were obtained, which were suitable for X-ray diffraction. (76.1 mg, 48.5 µmol, 66 %). The product **8** continues to react at room temperature over the course of a few hours and should be stored at −38 °C.

^{1}H-NMR (700.21 MHz, C_6D_6, 283 K): δ [ppm] = 0.23 (d, 6H, $^3J_{HH}$ = 6.7 Hz, H-18), 0.72 (s, 3H, H-8), 0.79 (s, 3H, H-8), 0.91 (d, 6H, $^3J_{HH}$ = 6.6 Hz, H-18), 1.05 (d, 6H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.15 (d, 6H, $^3J_{HH}$ = 6.7 Hz, H-18), 1.27 – 1.30 (m, 18H, H-20), 1.46 (d, 6H, $^3J_{HH}$ = 6.9 Hz, H-18), 1.47 – 1.50 (m, 12H, H-18 (6H) + H-20 (6H)), 1.65 (d, 6H, $^3J_{HH}$ = 6.6 Hz, H-18), 1.81 (d, 6H, $^3J_{HH}$ = 6.7 Hz, H-18), 2.79 (sept, 2H, $^3J_{HH}$ = 6.7 Hz, H-17), 2.86 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, H-19), 3.07 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, H-19), 3.14 – 3.18 (m, 2H, H-22), 3.32 (sept, 2H, $^3J_{HH}$ = 6.6 Hz, H-17), 3.58 (sept, 2H, $^3J_{HH}$ = 6.7 Hz, H-17), 3.80 (sept, 2H, $^3J_{HH}$ = 6.7 Hz, H-17), 4.93 – 4.97 (m, 2H, H-21), 5.91 (s, 2H, H-24), 6.55 (dd, 2H, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.0 Hz, H-4), 6.70 (t, 2H, $^3J_{HH}$ = 7.4 Hz, H-3), 6.83 (dd, 2H, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.0 Hz, H-2), 6.86 – 6.89 (m, 2H, H-26), 6.90 – 6.93 (m, 2H, H-27), 7.04 – 7.07 (m, 4H, H-12 + H-15 (2H)), 7.11 (dd, 2H, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.4 Hz, H-11), 7.14 (d, 2H, $^4J_{HH}$ = 1.5 Hz, H-15), 7.25 (d, 2H, $^4J_{HH}$ = 1.4 Hz, H-15), 7.32 (dd, 2H, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.4 Hz, H-11), 7.40 (d, 2H, $^4J_{HH}$ = 1.5 Hz, H-15). **^{13}C{^{1}H}-NMR** (176.07 MHz, C_6D_6, 283 K): δ [ppm] = 21.4 (C-8), 22.2 (C-18), 23.5 (C-20), 23.6 (C-18), 24.2 (C-18), 24.2 (C-20), 24.4 (C-18), 24.8 (C-20), 25.2 (C-20), 25.7 (C-18), 26.5 (C-18), 27.4 (C-18), 27.7 (C-18), 30.9 (C-17), 30.9 (C-17), 32.0 (C-17), 32.2 (C-17), 32.3 (C-8), 34.2 (C-19), 35.0 (C-19), 35.5 (C-7), 43.0 (C-22), 120.8 (C-15), 121.2 (C-15), 121.8 (C-15), 122.6 (C-15), 123.4

(C-27), 123.7 (C-3), 124.5 (C-24), 124.9 (C-4), 125.6 (C-21), 126.1 (C-12), 127.4 (C-26), 130.5 (C-25), 131.0 (C-5), 131.1 (C-1), 133.6 (C-2), 133.6 (C-11), 134.0 (C-11), 136.9 (C-23), 140.0 (C-13), 140.9 (C-13), 141.9 (C-9), 146.3 (C-14), 146.9 (C-14), 148.3 (C-16), 148.4 (C-10), 148.5 (C-14), 148.7 (C-14), 149.5 (C-16), 155.9 (C-6), 173.0 (C-28). **^{11}B{^{1}H}-NMR** (192.55 MHz, C_6D_6): δ [ppm] = −21.4 (s, br). **IR** (ATR, cm^{-1}): 2115 ($\nu_{C\text{-}O}$). **Elemental analysis calcd (%)** for $C_{102}H_{120}BClGe_2O_2$: C 78.06, H 7.71; found: C 78.88, H 7.74.



Synthesis of compound 9: Boradigermaallyl **1** (80.0 mg, 58.7 µmol, 1.00 equiv.) and biphenylene (8.93 µl, 58.7 µmol, 1.00 equiv.) were mixed together and *n*-pentane (3.50 ml) was added at room temperature. The turquoise reaction mixture was stirred for 2 weeks and a slow color change to green and finally orange was observed. After removing the solvent under reduced pressure, the residue was extracted with *n*-pentane. Small, suspended solids were filtered off and the yellow filtrate was concentrated under reduced pressure. Crystallization in *n*-pentane for three days at room temperature resulted in yellow crystals of **9**, suitable for X-ray structure analysis (64.8 mg, 38.0 µmol, 65 %.).

^{1}H-NMR (700.21 MHz, tol-$d_{8,}$ 253 K): δ [ppm] = 0.40 (d, 3H, $^{3}J_{HH}$ = 6.6 Hz, H-18), 0.46 (d, 3H, $^{3}J_{HH}$ = 6.6 Hz, H-18), 0.72 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 0.79 (d, 3H, $^{3}J_{HH}$ = 6.6 Hz, H-18), 0.82 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 0.94 – 0.98 (m, 9H, H-18 (6H) + H-20 (3H)), 1.05 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 1.08 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 1.18 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-18), 1.24 (d, 3H, $^{3}J_{HH}$ = 6.8 Hz, H-20), 1.27 – 1.29 (m, 9H, H-8 (6H), H-18 (3H)), 1.31 (d, 3H, $^{3}J_{HH}$ = 6.5 Hz, H-18), 1.33 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-18), 1.36 (d, 3H, $^{3}J_{HH}$ = 7.0 Hz, H-20), 1.39 (d, 3H, $^{3}J_{HH}$ = 7.0 Hz, H-20), 1.40 (d, 3H, $^{3}J_{HH}$ = 7.0 Hz, H-20), 1.48 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.50 – 1.53 (m, 6H, H-18 (6H)), 1.57 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-20), 1.71 (d, 3H, $^{3}J_{HH}$ = 6.9 Hz, H-18), 1.76 (d, 3H, $^{3}J_{HH}$ = 6.7 Hz, H-18), 2.08 – 2.12 (m, 1H, H-17, overlapped by solvent signal), 2.47 (sept., 1H, $^{3}J_{HH}$ = 6.8 Hz, H-19), 2.84 (sept., 1H, $^{3}J_{HH}$ = 6.9 Hz, H-19), 2.90 – 2.96 (m, 2H, H-17 (1H) + H-19 (1H)), 2.99 (sept., 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 3.12 (sept., 1H, $^{3}J_{HH}$ = 6.8 Hz, H-19), 3.15 – 3.24 (m, 2H, H-17 (2), 3.44 (sept., 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 3.50 (sept., 1H, $^{3}J_{HH}$ = 6.7 Hz, H-17), 3.60 (sept., 1H, $^{3}J_{HH}$ = 6.6 Hz, H-17), 3.75 (d, br, 1H, $^{3}J_{HH}$ = 5.6 Hz, H-21), 4.64 (s, 1H, H-32), 5.49 (d, 1H, $^{3}J_{HH}$ = 7.5 Hz, H-26), 6.34 – 6.37 (m, 2H, H-23 (1H) + H-29 (1H)), 6.43 – 6.46 (m, 1H, H-22), 6.59 – 6.65 (m, 2H, H-3 (1H) + H-28 (1H)), 6.73 – 6.76 (m, 1H, H-3), 6.80 – 6.84 (m, 3H, H-4 (1H) + H-15 (1H) + H-27 (1H)), 6.85 – 6.88 (m, 1H, H-11), 6.90 – 6.92 (m, 2H, H-11 (1H), H-12 (1H)), 6.92 – 6.95 (m, 2H, H-2 (1H), H-15 (1H)), 6.95 – 6.99 (m, 2H, H-4 (1H), H-15 (1H), overlapped by solvent signal), 7.01 – 7.04 (m, 1H, H-11, overlapped by solvent signal), 7.04 – 7.06 (m, 1H, H-2), 7.08 (t, 1H, $^{3}J_{HH}$ = 7.5 Hz, H-12), 7.14 – 7.16 (m, 1H, H-11), 7.19 – 7.21 (m, 3H, H-15 (3H)), 7.34 (s, br, 1H, H-15), 7.38 (s, br, 1H, H-15). **^{13}C-NMR** (176.07 MHz, tol-d_8, 253 K): δ [ppm] = 22.0 (C-18), 22.2 (C-20), 22.4 (C-20), 22.5 (C-18), 22.6 (C-18), 23.0 (C-18), 23.6 (C-20), 23.9 (C-18), 24.1 (C-18), 24.2 (C-20), 24.8 (C-20), 25.0 (C-18), 25.1 (C-18), 25.2

(C-18), 25.3 (C-20), 25.3 (C-20), 25.4 (C-18), 25.6 (C-18), 25.9 (C-18), 25.9 (C-18), 26.2 (C-18), 26.6 (C-20), 26.9 (C-18), 27.1 (C-18), 30.5 (C-17), 30.8 (C-17), 30.9 (C-17), 31.7 (C-17), 31.8 (C-17), 31.9 (2 x C-17), 32.1 (C-17), 33.1 (C-8), 33.7 (C-19), 33.8 (C-19), 33.9 (C-8), 34.1 (C-7), 34.2 (C-19), 35.0 (C-19), 43.2 (C-21), 69.0 (C-24), 118.1 (C-32), 119.0 (C-29), 119.4 (C-15), 120.0 (C-15), 121.2 (2 x C-15), 121.7 (C-15), 122.6 (C-15), 122.8 (C-3), 122.9 (C-3), 123.0 (C-15), 123.4 (C-15), 124.1 (C-26), 126.7 (C-28), 126.8 (C-12), 127.1 (C-1), 128.0 (C-12, overlapped by solvent signal), 128.0 (C-4, overlapped by solvent signal), 128.2 (C-5), 128.4 (C-4), 129.3 (C-5), 130.2 (C-1), 130.4 (C-27), 130.9 (C-11), 131.9 (C-22), 132.5 (C-11), 133.1 (C-23), 133.7 (C-2 + C-11), 133.9 (C-2), 134.1 (C-11), 137.0 (C-13), 139.2 (C-13), 139.6 (C-13), 139.8 (C-9), 141.5 (C-9), 142.0 (C-13), 142.2 (C-30), 145.3 (C-14), 145.6 (C-14), 145.8 (C-14), 145.9 (C-14), 146.2 (C-10), 146.7 (C-10), 146.9 (C-16), 146.9 (C-14), 147.0 (C-14), 147.4 (C-14), 147.6 (C-10), 148.5 (C-16), 148.5 (C-25), 148.6 (C-14), 149.1 (C-16), 149.5 (C-14), 149.6 (C-10), 151.7 (C-6), 152.1 (C-6), 168.2 (C-31). **^{11}B-MAS-NMR** (96.29 MHz): δ [ppm] = 71.0. **UV/Vis** (*n*-pentane, c = 0.048 mmol·L^{-1}): λ [nm] (ε [L·mol^{-1}cm^{-1}): 345 (11800), 320 (16400). **Elemental analysis cacld (%) for** $C_{99}H_{118}BClGe_2O$: C 78.46, H 7.85; found: C 79.09, H 7.73.

Crystal structure determination

Table S1: Data of crystal structure determination.

	2	**3**	**4**	**5**
empirical formula	$C_{93}H_{122}BClGe_2O$ (Et_2O)	$C_{95}H_{118}BClGe_2O$	$C_{95}H_{116}BClGe_2O$ 2x (Et_2O)	$C_{95}H_{116}BClGe_2O$
M [g/mol]	1521.51	1467.38	1613.61	1465.37
T [K]	100(2)	100(2)	130(2)	100(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073
crystal system	triclinic	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
Z	2	2	2	2
a [Å]	13.3309(4)	13.7734(4)	14.4877(4)	13.5962(4)
b [Å]	17.1204(5)	16.6004(5)	18.0318(4)	16.6710(5)
c [Å]	20.0227(6)	20.0960(7)	18.9385(5)	20.1773(6)
α [°]	78.851(2)	83.116(2)	77.2310(10)	81.8234(16)
β [°]	72.034(2)	85.997(2)	89.5030(10)	87.2510(15)
γ [°]	84.771(2)	84.814(2)	73.8950(10)	84.0915(14)
V [Å^3]	4262.5(2)	4534.9(2)	4628.4(2)	4500.3(2)
D_c [g/cm^3]	1.185	1.075	1.158	1.081
μ [mm^{-1}]	0.784	0.734	0.726	0.740
F(000)	1632	1564	1728	1560
crystal size [mm]	0.293 x 0.235 x 0.200	0.26 x 0.25 x 0.22	0.436 x 0.429 x 0.392	0.31 x 0.28 x 0.26
θ range [°]	2.438 – 30.529	2.785 – 26.551	2.415 – 29.641	2.530 – 28.796
limiting indices	−19 ≤ h ≤ 19 −24 ≤ k ≤ 24 −28 ≤ l ≤ 28	−16 ≤ h ≤ 17 −20 ≤ k ≤ 20 −25 ≤ l ≤ 25	−20 ≤ h ≤ 20 −25 ≤ k ≤ 25 −26 ≤ l ≤ 26	−18 ≤ h ≤ 18 −22 ≤ k ≤ 22 −27 ≤ l ≤ 26
reflections collected	89239	66600	292533	127644
independent reflections	25701	18029	25905	23374
R_{int}	0.0501	0.0619	0.0320	0.0537
Completeness [%]	98.6	95.3	99.2	99.5
absorption correction	multi-scan	multi-scan	multi-scan	multi-scan
max., min. transmission	0.7034, 0.7461	0.6050, 0.7454	0.9387, 1.0000	0.6851, 0.7458
parameter/restraints	956 / 0	976 / 399	1030 / 139	930 / 0
R_1, ωR_2 [I > 2σ(I)]	0.0412, 0.0957	0.0638, 0.1498	0.0378, 0.0977	0.0377, 0.1042
R_1, ωR_2 (all data)	0.0637, 0.1049	0.1038, 0.1678	0.0463, 0.1041	0.0536, 0.1114
GooF on F^2	1.019	1.040	1.032	1.038
peak / hole [e·Å^{-3}]	1.317, −0.555	1.937, −1.008	1.481, −1.175	0.467, −0.389
CCDC	2418123	2418127	2418126	2418129

Table S2: Data of crystal structure determination.

	6	**7**	**8**	**9**
empirical formula	$C_{96}H_{116}BClGe_2O_2$ (Et_2O)	$C_{96}H_{116}BClGe_2O_2$ 2x (*n*-pentane)	$C_{102}H_{120}BClGe_2O$ 2.5x (*n*-pentane)	$C_{99}H_{118}BClGe_2O$
M [g/mol]	1568.50	1637.61	1749.78	1515.42
T [K]	120(2)	120 (2)	120 (2)	100(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073
crystal system	triclinic	monoclinic	monoclinic	triclinic
space group	$P\bar{1}$	$P2_1/n$	$P2/c$	$P\bar{1}$
Z	2	4	4	2
a [Å]	14.1976(3)	19.5707(6)	25.9105(14)	15.9892(3)
b [Å]	14.5282(3)	18.9384(6)	14.4062(8)	19.2578(3)
c [Å]	22.8599(4)	26.3009(8)	28.4018(16)	20.5718(4)
α [°]	87.8450(10)	90	90	102.6310(10)
β [°]	74.4580(10)	107.021(2)	109.755(3)	112.2980(10)
γ [°]	75.2490(10)	90	90	106.5770(10)
V [$Å^3$]	4390.70(15)	9321.1(5)	9977.6(10)	5221.48(17)
D_c [g/cm^3]	1.186	1.167	1.165	0.964
μ [mm^{-1}]	0.764	0.722	0.678	0.639
F(000)	1672	3512	3756	1612
crystal size [mm]	0.30 x 0.28 x 0.27	0.31 x 0.27 x 0.26	0.30 x 0.28 x 0.26	0.27 x 0.26 x 0.25
θ range [°]	2.956 – 27.990	1.530 – 27.619	1.469 – 30.533	1.954 – 30.434
	−18 ≤ h ≤ 18	−25 ≤ h ≤ 25	−37 ≤ h ≤ 36	−22 ≤ h ≤ 22
limiting indices	−19 ≤ k ≤ 18	−24 ≤ k ≤ 24	−20 ≤ k ≤ 20	−27 ≤ k ≤ 27
	−30 ≤ l ≤ 30	−34 ≤ l ≤ 34	−38 ≤ l ≤ 40	−29 ≤ l ≤ 29
reflections collected	105316	195734	331399	281112
independent reflections	20982	21434	30530	31410
R_{int}	0.0625	0.0397	0.0549	0.0335
Completeness [%]	99.1	98.9	99.9	99.2
absorption correction	multi-scan	multi-scan	multi-scan	multi-scan
max., min. transmission	0.6961, 0.7456	0.6666, 0.7456	0.6299, 0.7461	0.7133, 0.7461
parameter/restraints	992 / 0	1039 / 0	1363 / 960	984 / 75
R_1, ωR_2 [$I > 2\sigma(I)$]	0.0555, 0.1163	0.0351, 0.0875	0.0578, 0.1256	0.0487, 0.1290
R_1, ωR_2 (all data)	0.0895, 0.1299	0.0544, 0.0992	0.0738, 0.1315	0.0632, 0.1407
GooF on F^2	1.015	1.027	1.151	1.047
peak / hole [$e \cdot Å^{-3}$]	2.525, −1.659	0.920, −0.480	1.062, −1.275	1.660, −2.192
CCDC	2418124	2418130	2418128	2418125

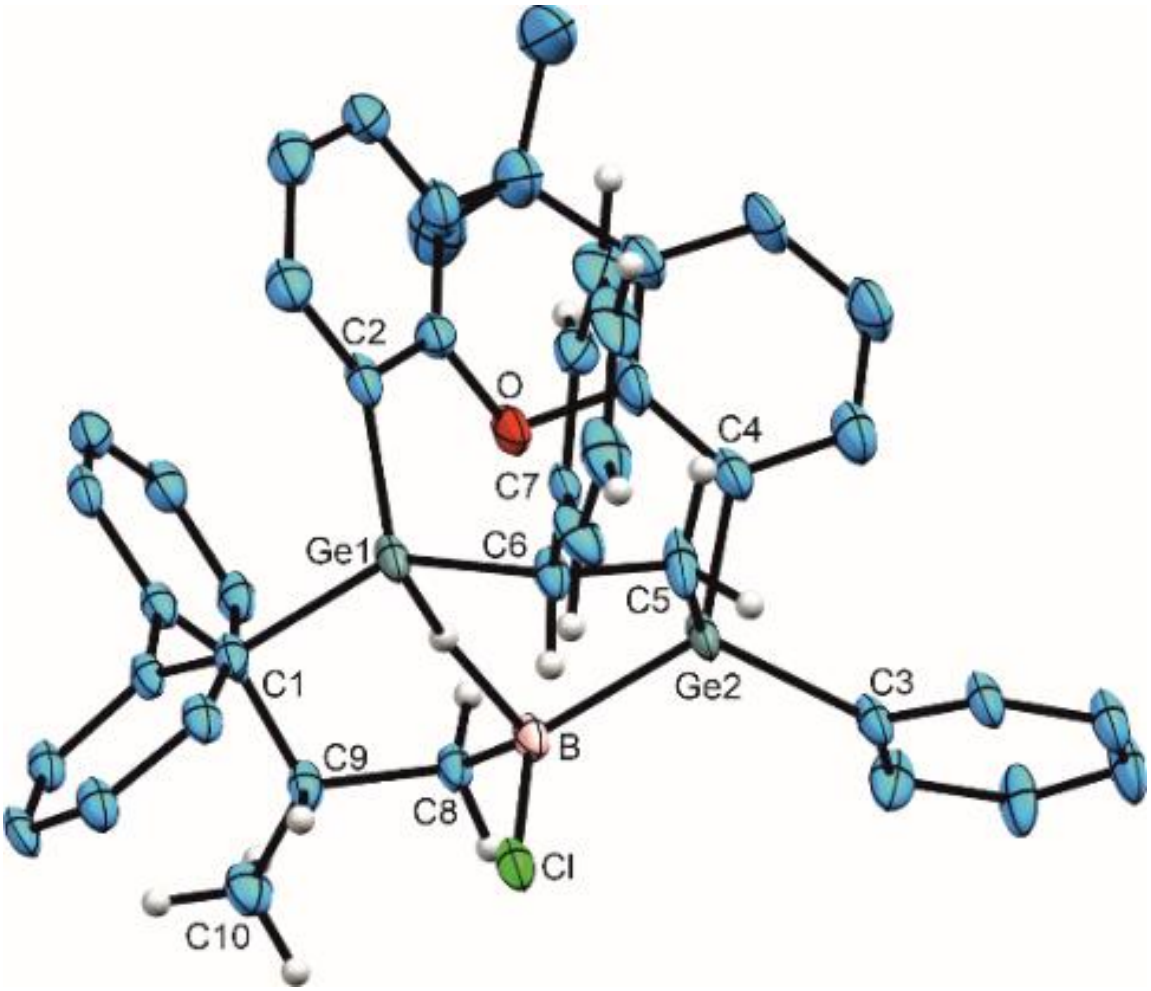


Figure S1. ORTEP of the molecular structure of **3**. Thermal ellipsoids are shown at 50 % probability level. Hydrogen atoms, ^{i}Pr and Trip groups except the styrene H-atoms and the reacting ^{i}Pr-group have been omitted. Selected interatomic distances [Å]: Ge1-C1 1.973(4), Ge1-C2 1.937(4), Ge1-C6 1.984(4), Ge2-C3 1.994(4), Ge2-C4 1.980(4), Ge2-C5 1.995(4), Ge2-B 2.081(4), C5-C6 1.562(5), B-C8 1.553(6), B-Cl 1.854(5).

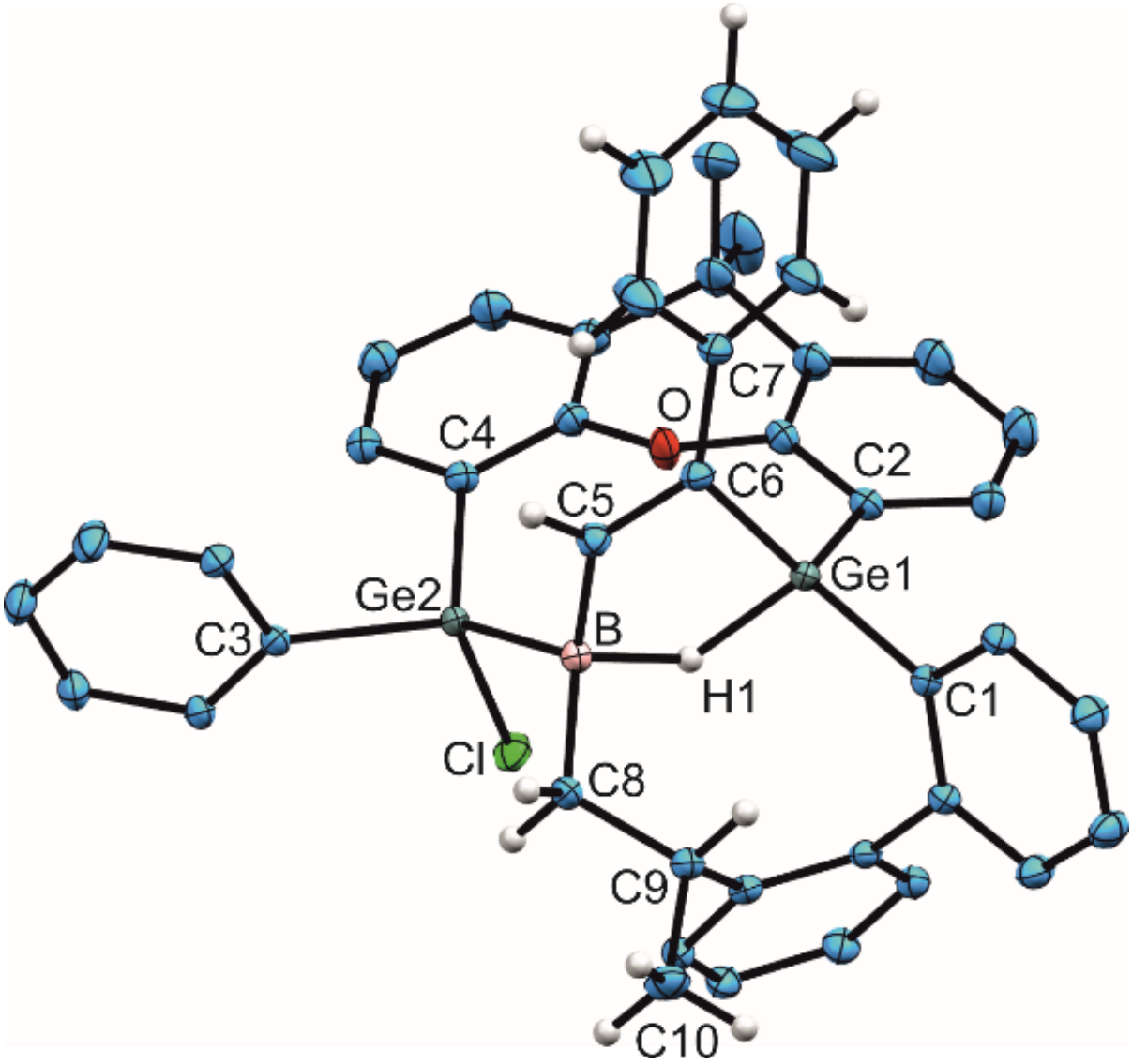


Figure S2. ORTEP of the molecular structure of **4**. Thermal ellipsoids are shown at 50 % probability level. Hydrogen atoms, ^{i}Pr and Trip groups except the phenylalkyne H-atoms and the reacting ^{i}Pr group have been omitted. Selected interatomic distances [Å]: Ge1-C1 1.9550(14), Ge1-C2 1.9331(15), Ge1 C6 1.9356(14), Ge2-C3 2.0077(14), Ge2-C4 1.9834(14), Ge2-Cl 2.2042(4), Ge2-B 2.1280(16), B-C5 1.576(2), B-C8 1.608(2), C5-C6 1.348(2), B-H 1.46(2), Ge1-H 1.64(2).

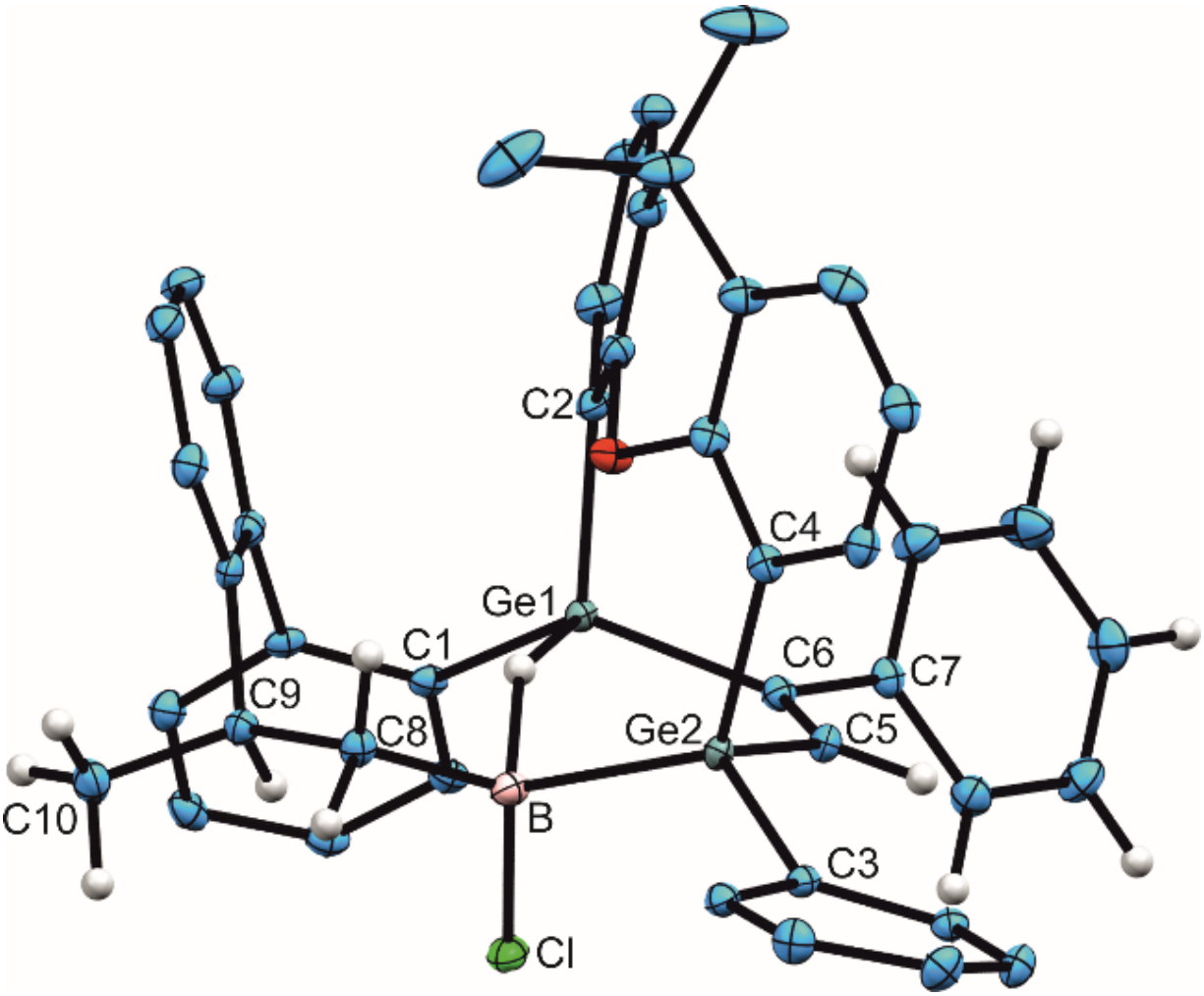
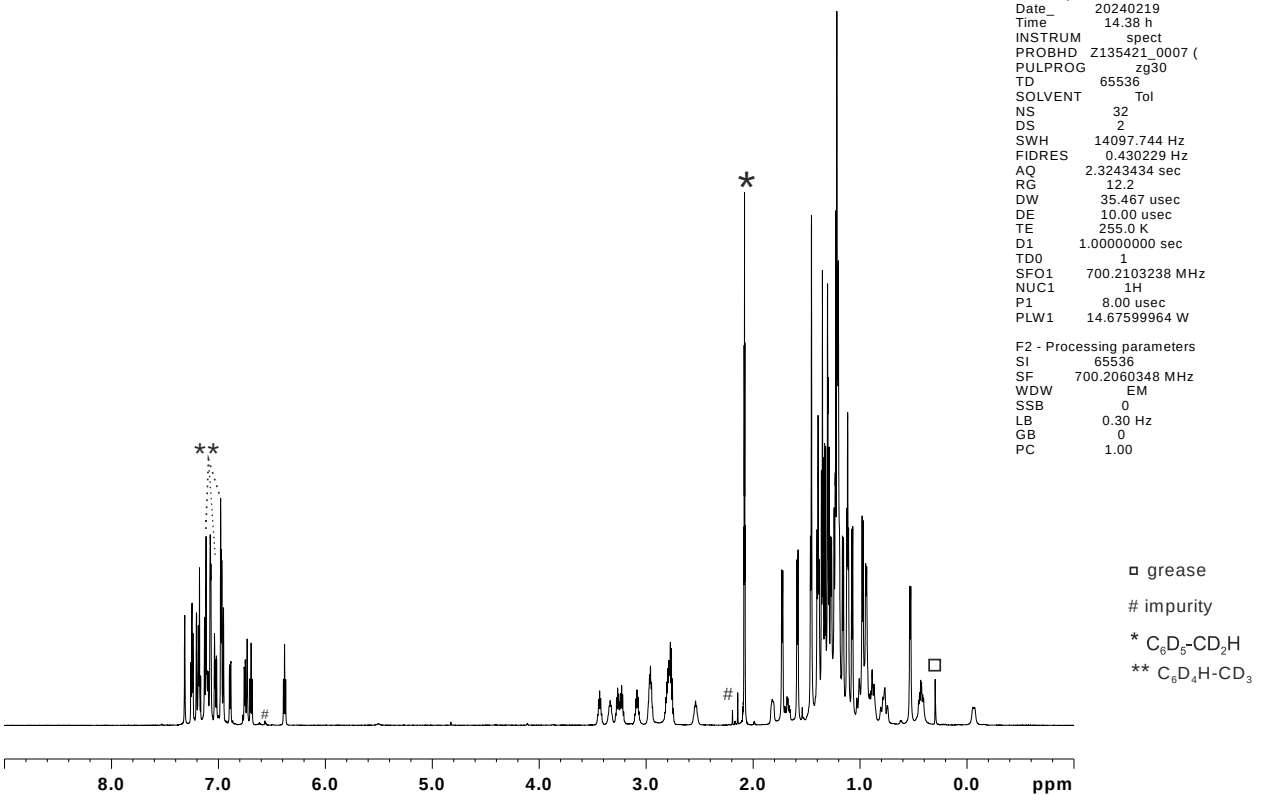


Figure S3. ORTEP of the molecular structure of **5**. Thermal ellipsoids are shown at 50 % probability level. Hydrogen atoms, ^{i}Pr and Trip groups except the phenylalkyne H-atoms and the reacting ^{i}Pr group have been omitted. Selected interatomic distances [Å]: Ge1-C1 1.9704(17), Ge1-C2 1.9579(17), Ge1-C6 1.9747(18), Ge2-C3 1.9931(17), Ge2-C4 1.9897(17), Ge2-C5 1.9820(18), Ge2-B 2.073(2), B-Cl 1.838(2), B-C8 1.571(3), B-H 1.56(2), Ge1-H 1.54(2), C5-C6 1.345(2).

NMR spectroscopy

NMR spectra of compound **2**.



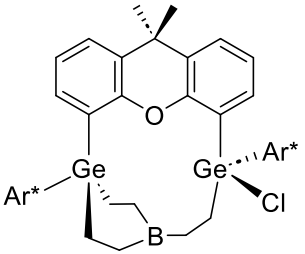
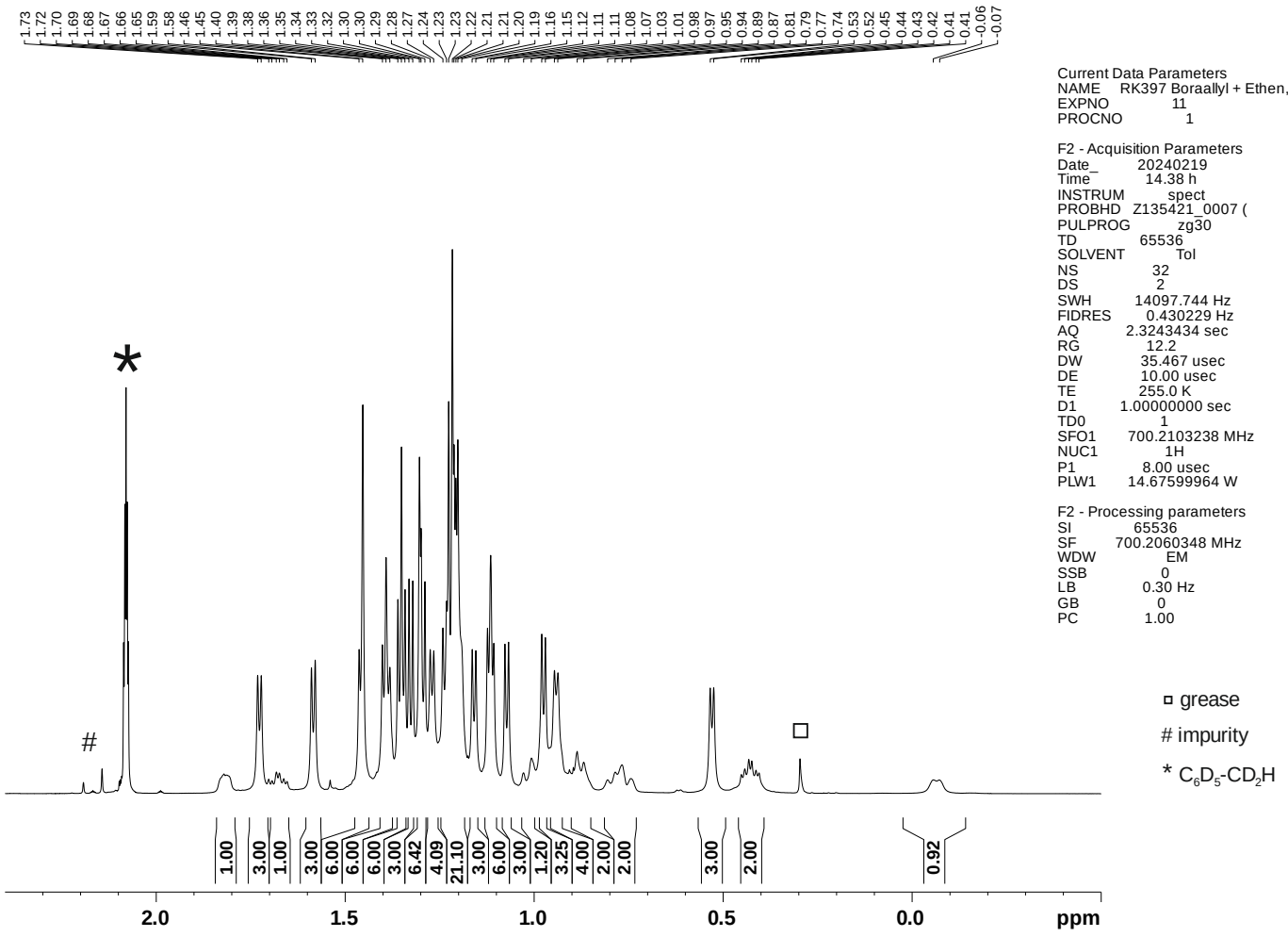


Figure S4. ^{1}H NMR spectrum of compound **2**.



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PROCNO 1

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▫ grease
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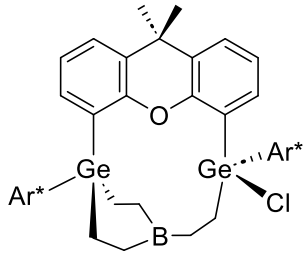
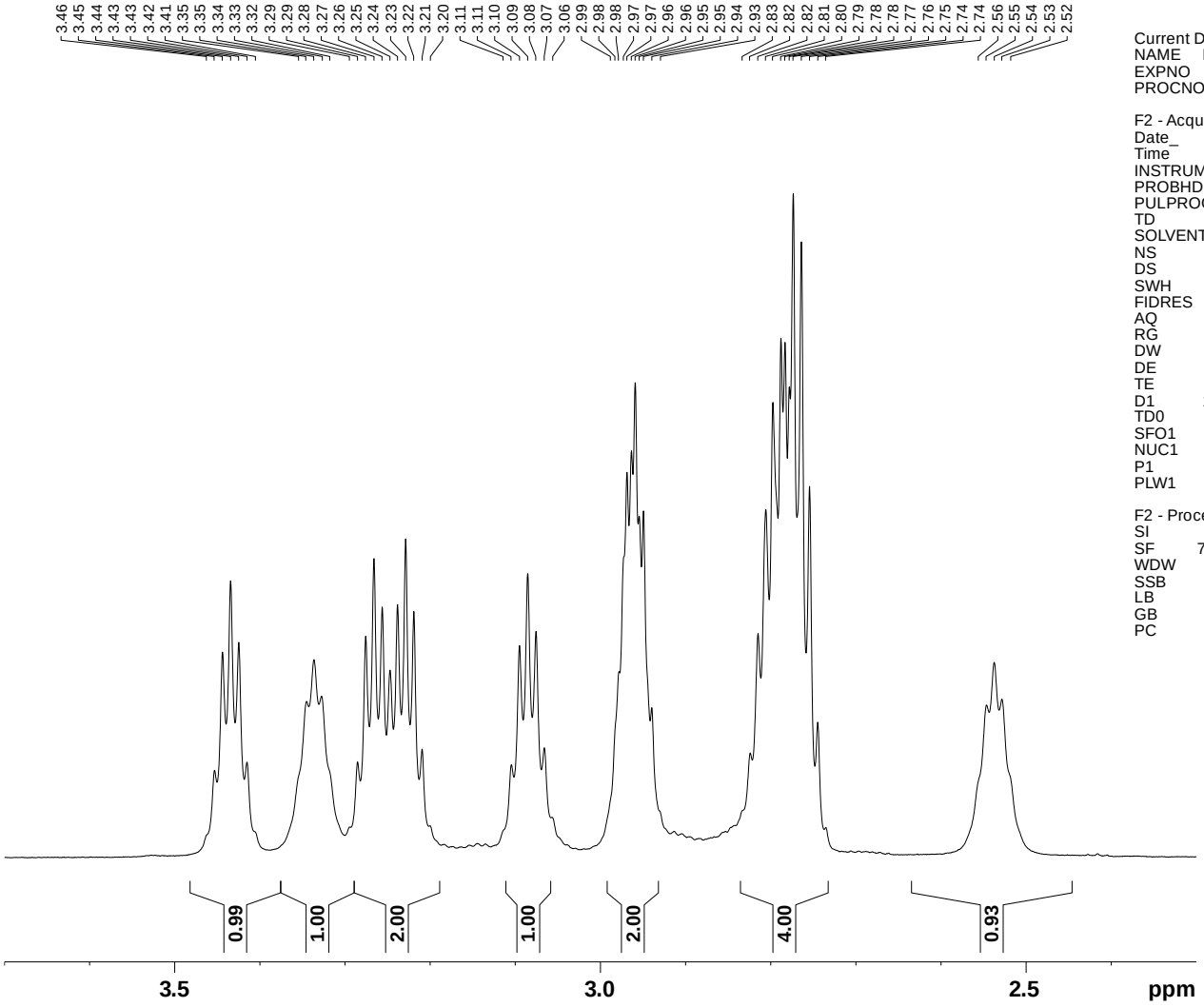


Figure S5. ^{1}H NMR spectrum of compound **2** (−0.5 – 2.4 ppm).



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SOLVENT Tol
NS 32
DS 2
SWH 14097.744 Hz
FIDRES 0.430229 Hz
AQ 2.3243434 sec
RG 12.2
DW 35.467 usec
DE 10.00 usec
TE 255.0 K
D1 1.00000000 sec
TD0 1
SFO1 700.2103238 MHz
NUC1 1H
P1 8.00 usec
PLW1 14.67599964 W

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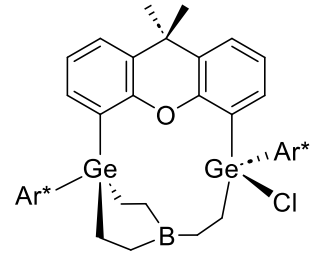
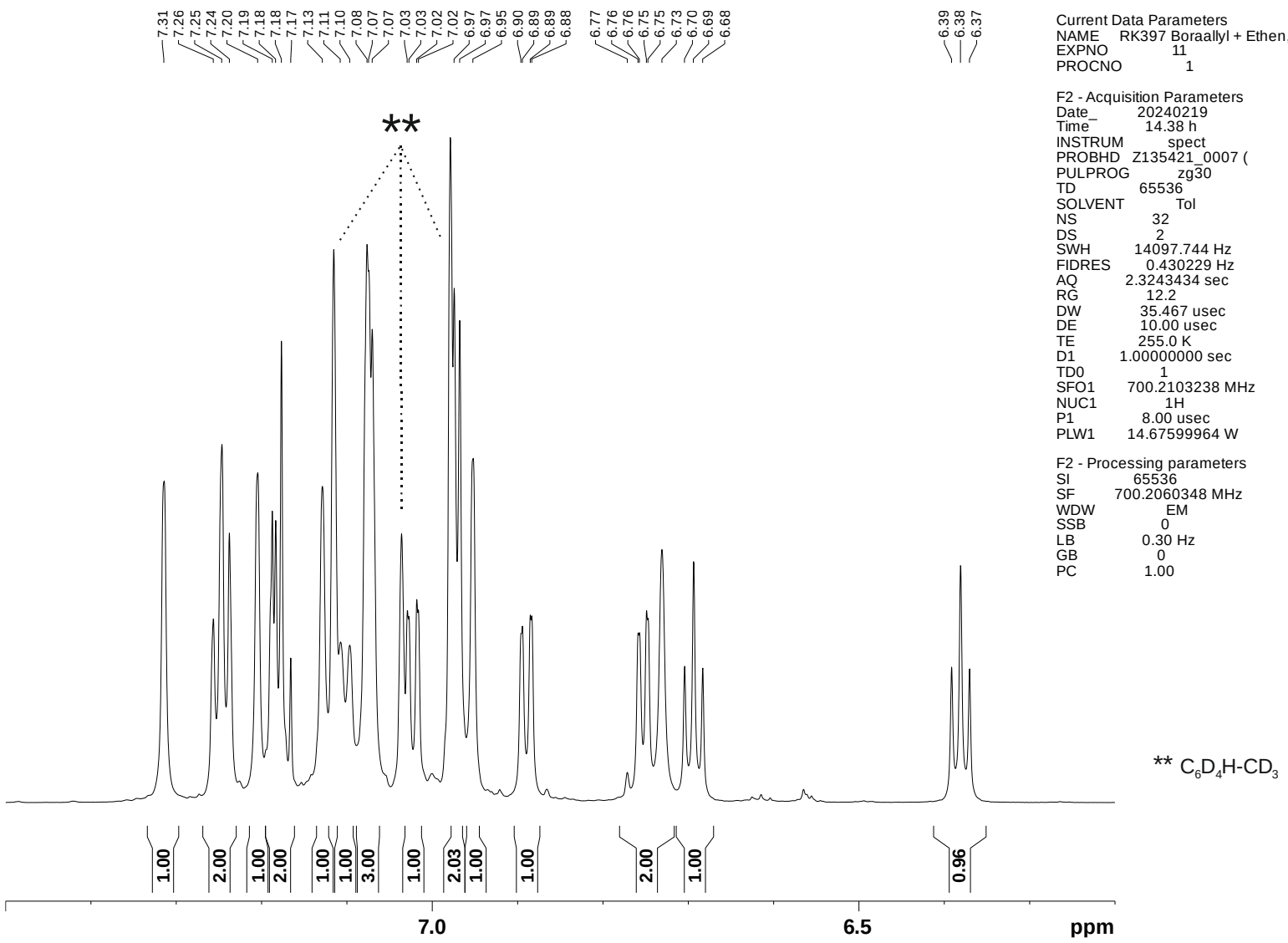


Figure S6. ^{1}H NMR spectrum of compound **2** (2.3 – 3.7 ppm).



Current Data Parameters
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EXPNO 11
PROCNO 1

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TE 255.0 K
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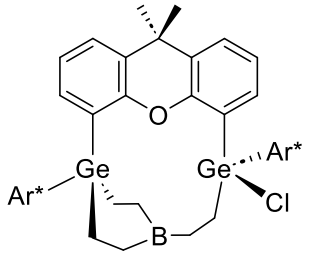
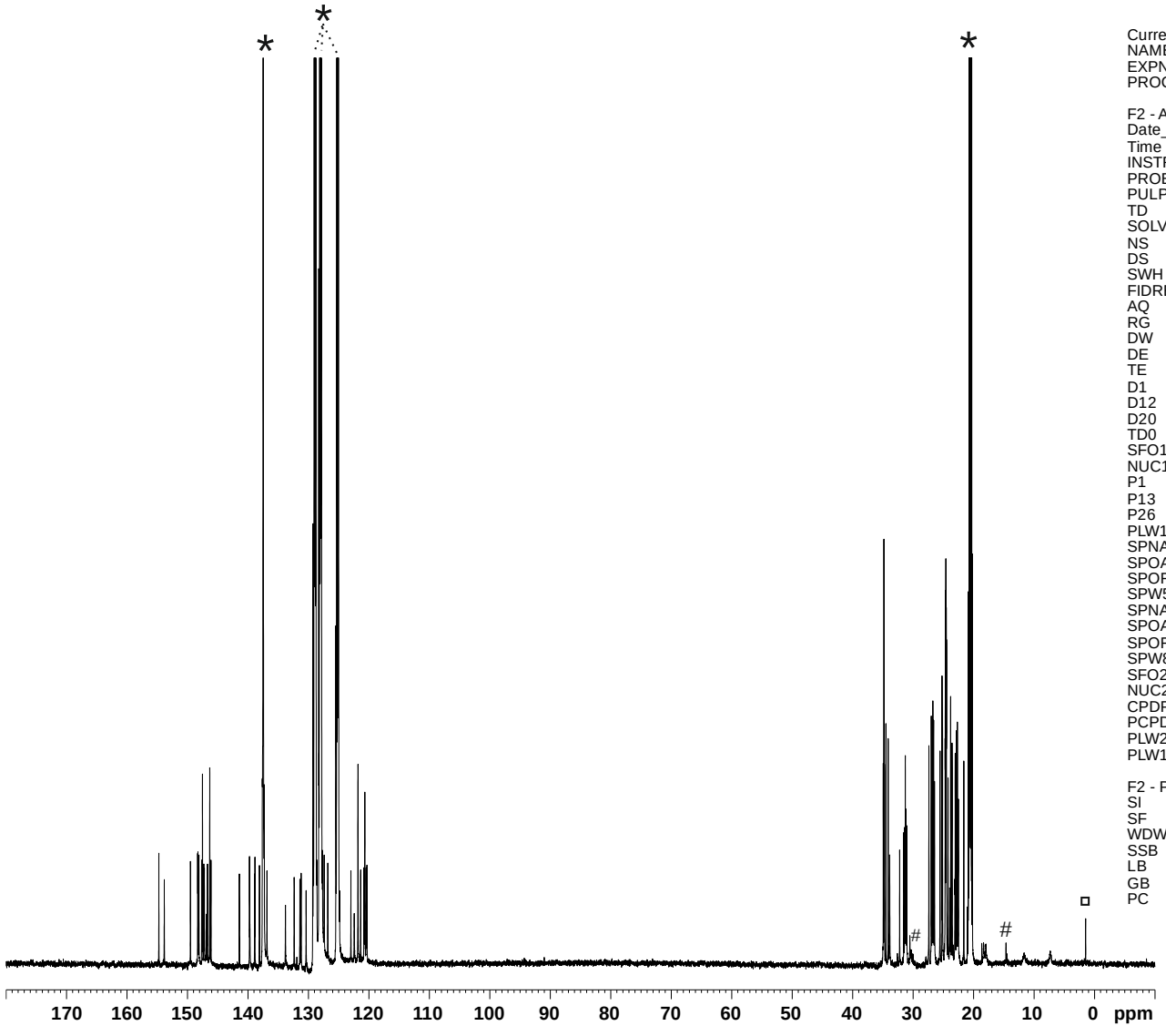


** C_6D_4H-CD_3

Figure S7. ^{1}H NMR spectrum of compound **2** (6.2 – 7.5 ppm).



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PROCNO 1

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TD0 1
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NUC1 13C
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P13 2000.00 usec
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PCPD2 65.00 usec
PLW2 14.67599964 W
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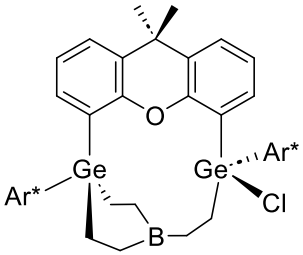
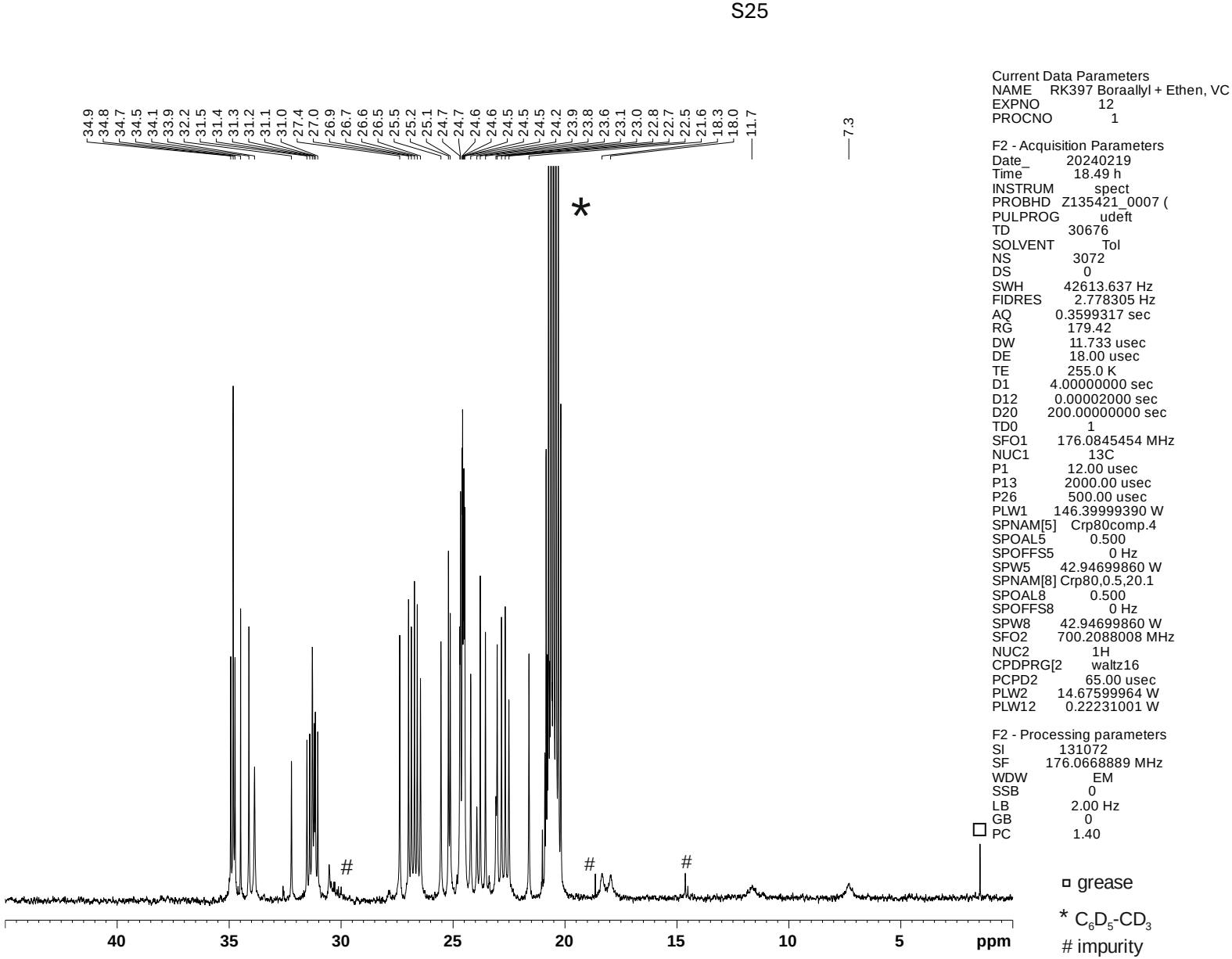


▫ grease

impurity

* C_6D_5-CD_3

Figure S8. $^{13}C\{^1H\}$ NMR spectrum of compound **2**.



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EXPNO 12
PROCNO 1

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PULPROG udeft
TD 30676
SOLVENT Tol
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 255.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0845454 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
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SPOFFS5 0 Hz
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SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

▫ grease
* C_6D_5-CD_3
# impurity

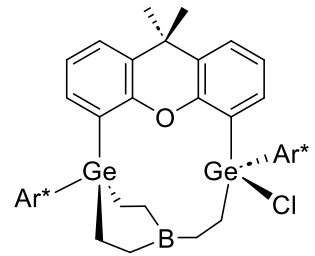
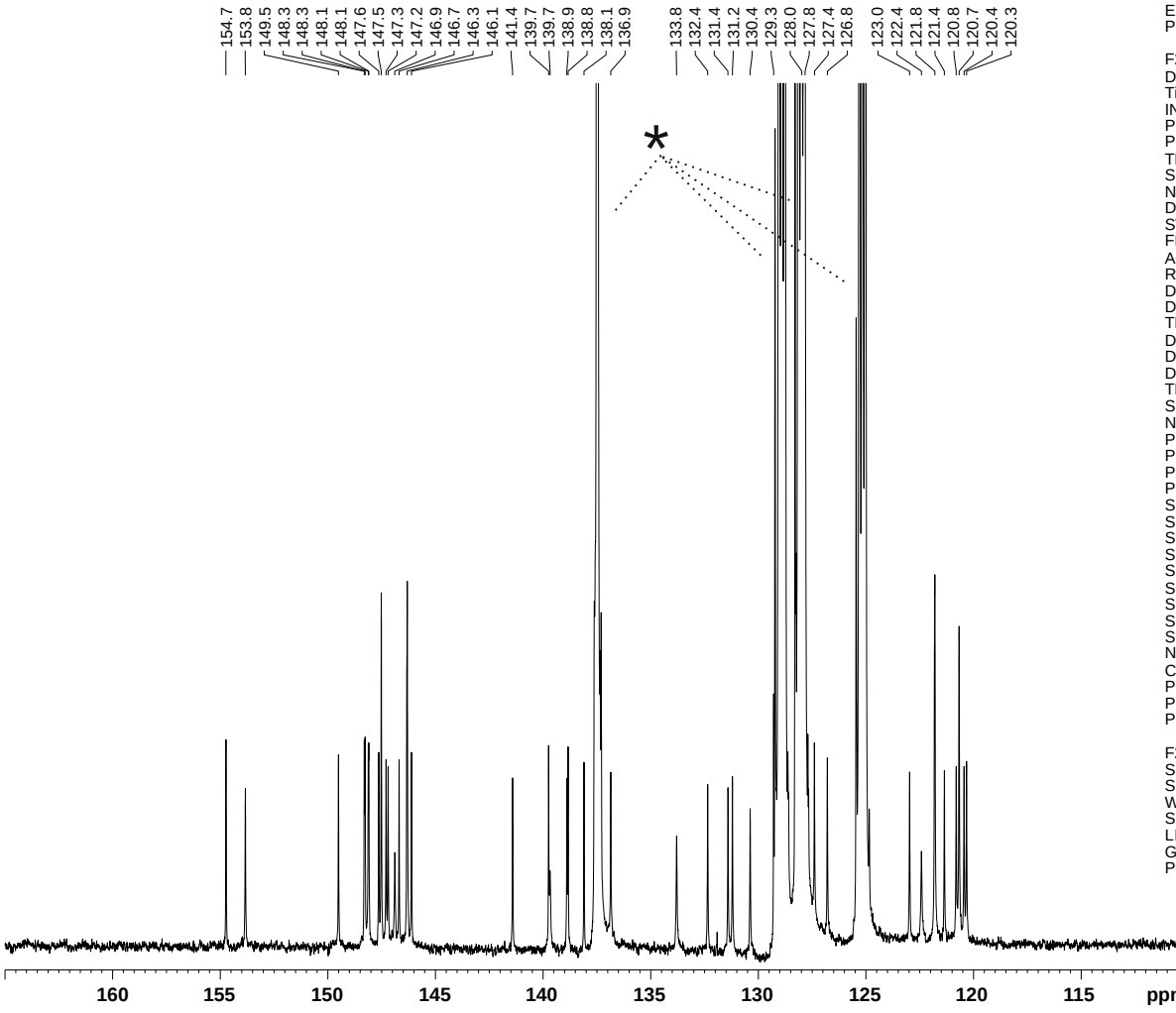


Figure S9. $^{13}C\{^1H\}$ NMR spectrum of compound **2** (0 – 45 ppm).



Current Data Parameters
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EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
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Time 18.49 h
INSTRUM spect
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TD 30676
SOLVENT Tol
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 255.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0845454 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
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SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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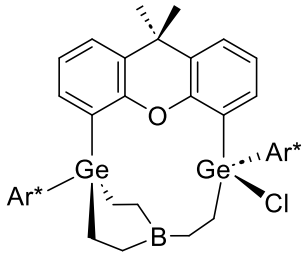
SF 176.0668889 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



* C_6D_5-CD_3

Figure S10. $^{13}C\{^1H\}$ NMR spectrum of compound **2** (110 – 165 ppm).

NMR spectra of compound **3**.

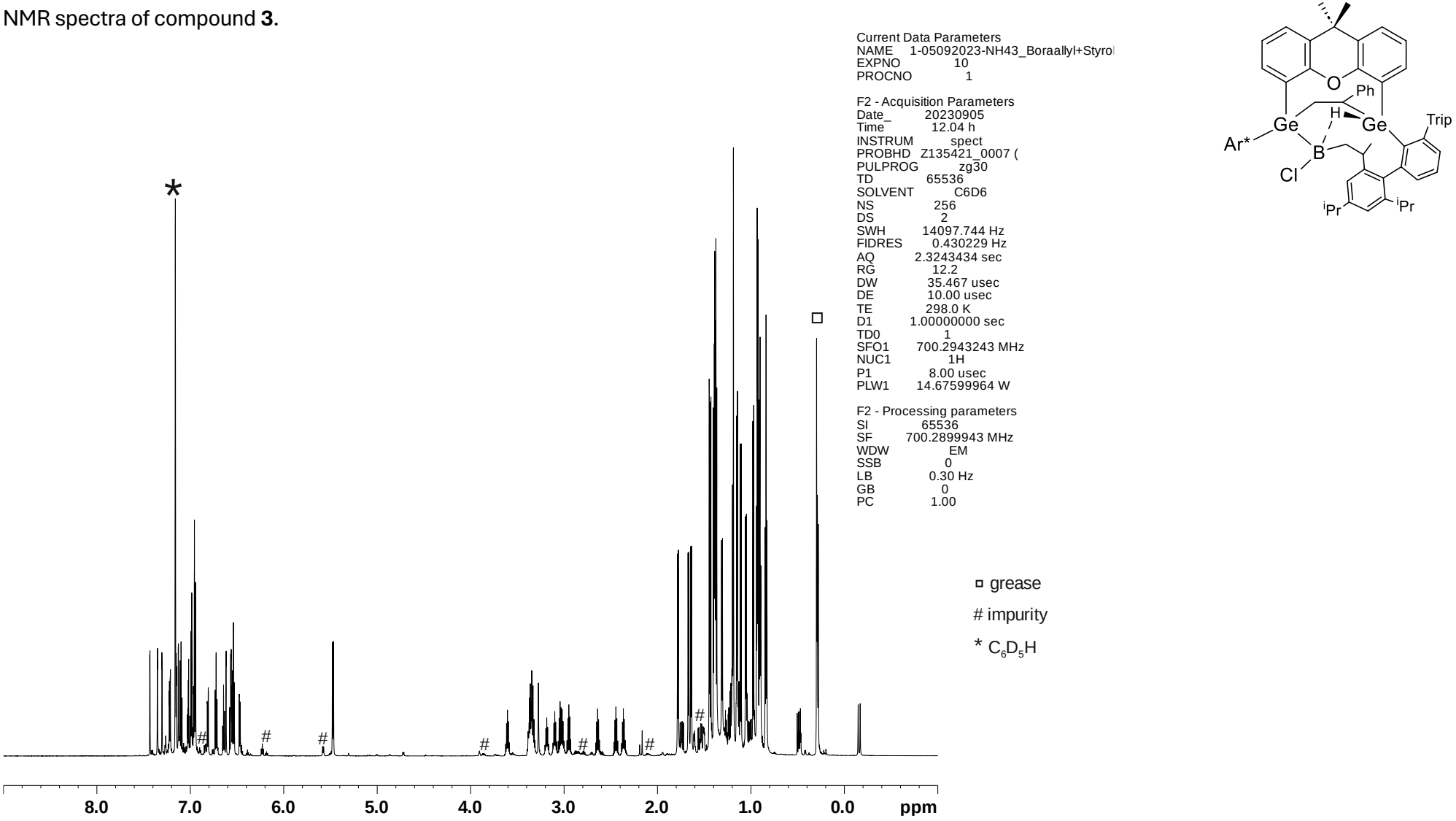


Figure S11. ^{1}H NMR spectrum of compound **3**.

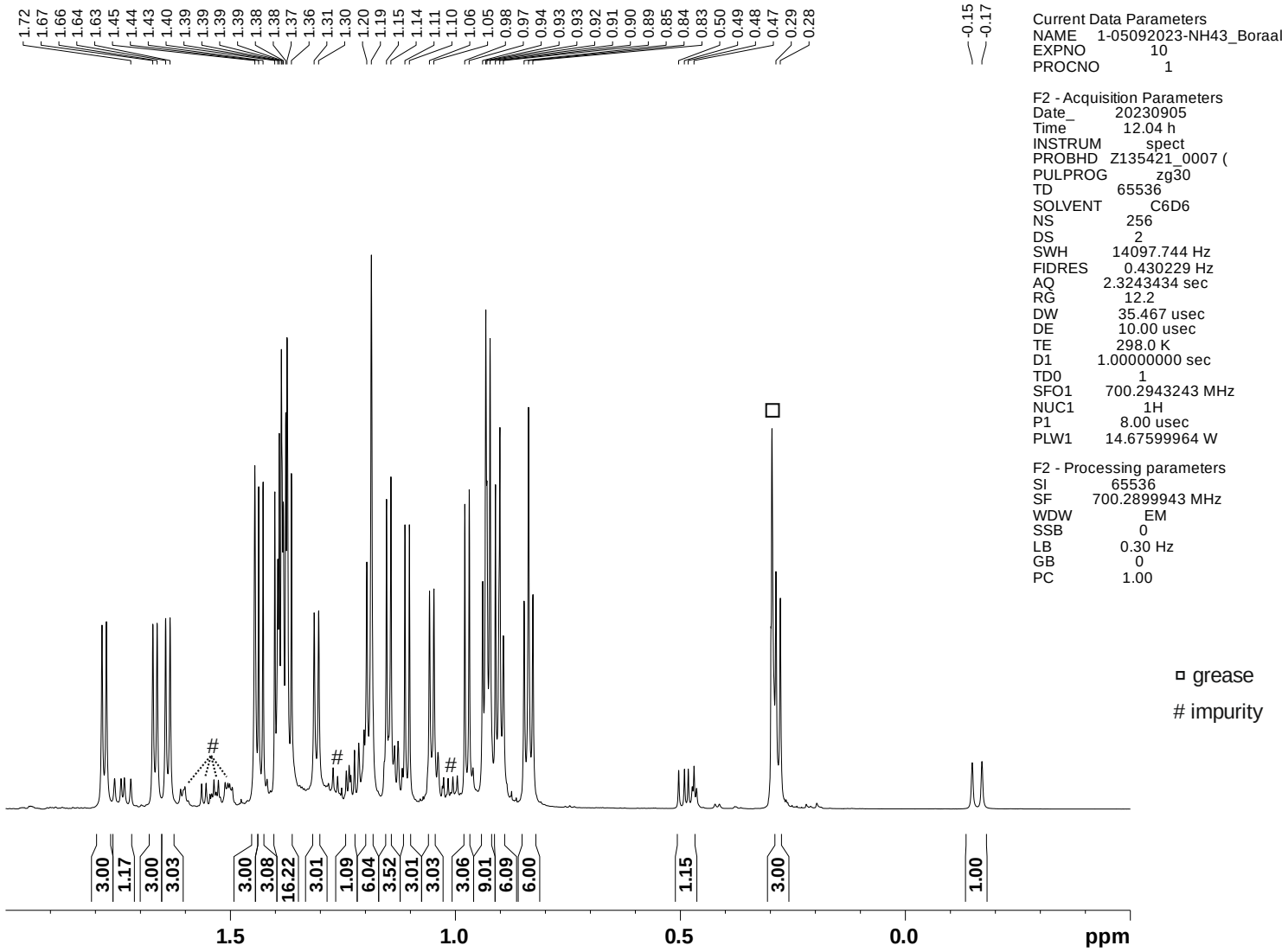


Figure S12. ^{1}H NMR spectrum of compound **3** (−0.5 – 2.0 ppm).

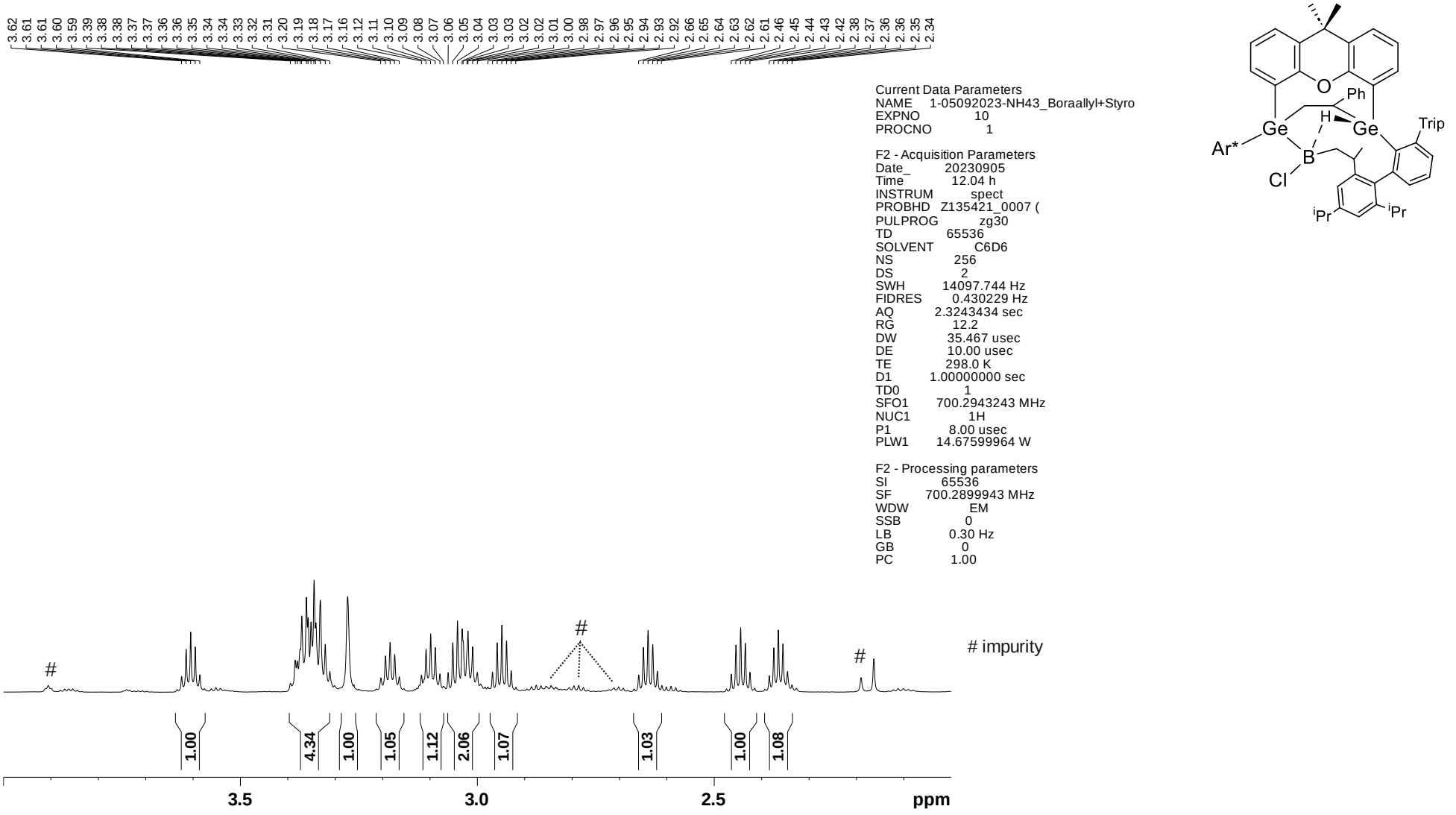


Figure S13. ^{1}H NMR spectrum of compound **3** (2.0 – 4.0 ppm).

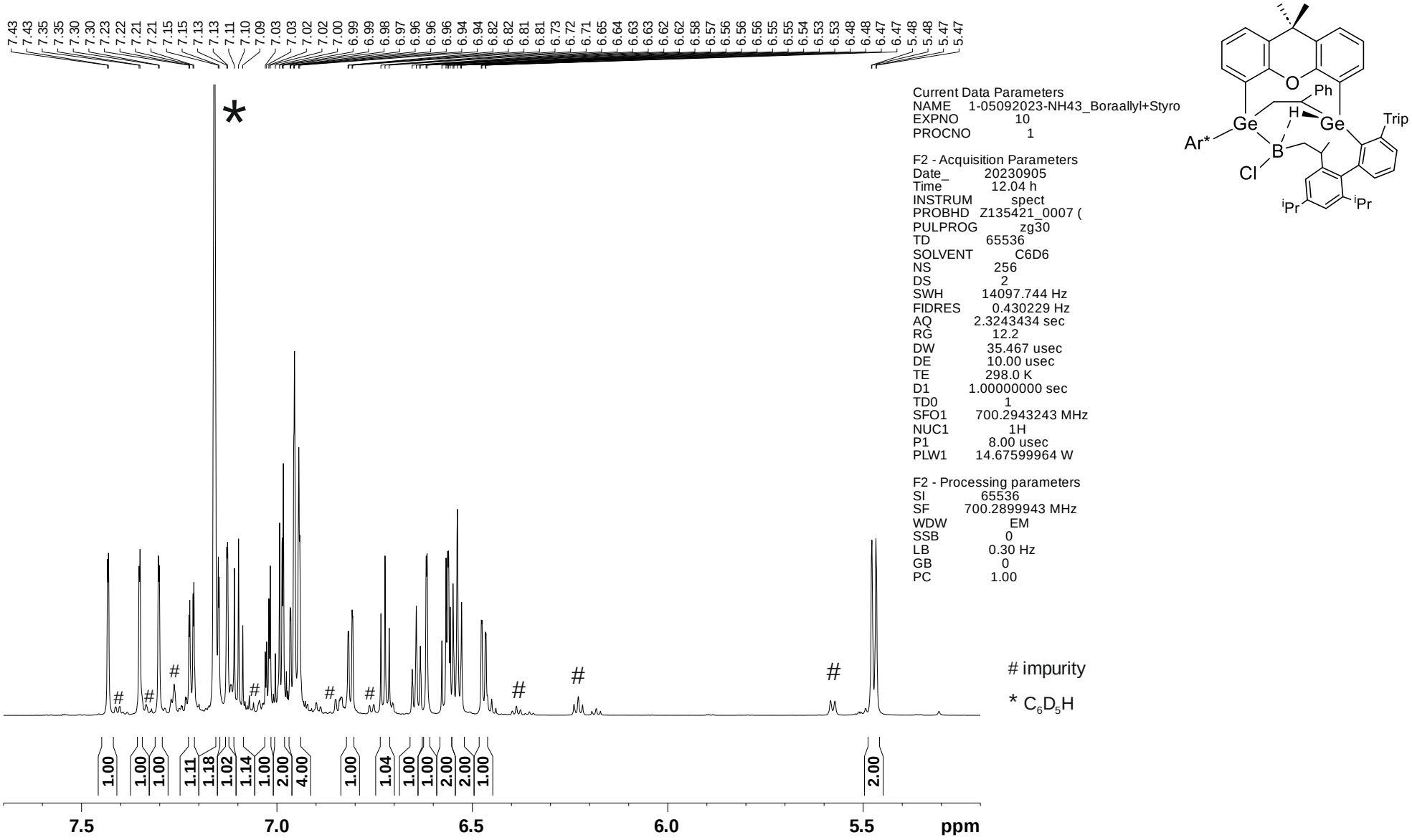
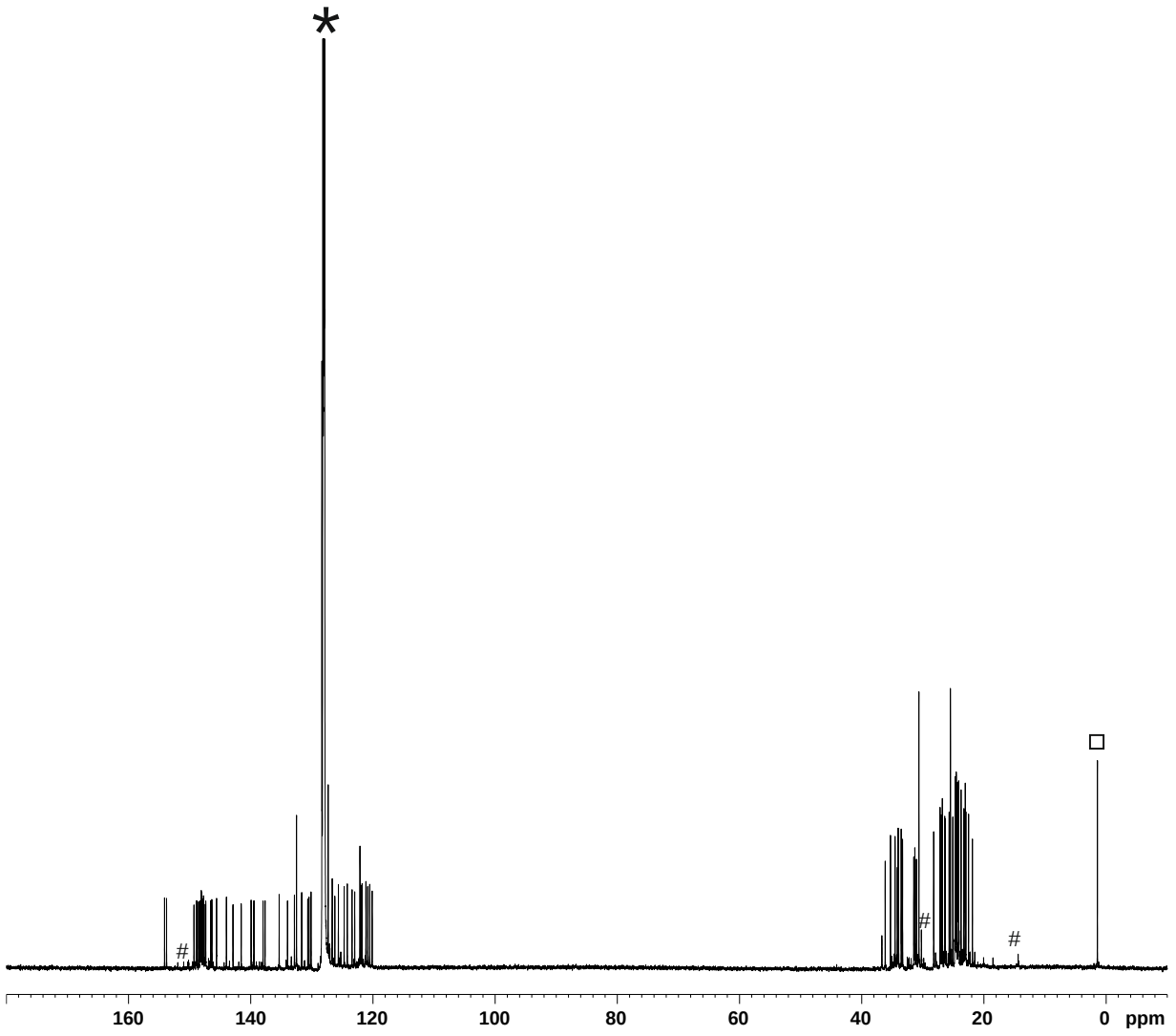


Figure S14. ^{1}H NMR spectrum of compound **3** (5.2 – 7.7 ppm).



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EXPNO 11
PROCNO 1

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TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.1056694 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2928012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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SSB 0
LB 2.00 Hz
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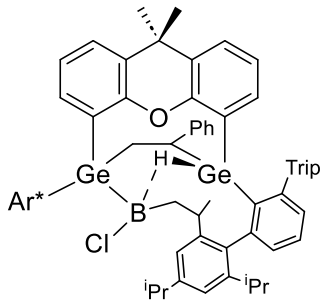
PC 1.40

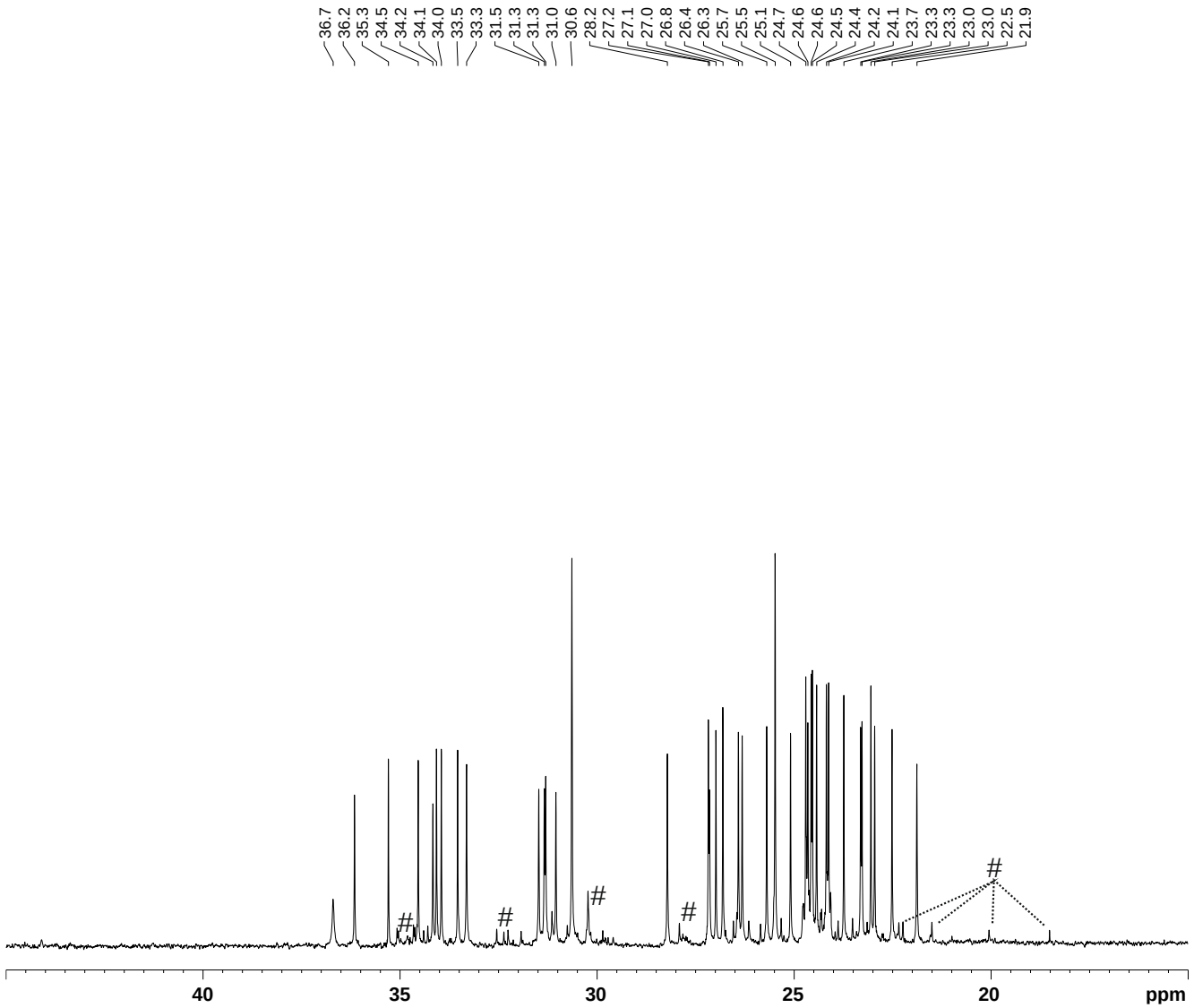


□ grease

impurity

* C_6D_6

Figure S15. $^{13}C\{^1H\}$ NMR spectrum of compound **3**.



impurity

Current Data Parameters
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EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 17.36 h
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TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.1056694 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
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SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2928012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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SF 176.0879952 MHz
WDW EM
SSB 0
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PC 1.40

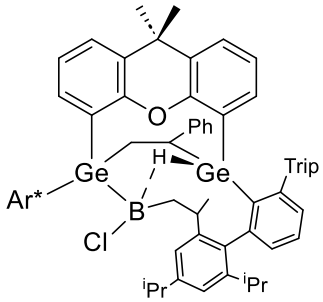
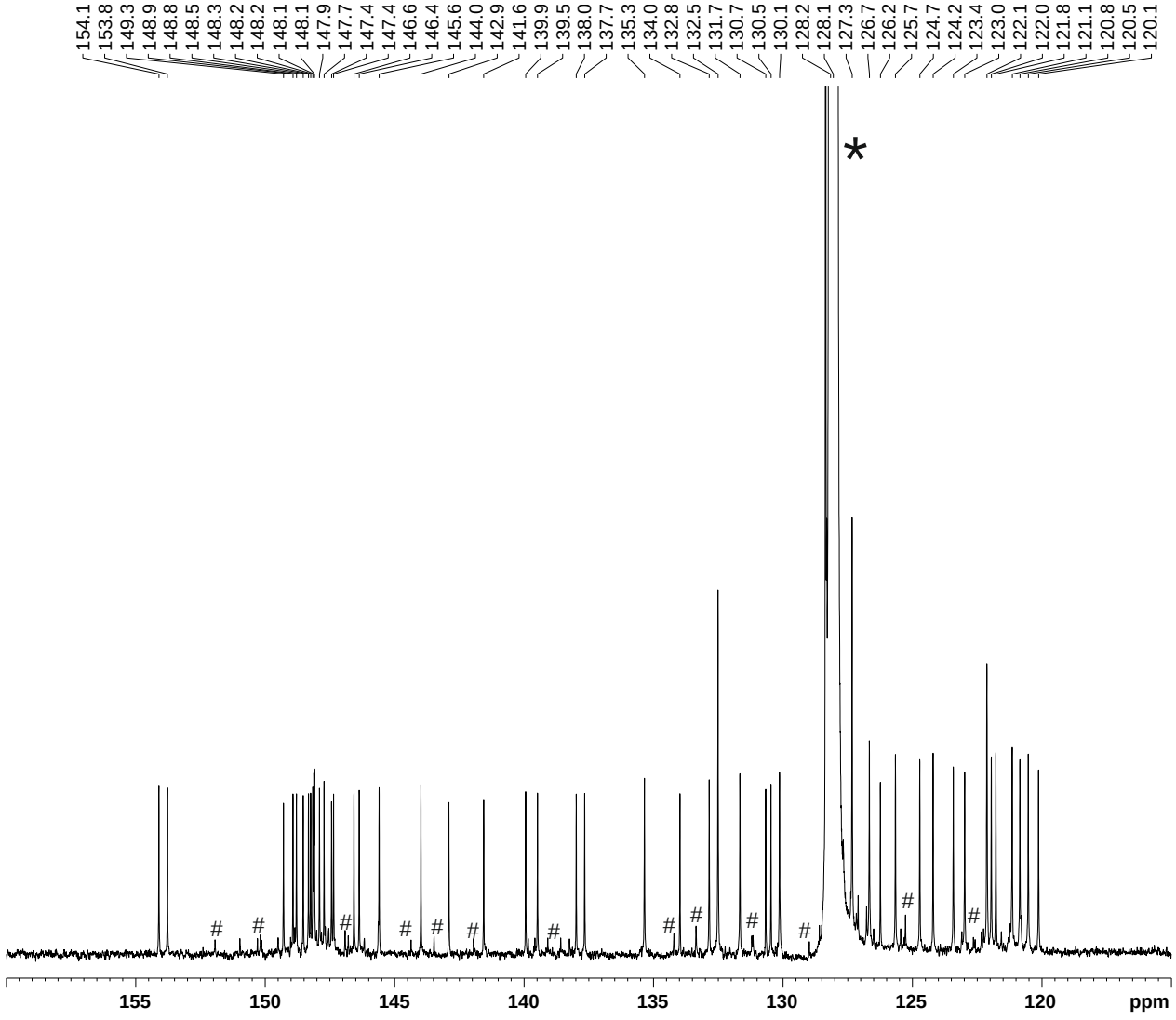


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** (15 – 45 ppm).



Current Data Parameters
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EXPNO 11
PROCNO 1

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PULPROG udeft
TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.1056694 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
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SPOFFS5 0 Hz
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SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2928012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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SF 176.0879952 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

impurity

* C_6D_6

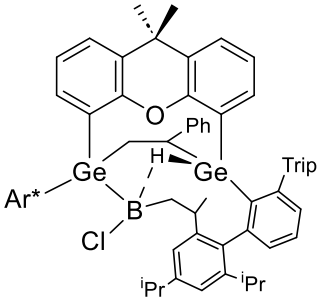
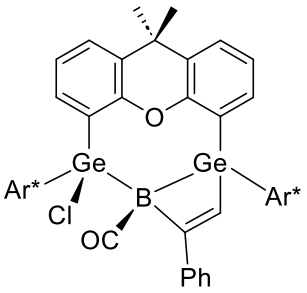


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** (115 – 160 ppm).

NMR spectra of compound **6**.



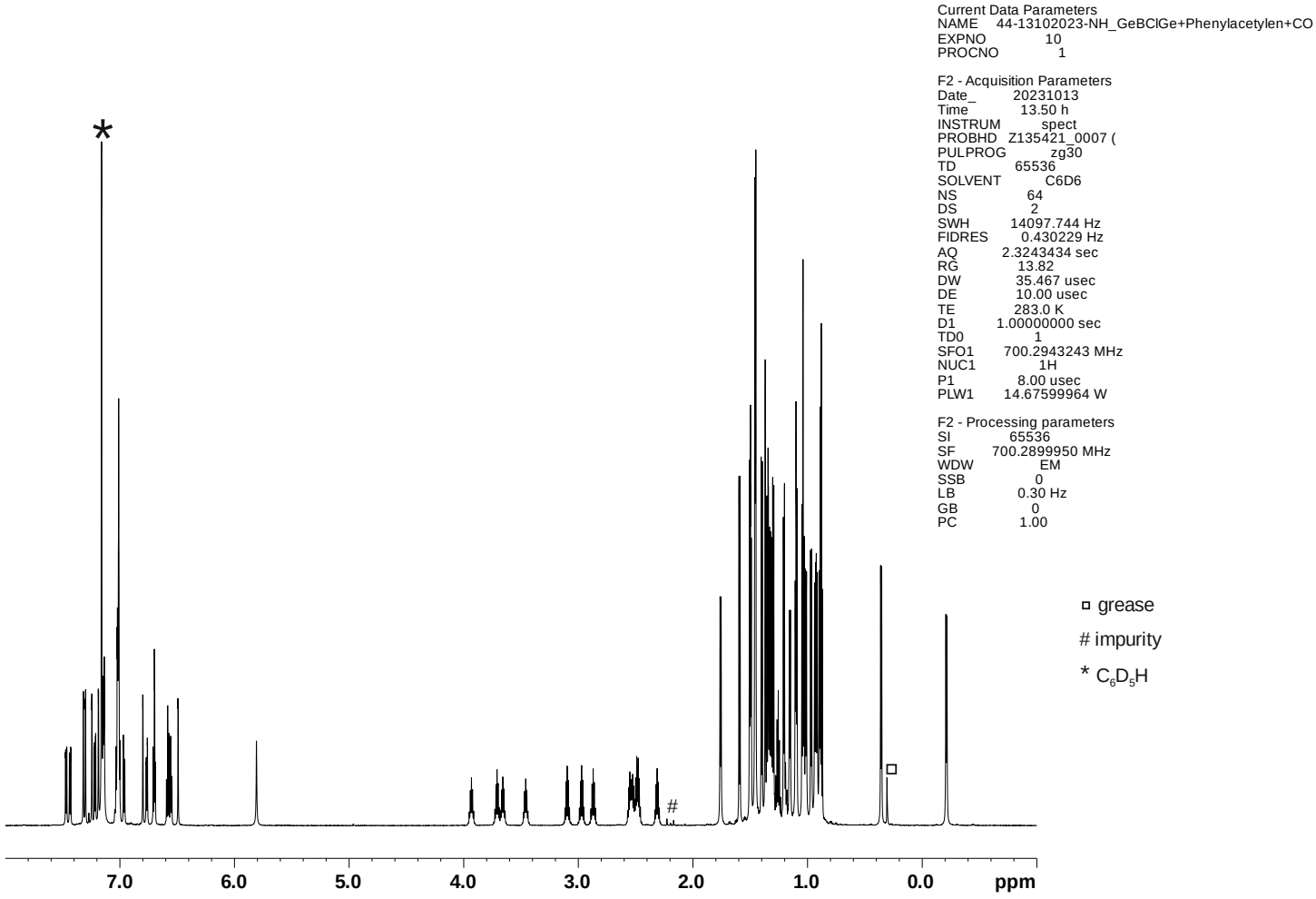


Figure S18. ^{1}H NMR spectrum of compound **6**.

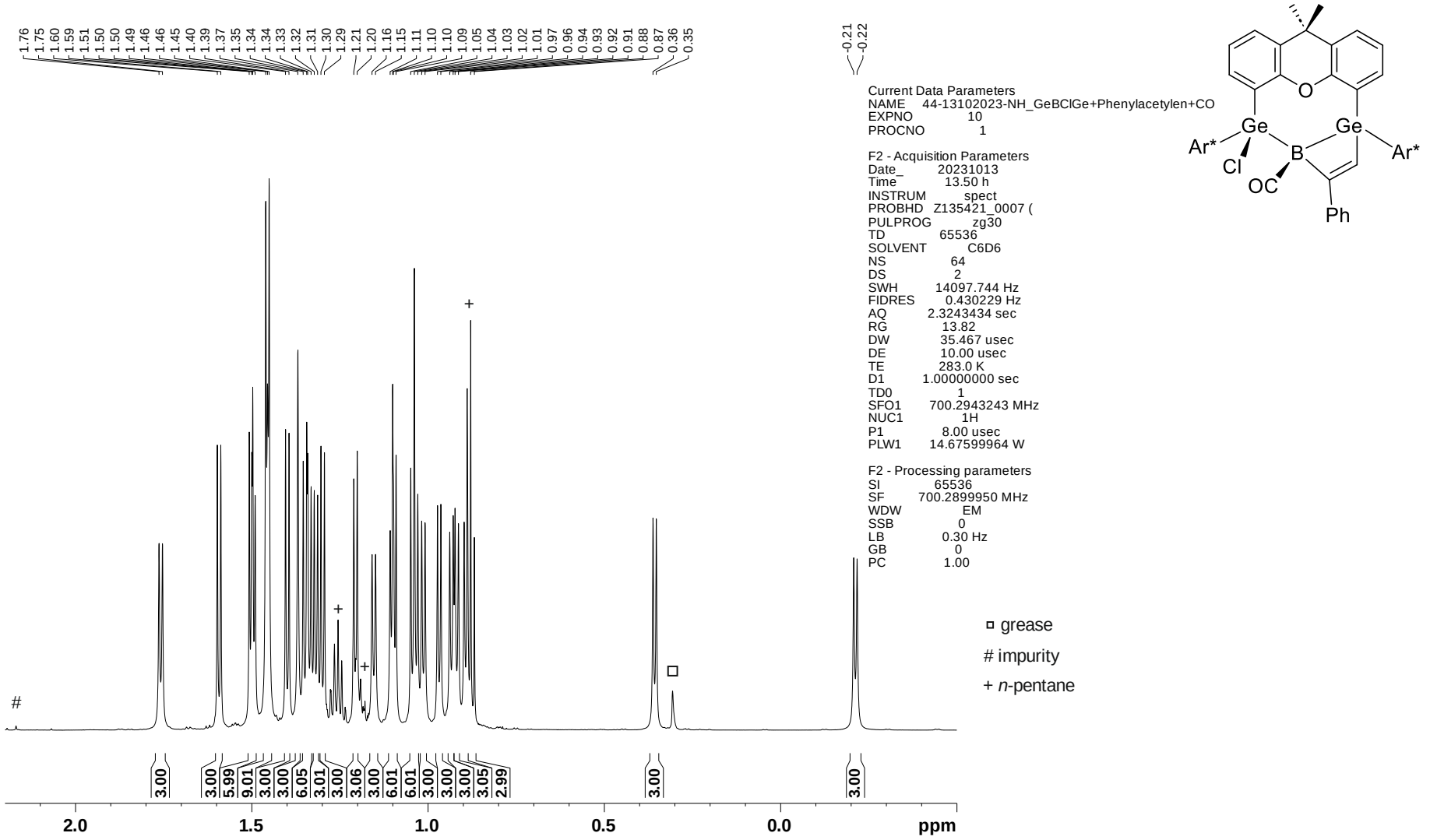
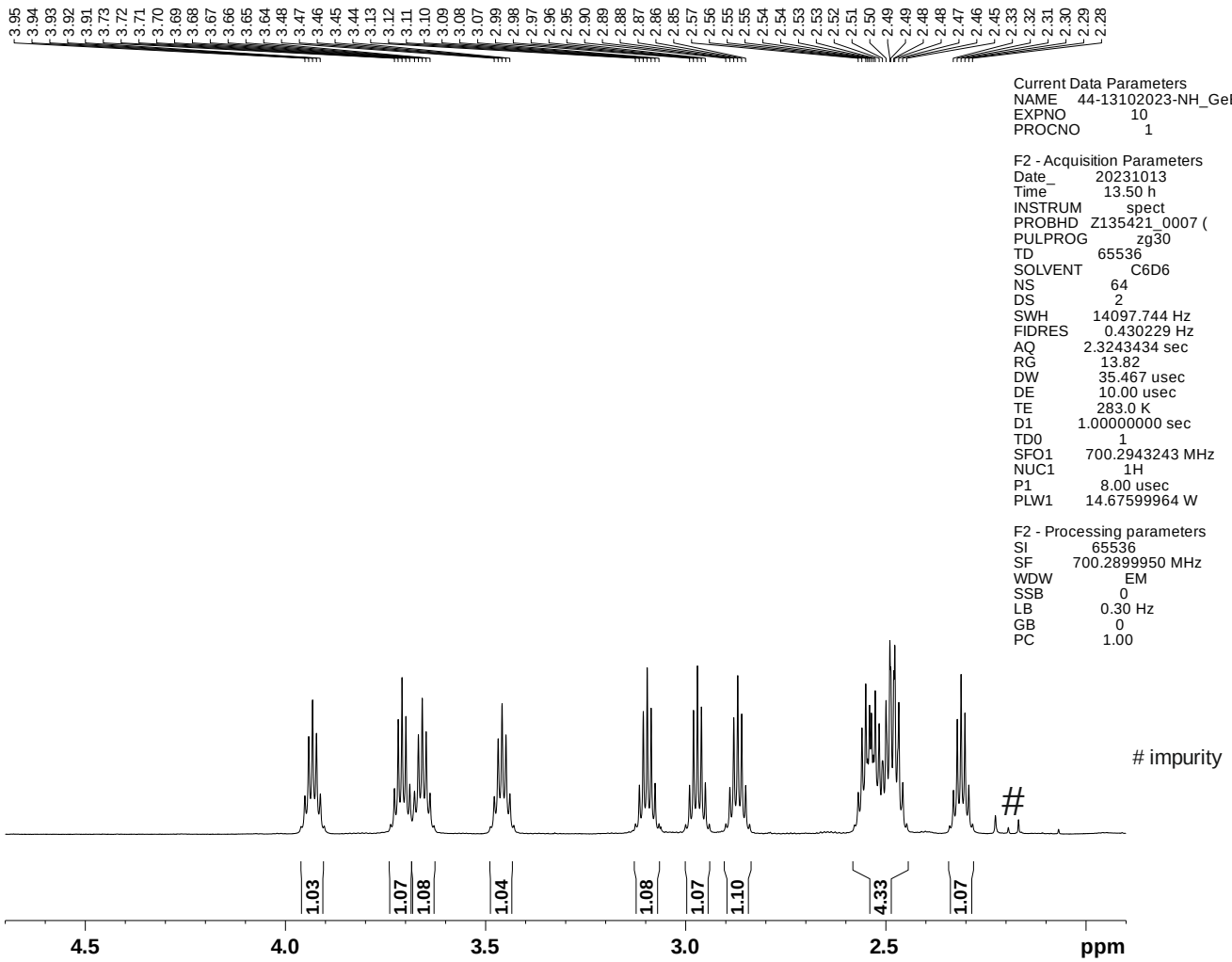


Figure S19. ^{1}H NMR spectrum of compound **6** (−0.5 – 2.2 ppm).



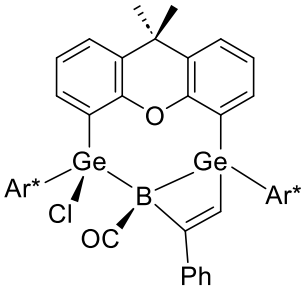


Figure S20. ^{1}H NMR spectrum of compound **6** (1.9 – 4.7 ppm).

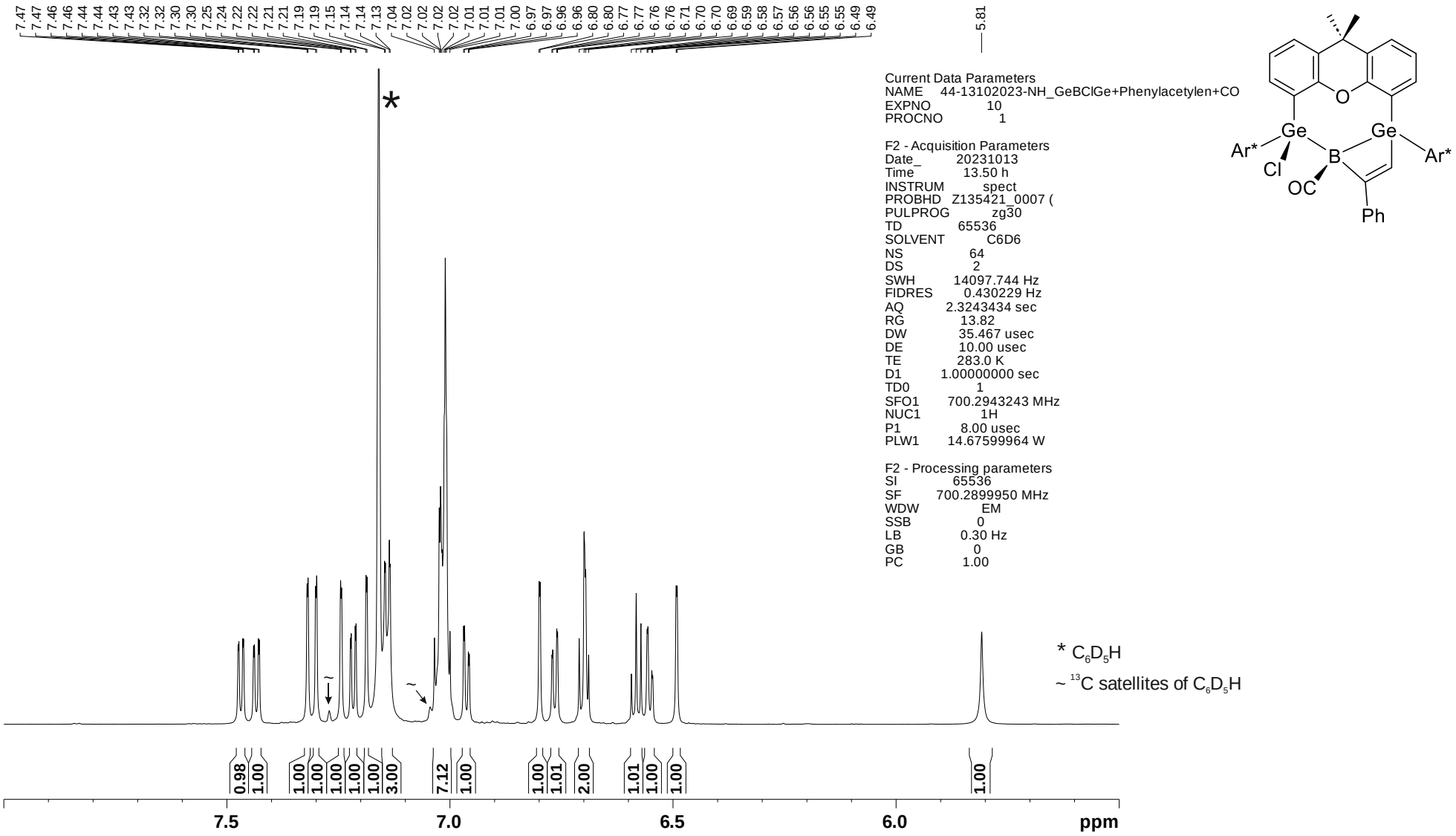
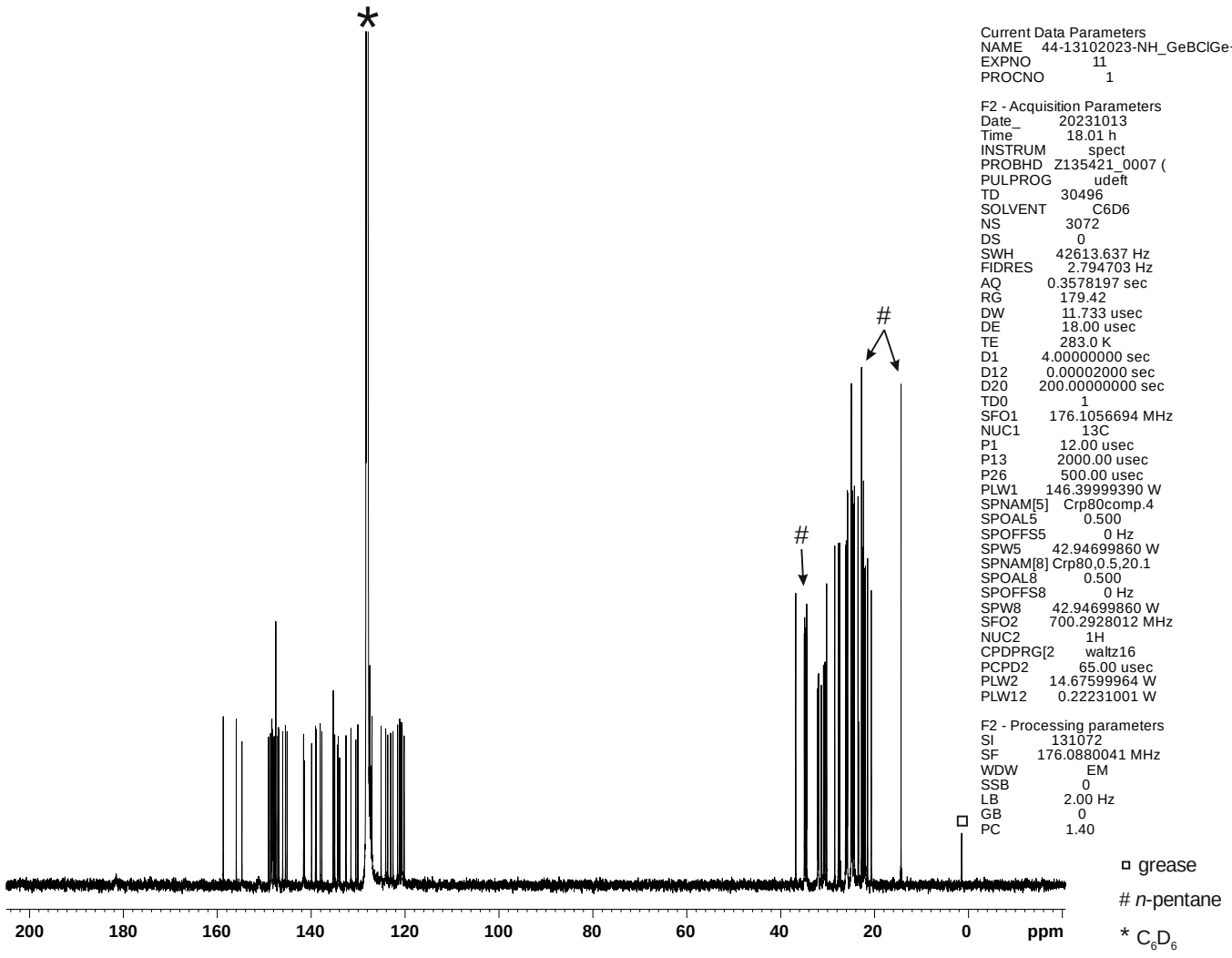


Figure S21. ^{1}H NMR spectrum of compound **6** (5.5 – 8.0 ppm).



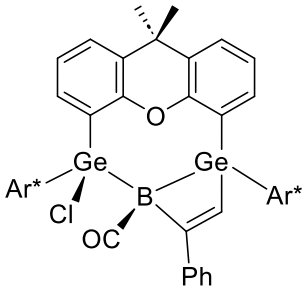
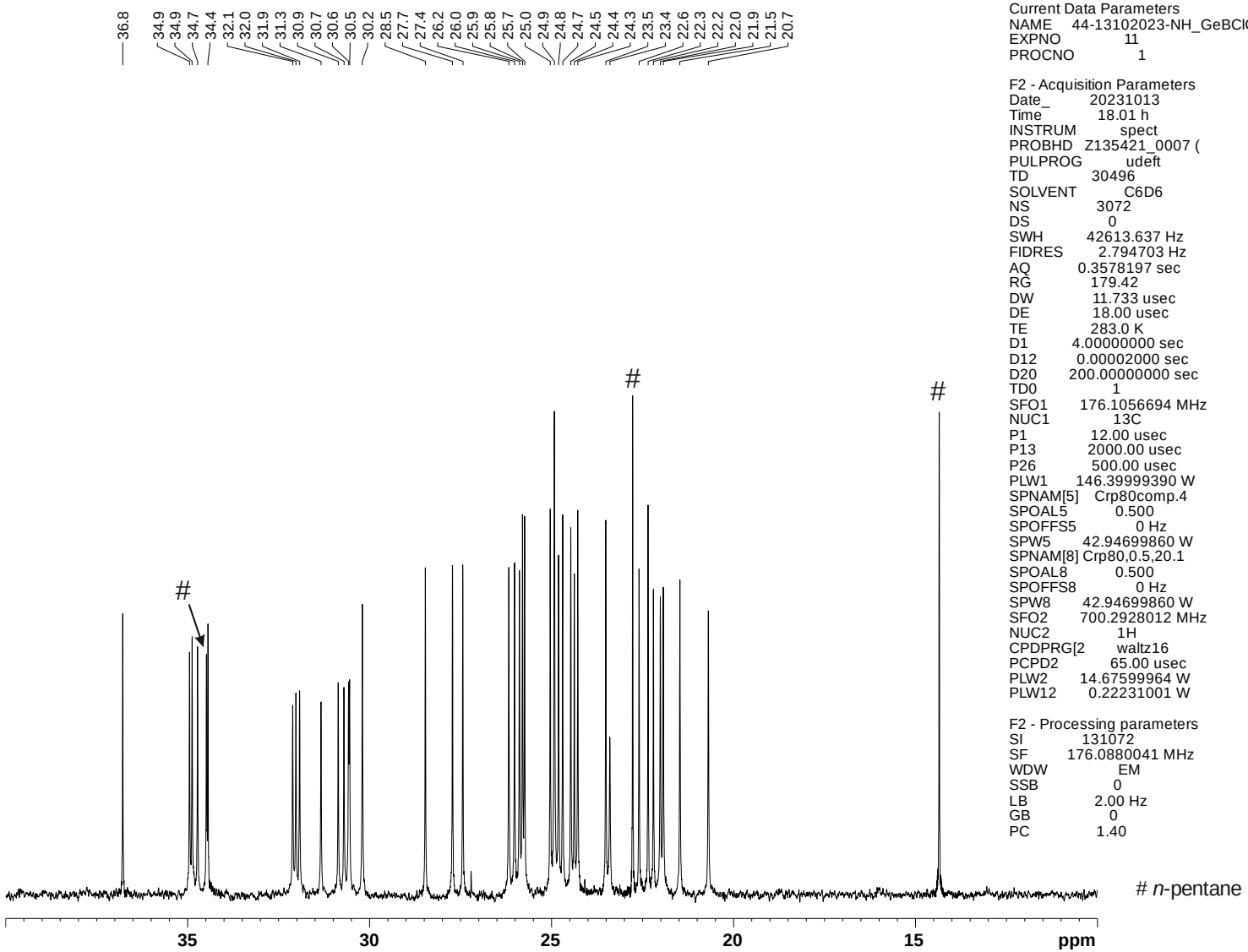


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6**.



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PROCNO 1

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TD 30496
SOLVENT C6D6
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FIDRES 2.794703 Hz
AQ 0.3578197 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 283.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.1056694 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2928012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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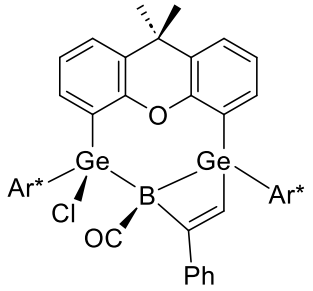
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



n-pentane

Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** (10 – 40 ppm).

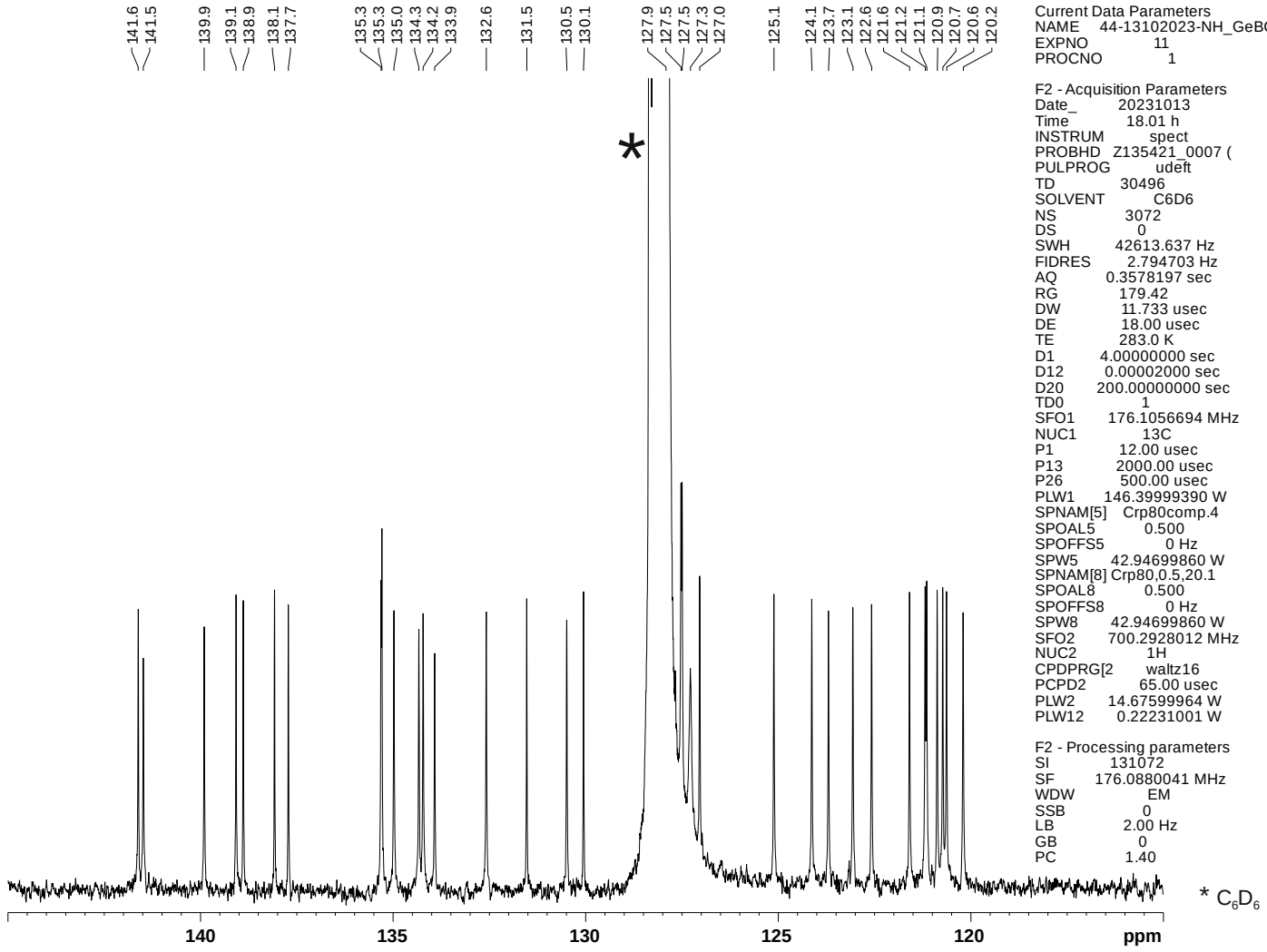
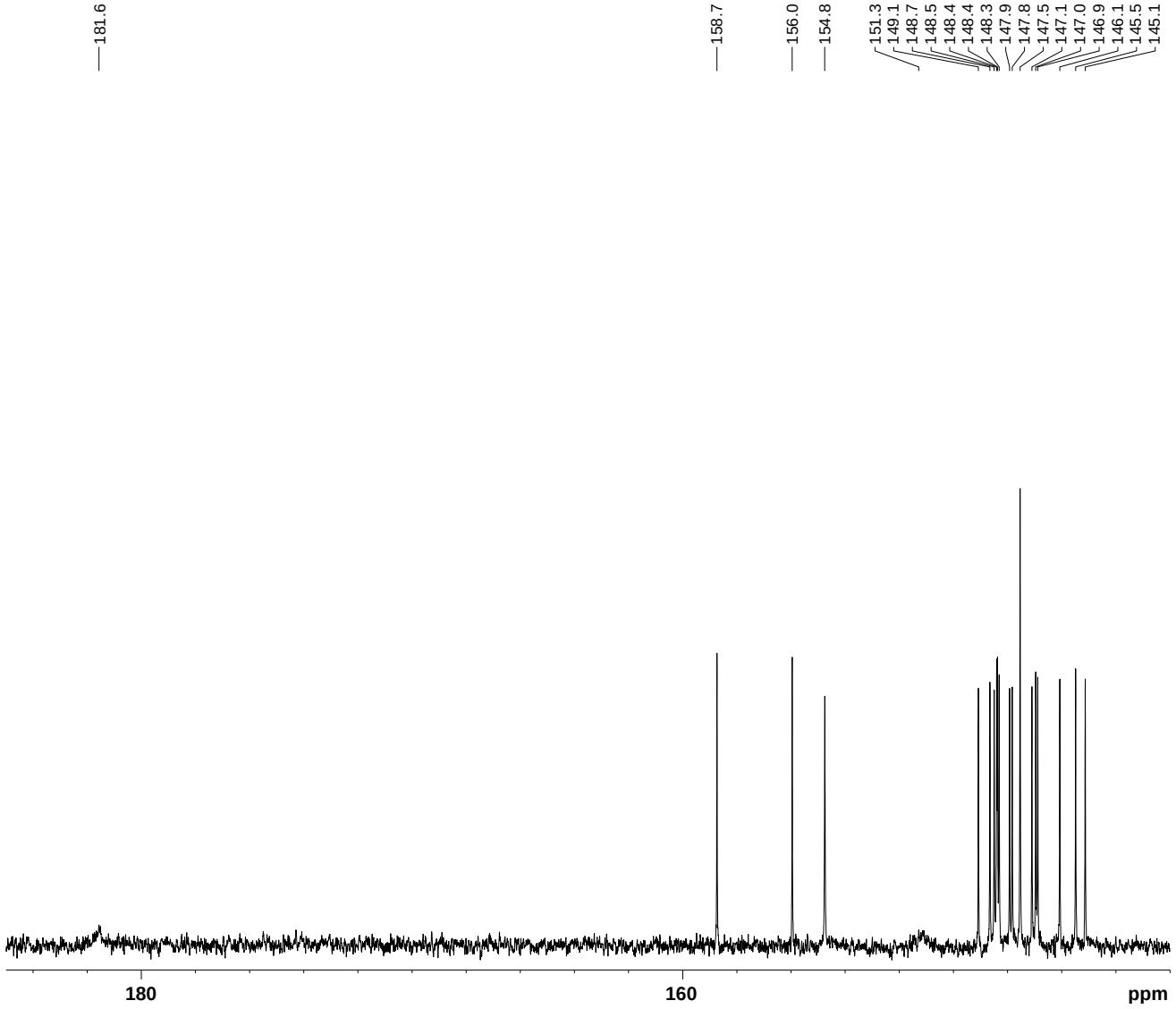


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** (115 – 145 ppm).



Current Data Parameters
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EXPNO 11
PROCNO 1

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TD 30496
SOLVENT C6D6
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.794703 Hz
AQ 0.3578197 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 283.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.1056694 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2928012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

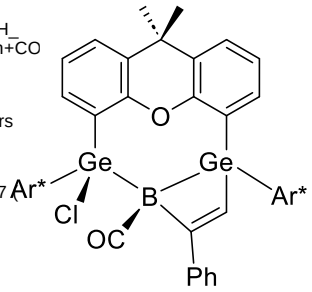
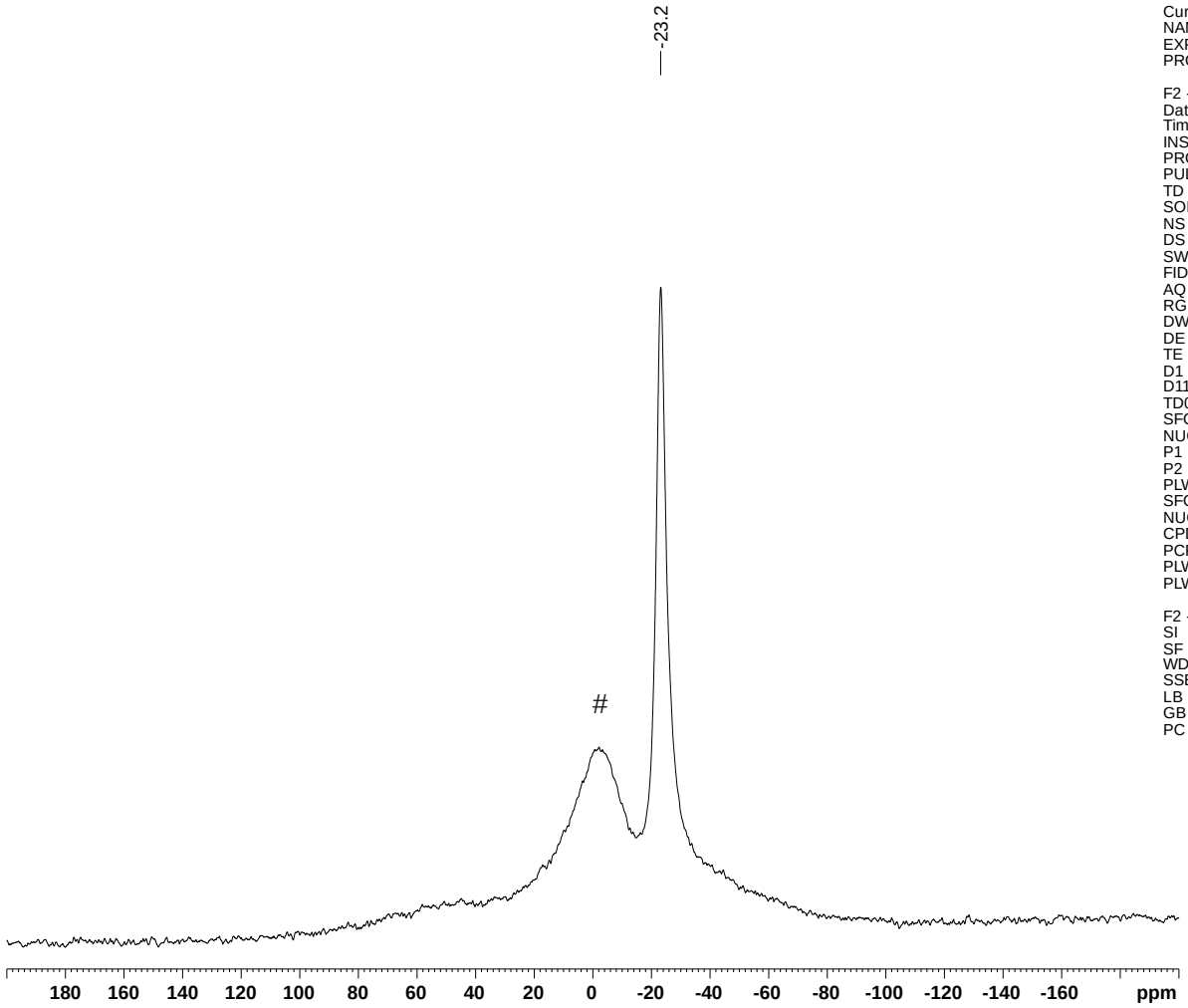


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** (142 – 185 ppm).



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EXPNO 11
PROCNO 1

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TD 8192
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FIDRES 11.737530 Hz
AQ 0.0851968 sec
RG 161.31
DW 10.400 usec
DE 6.50 usec
TE 298.0 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1
SFO1 96.2936310 MHz
NUC1 11B
P1 5.75 usec
P2 11.50 usec
PLW1 70.00000000 W
SFO2 300.1314106 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.26509953 W
PLW12 0.20000000 W

F2 - Processing parameters
SI 32768
SF 96.2936310 MHz
WDW EM
SSB 0
LB 50.00 Hz
GB 0
PC 1.40

glass

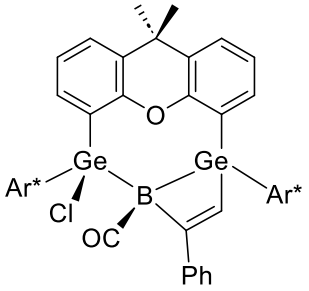
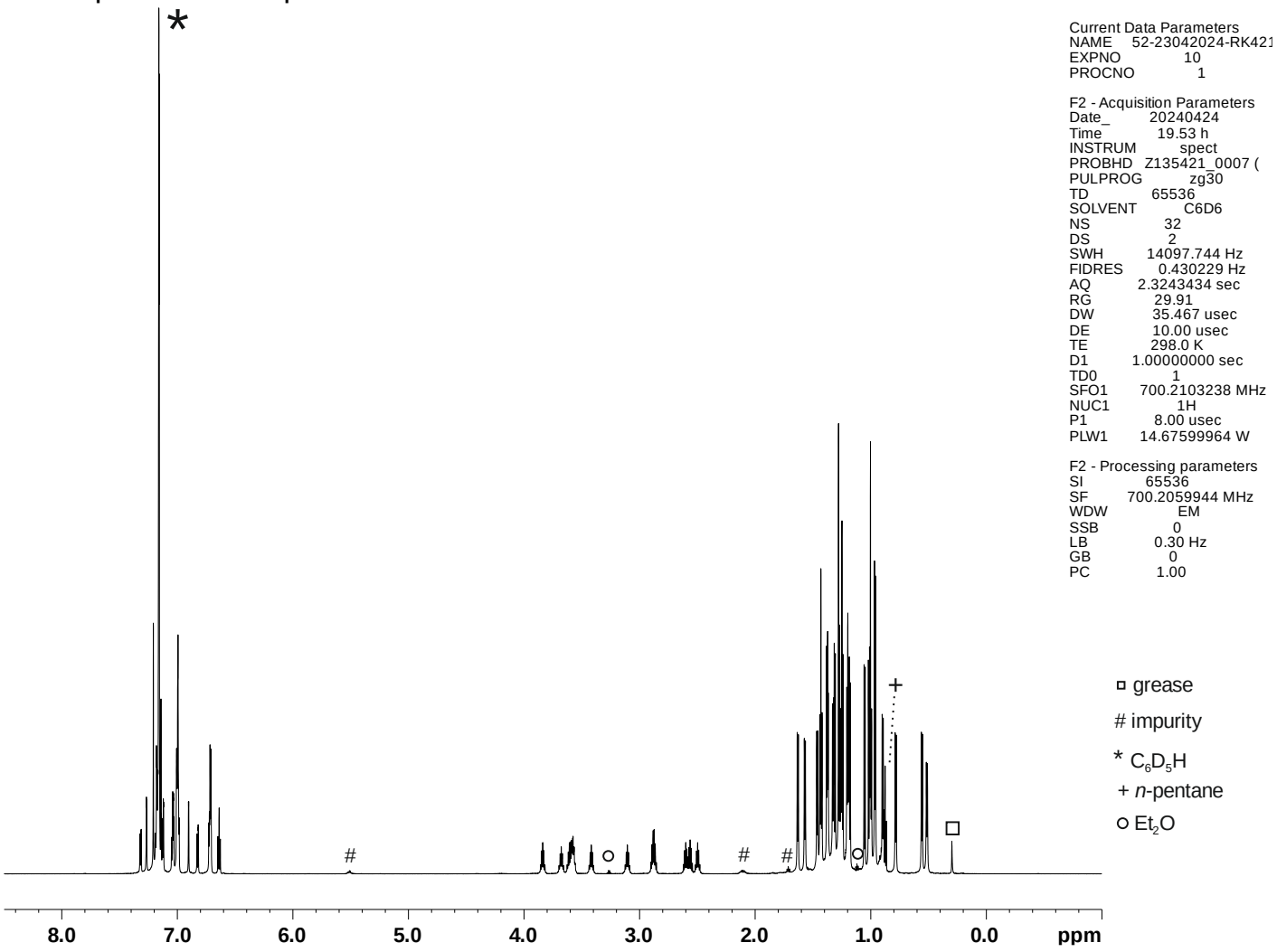


Figure S26. $^{11}B\{^{1}H\}$ NMR spectrum of compound **6**.

NMR spectra of compound **7**.



Current Data Parameters
NAME 52-23042024-RK421
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 19.53 h
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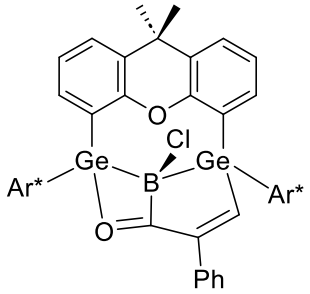
PROBHD Z135421_0007 (
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 32
DS 2
SWH 14097.744 Hz
FIDRES 0.430229 Hz
AQ 2.3243434 sec
RG 29.91
DW 35.467 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 700.2103238 MHz
NUC1 1H
P1 8.00 usec
PLW1 14.67599964 W

F2 - Processing parameters
SI 65536
SF 700.2059944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



▫ grease
impurity
* C_6D_5H
+ *n*-pentane
o Et_2O

Figure S27. ^{1}H NMR spectrum of compound **7**.

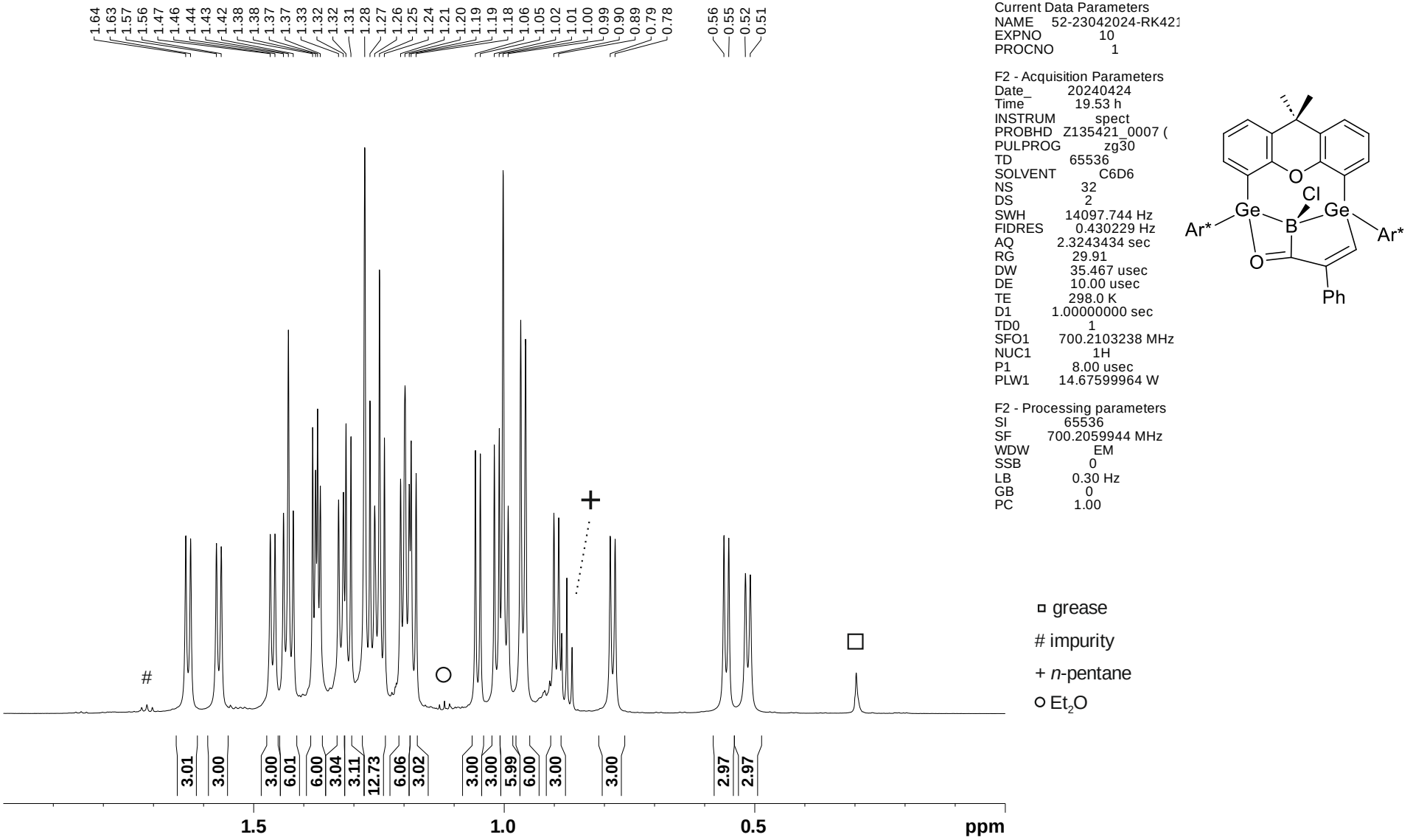


Figure S28. ^{1}H NMR spectrum of compound **7** (0 – 2.0 ppm).

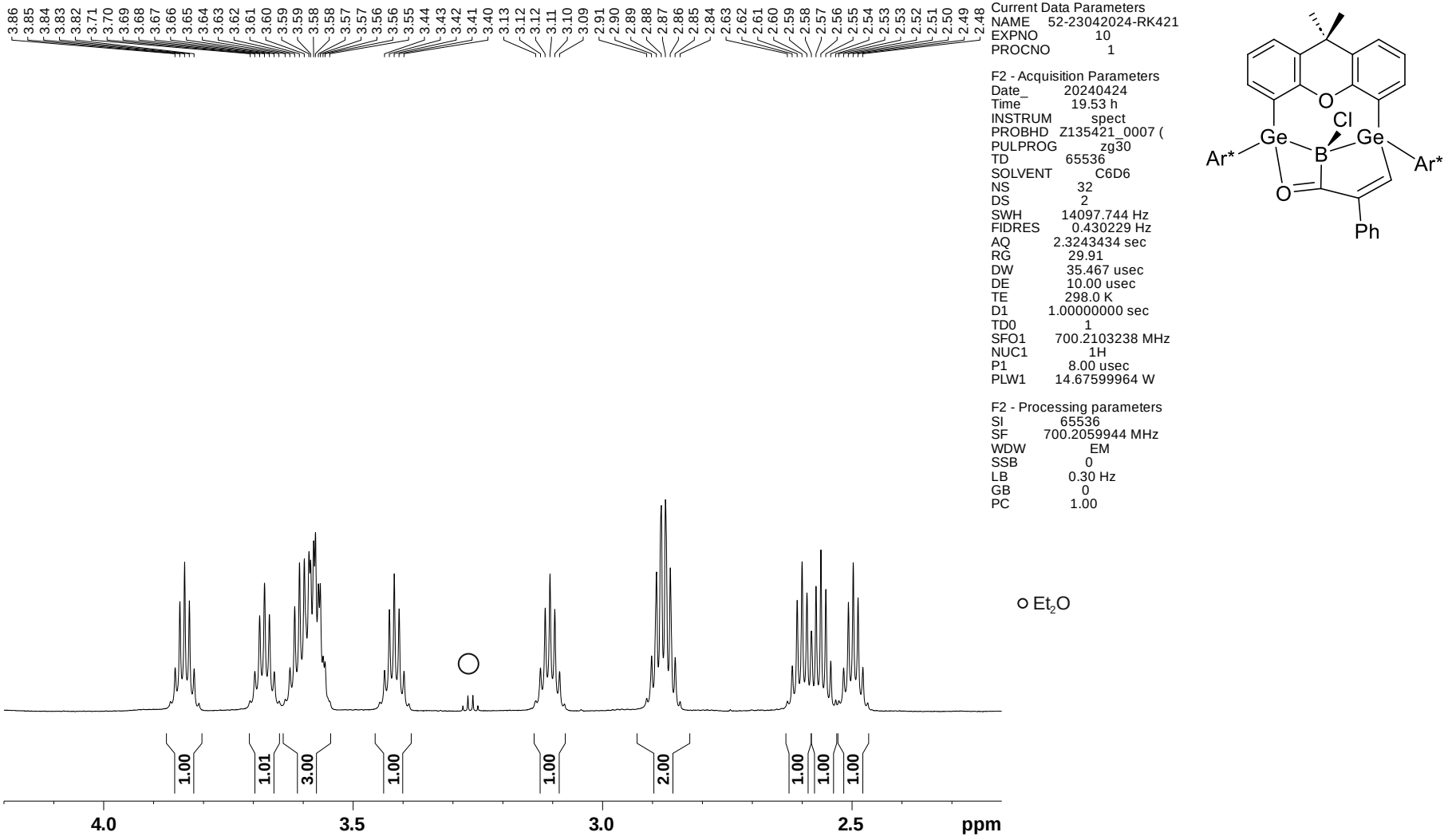


Figure S29. ^{1}H NMR spectrum of compound **7** (2.2 – 4.2).

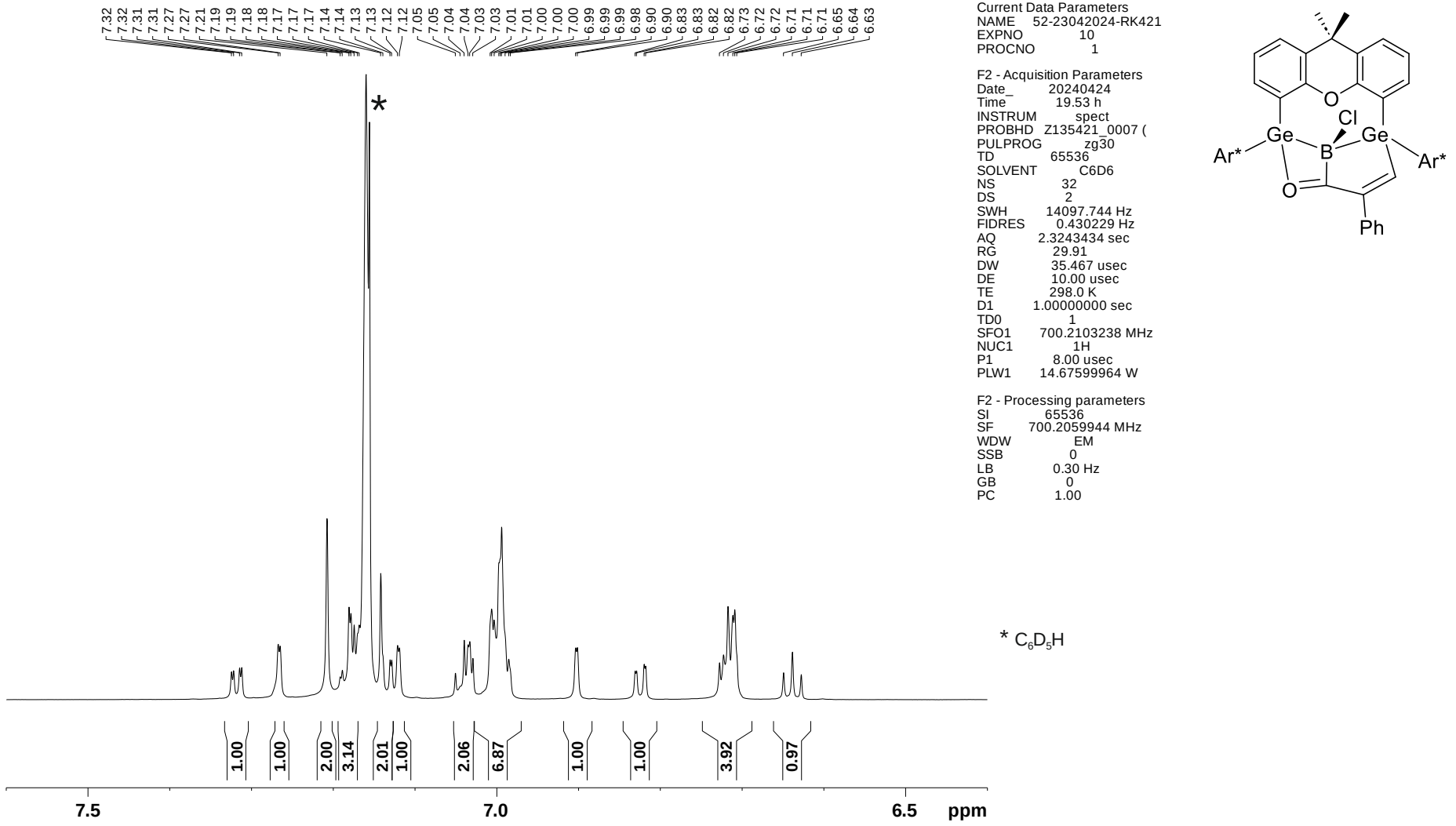
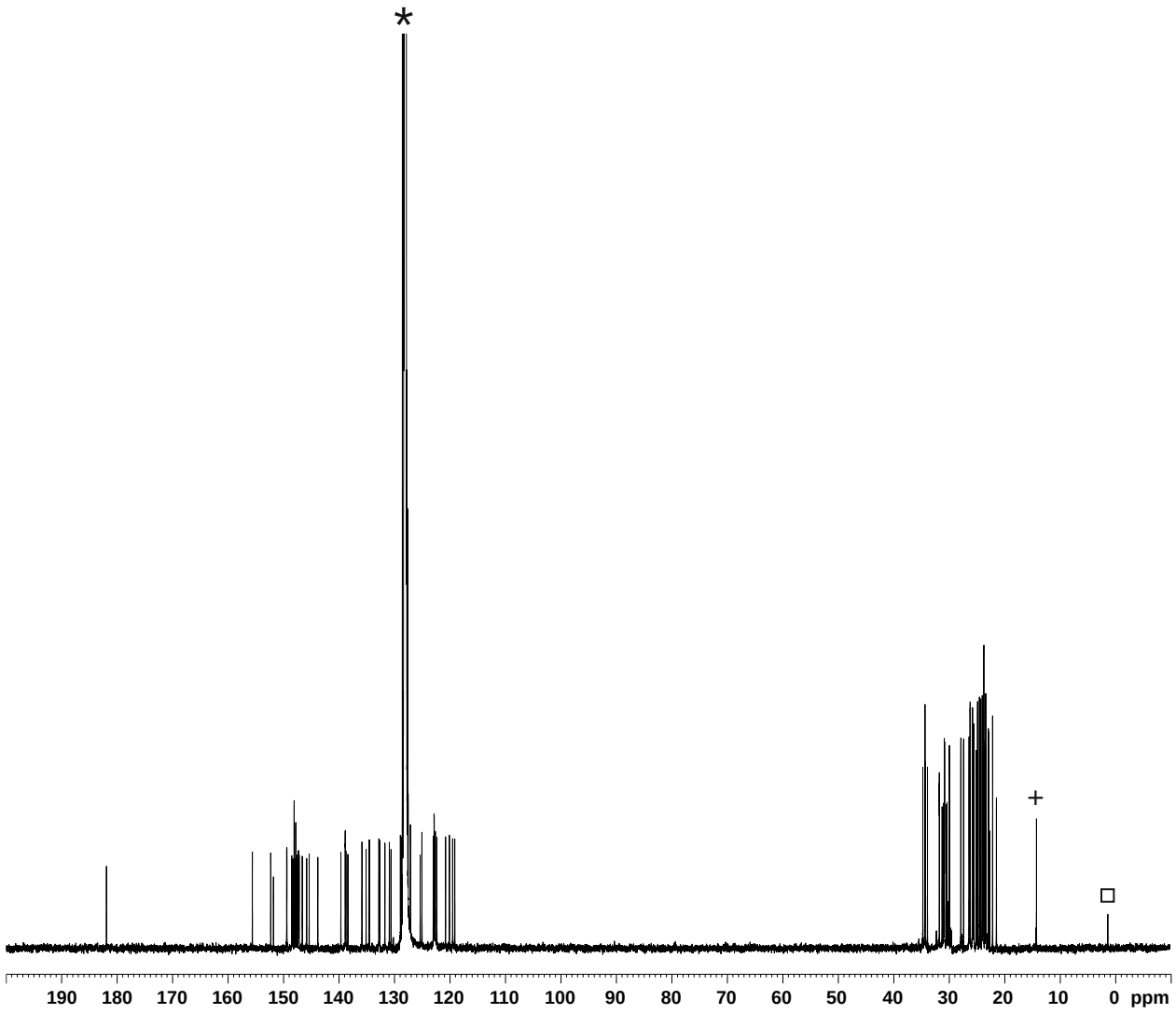


Figure S30. ^{1}H NMR spectrum of compound **7** (6.4 – 7.6 ppm).



Current Data Parameters
NAME 52-23042024-RK421
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 7.08 h
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PULPROG udeft
TD 35340
SOLVENT C6D6
NS 8453
DS 0
SWH 49342.105 Hz
FIDRES 2.792423 Hz
AQ 0.3581120 sec
RG 179.42
DW 10.133 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0898274 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
SF 176.0668739 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

▫ grease

* C_6D_6

+ *n*-pentane

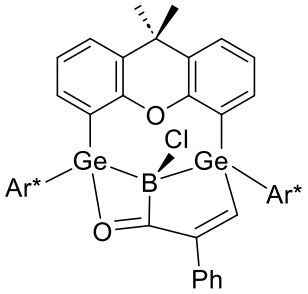
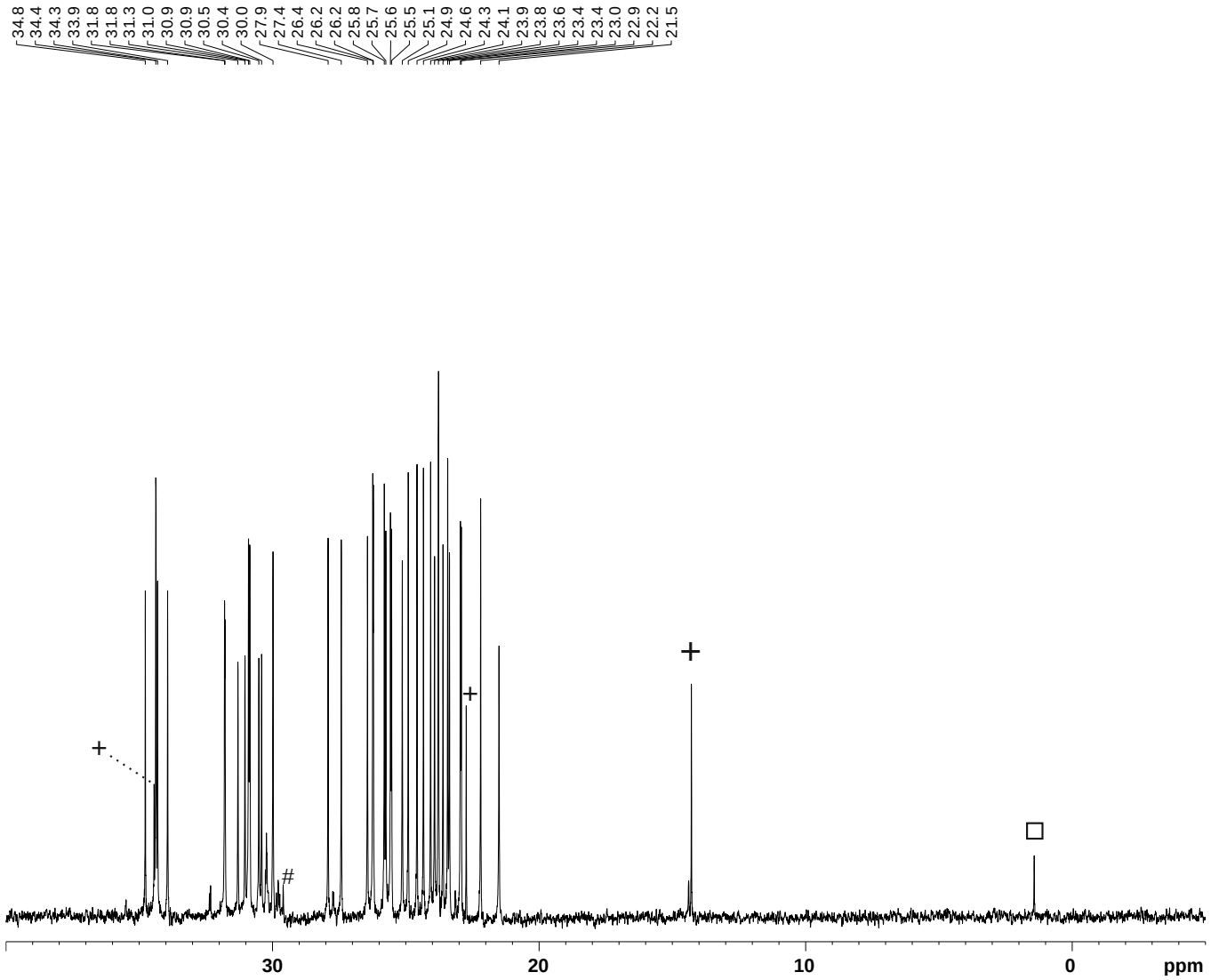


Figure S31. $^{13}C\{^1H\}$ NMR spectrum of compound **7**.



Current Data Parameters
NAME 52-23042024-RK421
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240425
Time 7.08 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 35340
SOLVENT C6D6
NS 8453
DS 0
SWH 49342.105 Hz
FIDRES 2.792423 Hz
AQ 0.3581120 sec
RG 179.42
DW 10.133 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0898274 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
SF 176.0668739 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

□ grease

impurity

+ *n*-pentane

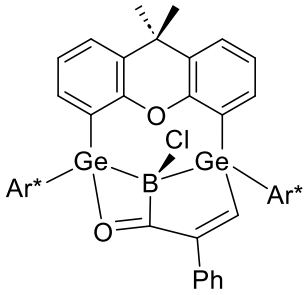


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of compound **7** (−5 – 40 ppm).

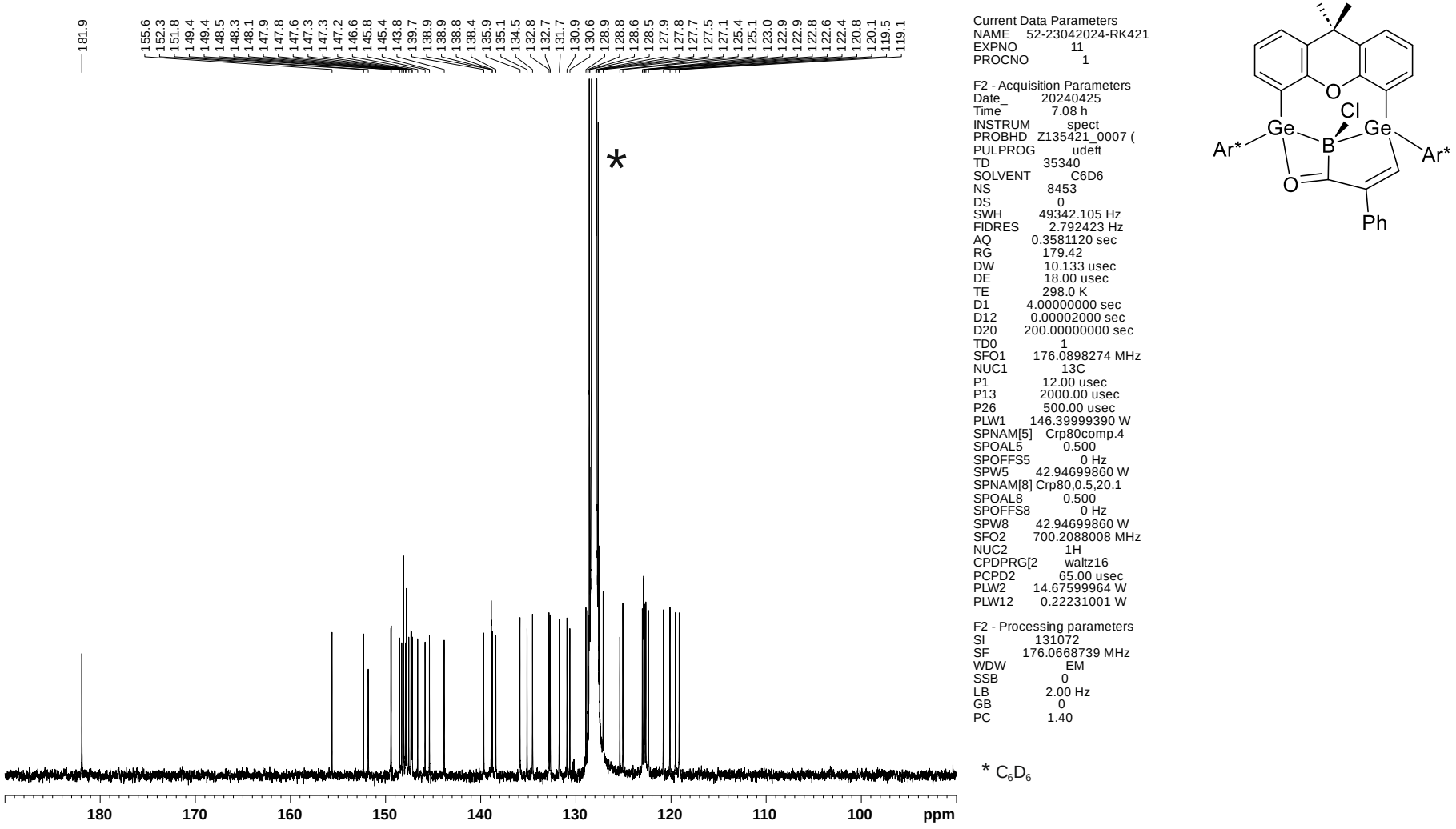
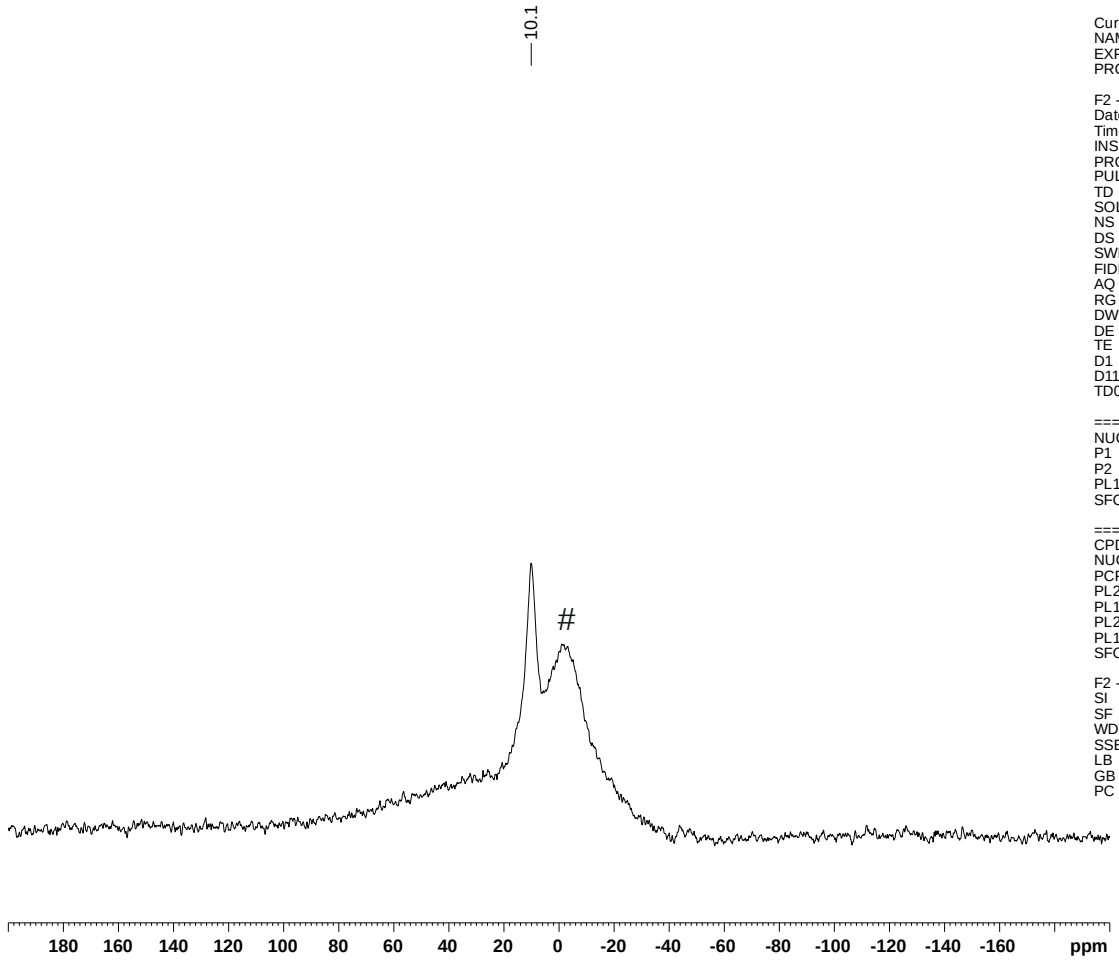


Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of compound **7** (90 – 190 ppm).



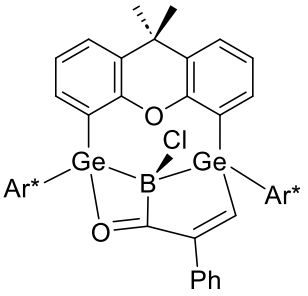


Figure S34. $^{11}B\{^{1}H\}$ NMR spectrum of compound **7**.

NMR spectra of compound **8**.

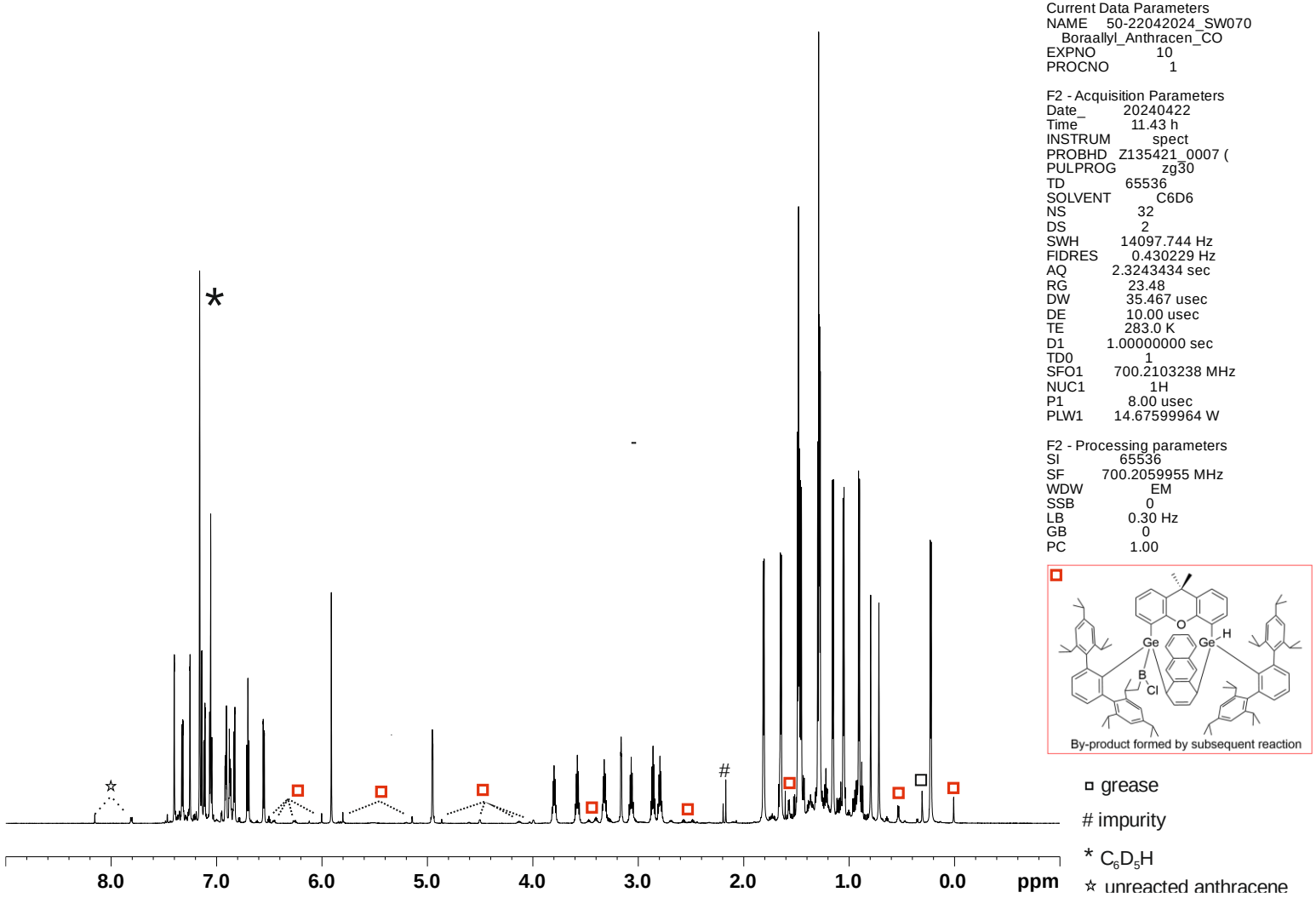


Figure S35. ^{1}H NMR spectrum of compound **8**.

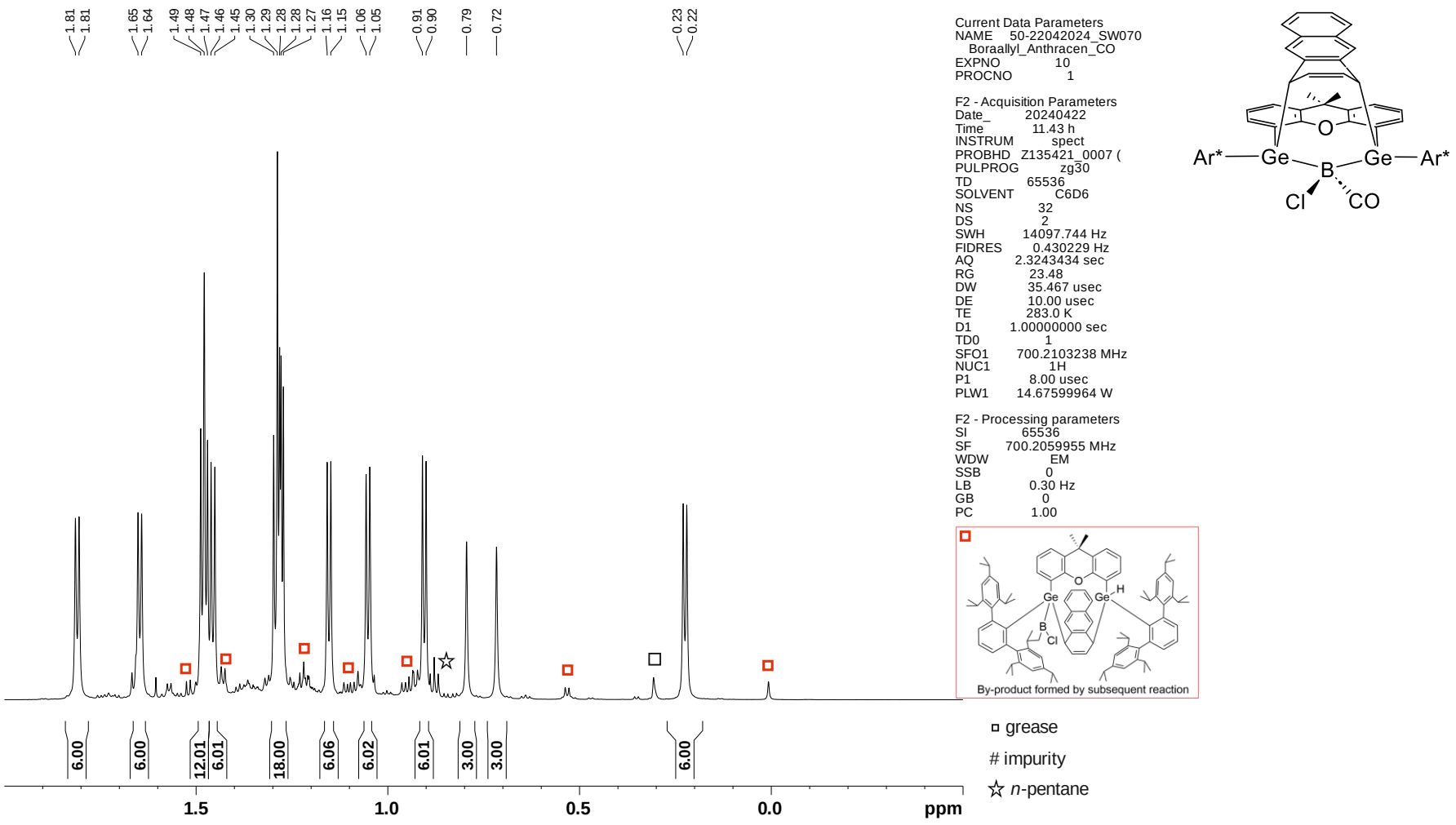


Figure S36. ^{1}H NMR spectrum of compound **8** (−0.5 – 2.0 ppm).

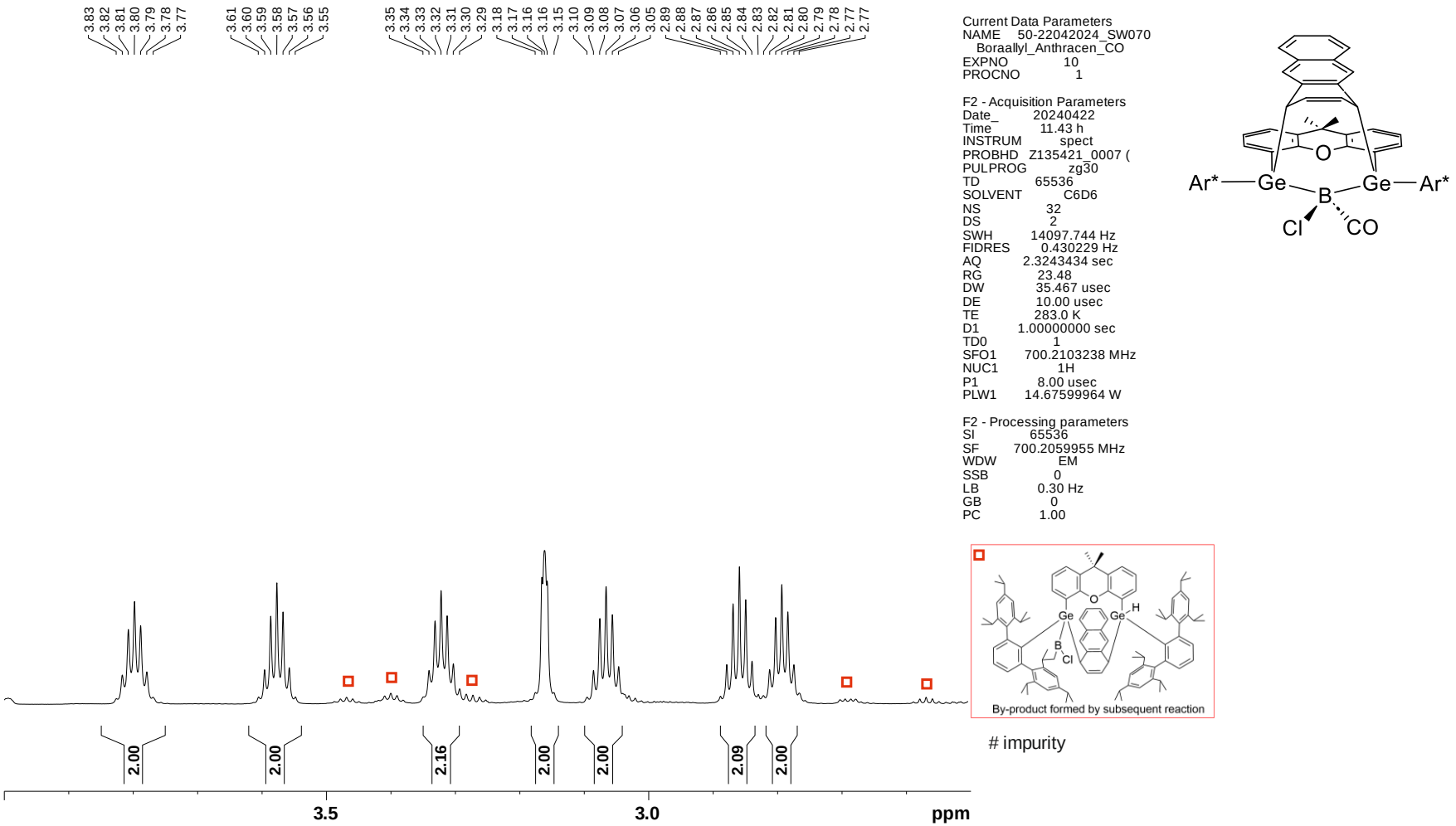


Figure S37. ^{1}H NMR spectrum of compound **8** (2.5 – 4.0 ppm).

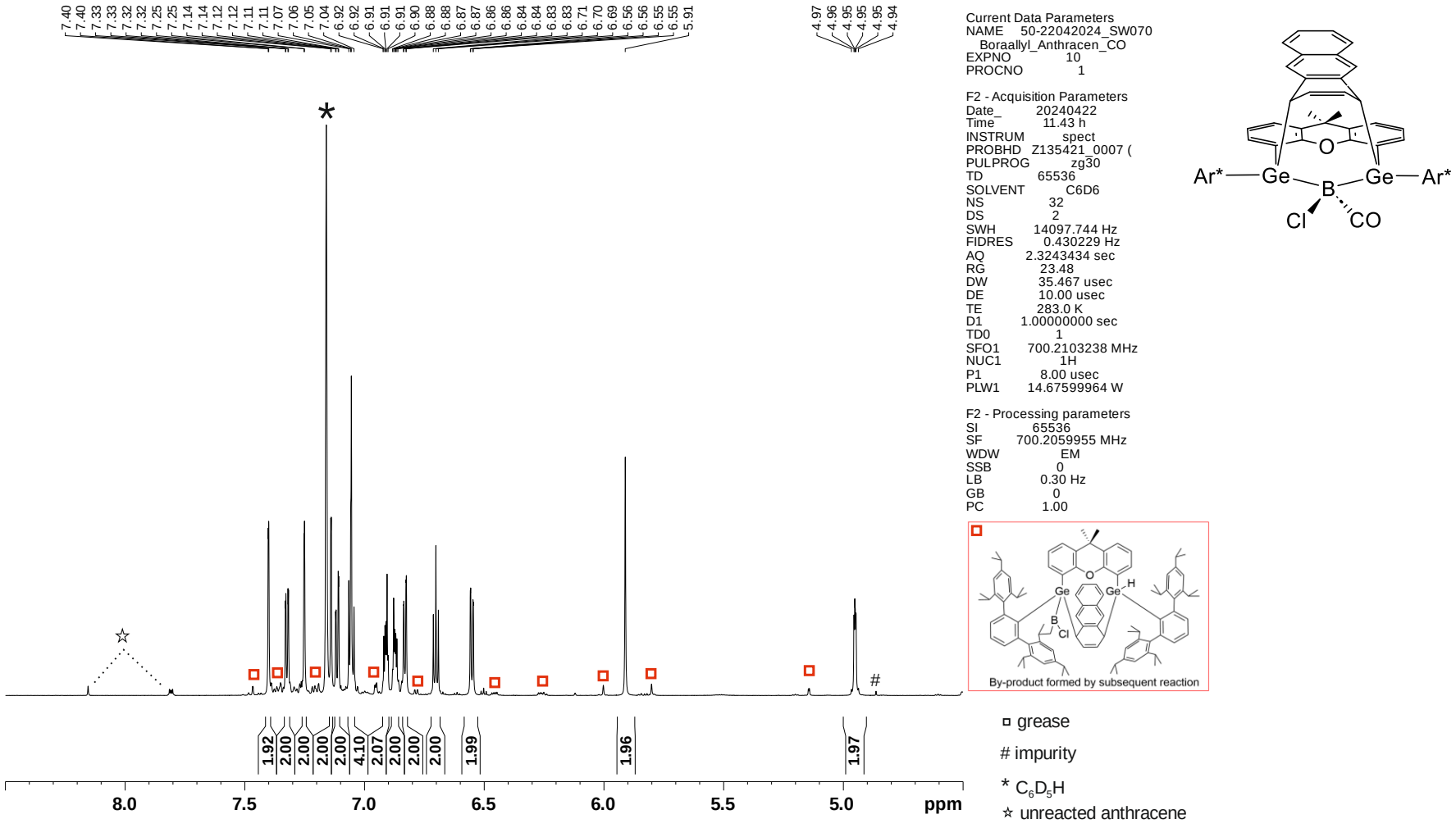
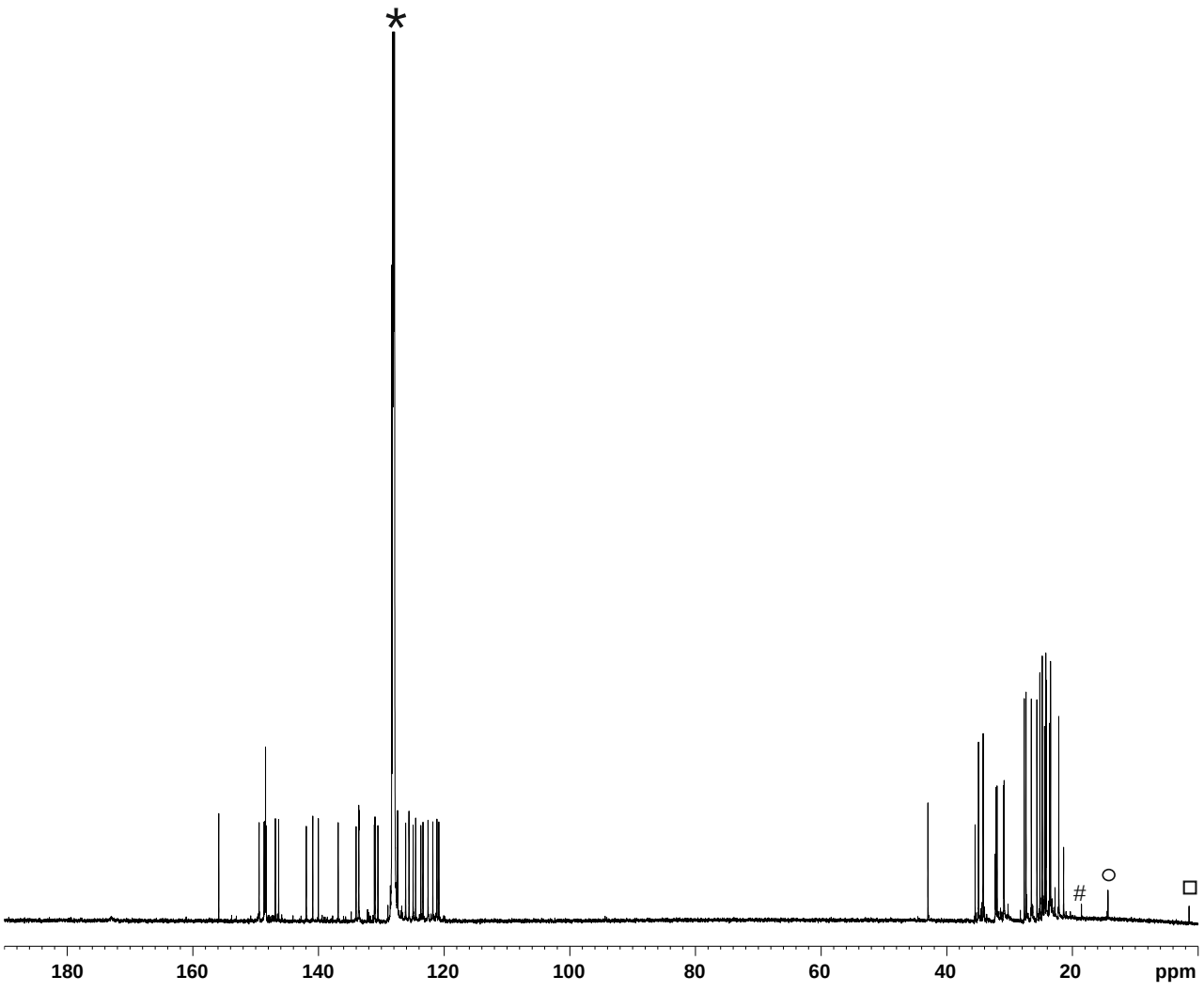


Figure S38. ^{1}H NMR spectrum of compound **8** (4.5 – 8.5 ppm).



Current Data Parameters
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Boraallyl_Anthracen_CO
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 17.14 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 283.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0880668 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
SF 176.0668821 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

impurity
* C_6D_6
□ grease
○ *n*-pentane

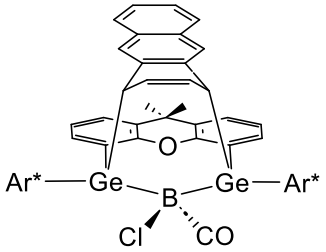
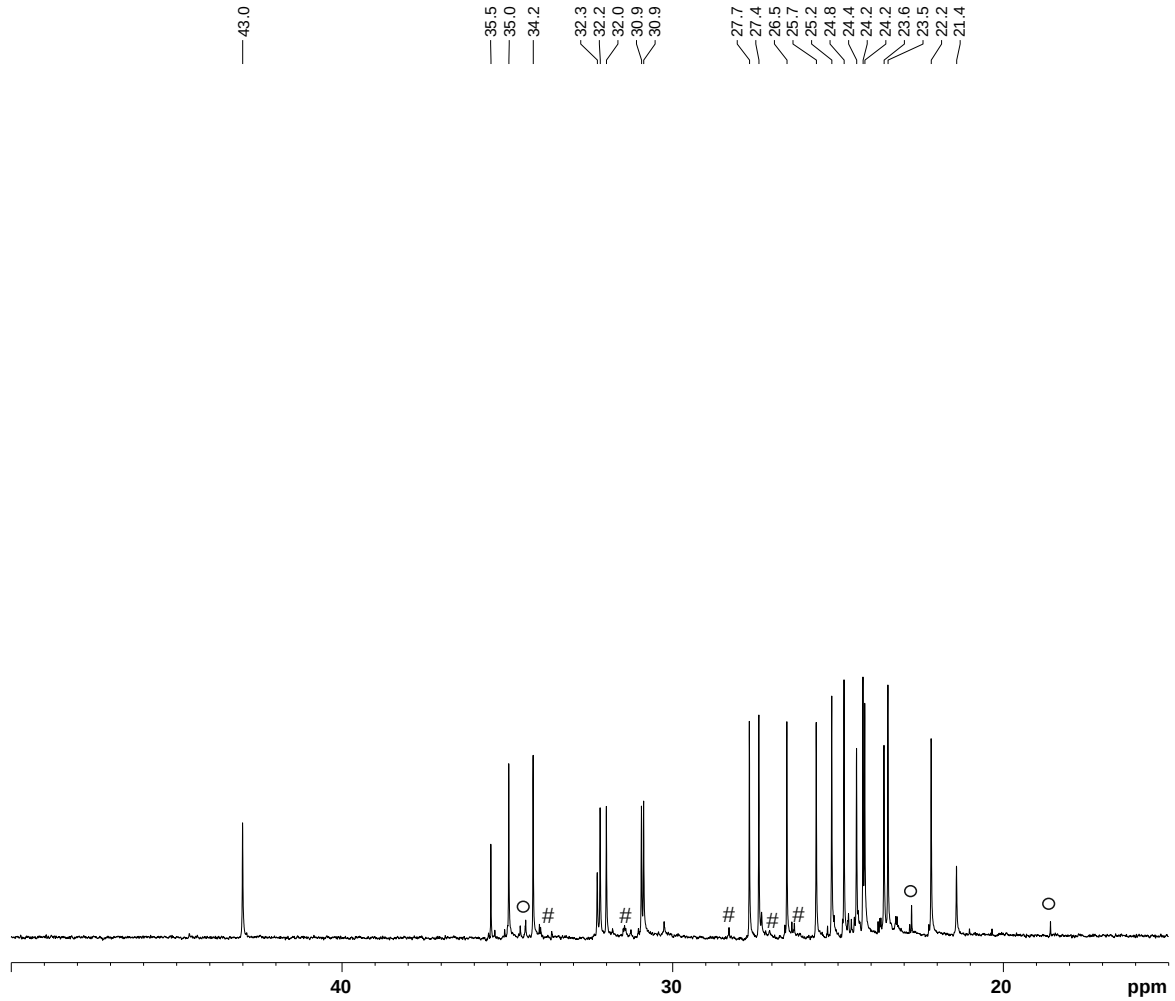


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8**.



Current Data Parameters
NAME 50-22042024_SW070 Boraallyl_Anthracen_CO
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 17.14 h
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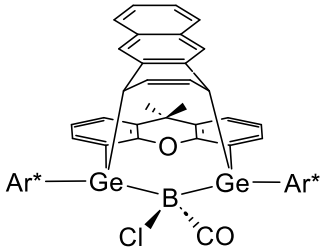
PULPROG udeft
TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 283.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0880668 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

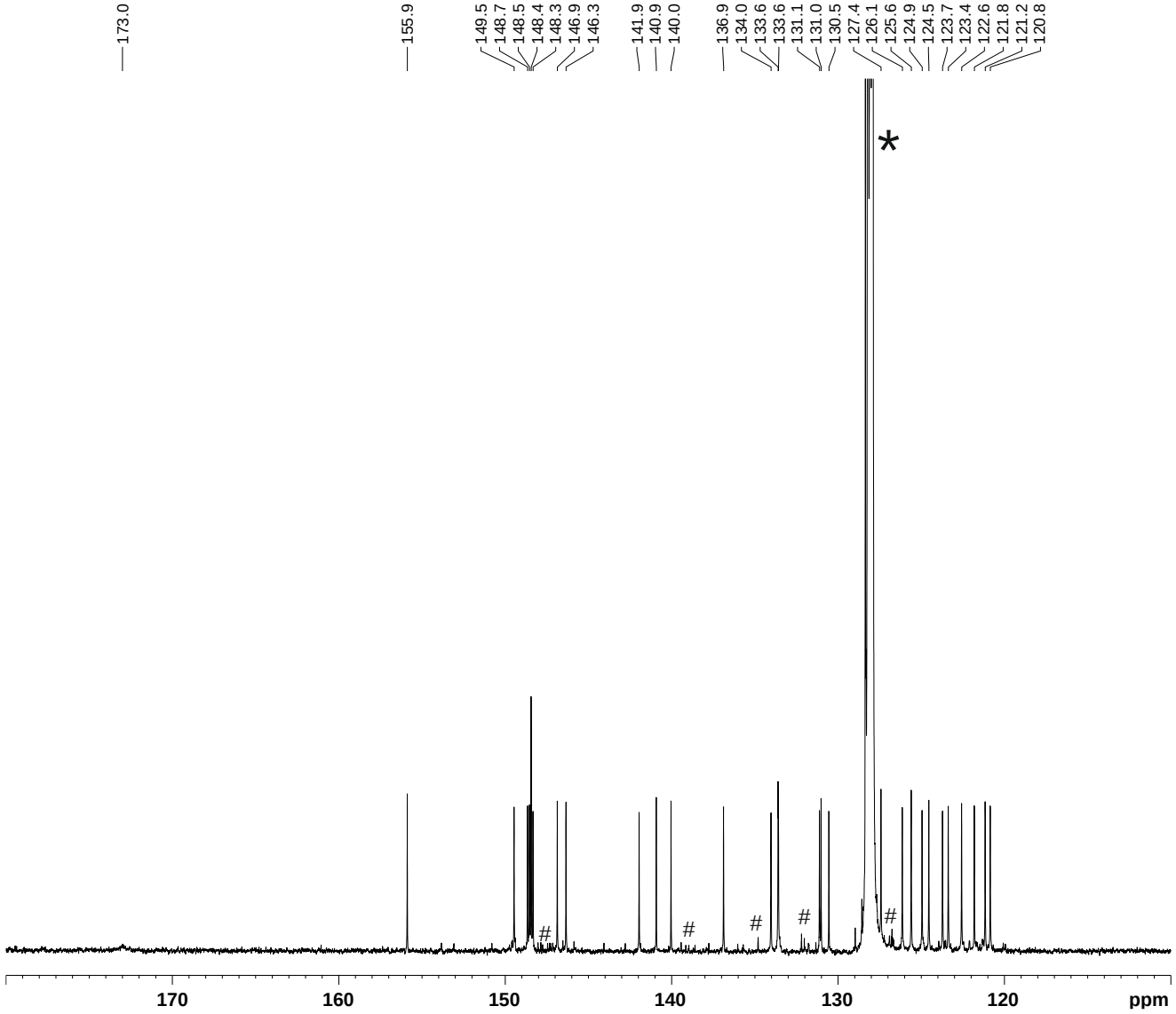
F2 - Processing parameters
SI 131072
SF 176.0668821 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



impurity/by-product see ^{1}H

○ *n*-pentane

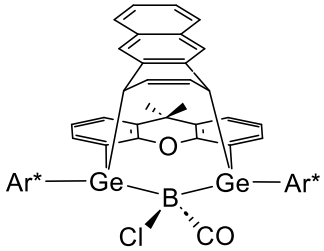
Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8** (15 – 50 ppm).



Current Data Parameters
NAME 50-22042024_SW070 Boraallyl_Anthracen_CO
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240422
Time 17.14 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 30676
SOLVENT C6D6
NS 4096
DS 0
SWH 42613.637 Hz
FIDRES 2.778305 Hz
AQ 0.3599317 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 283.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0880668 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
SF 176.0668821 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



impurity/by-product see ^{1}H

* C_6D_6

Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8** (110 – 180 ppm).

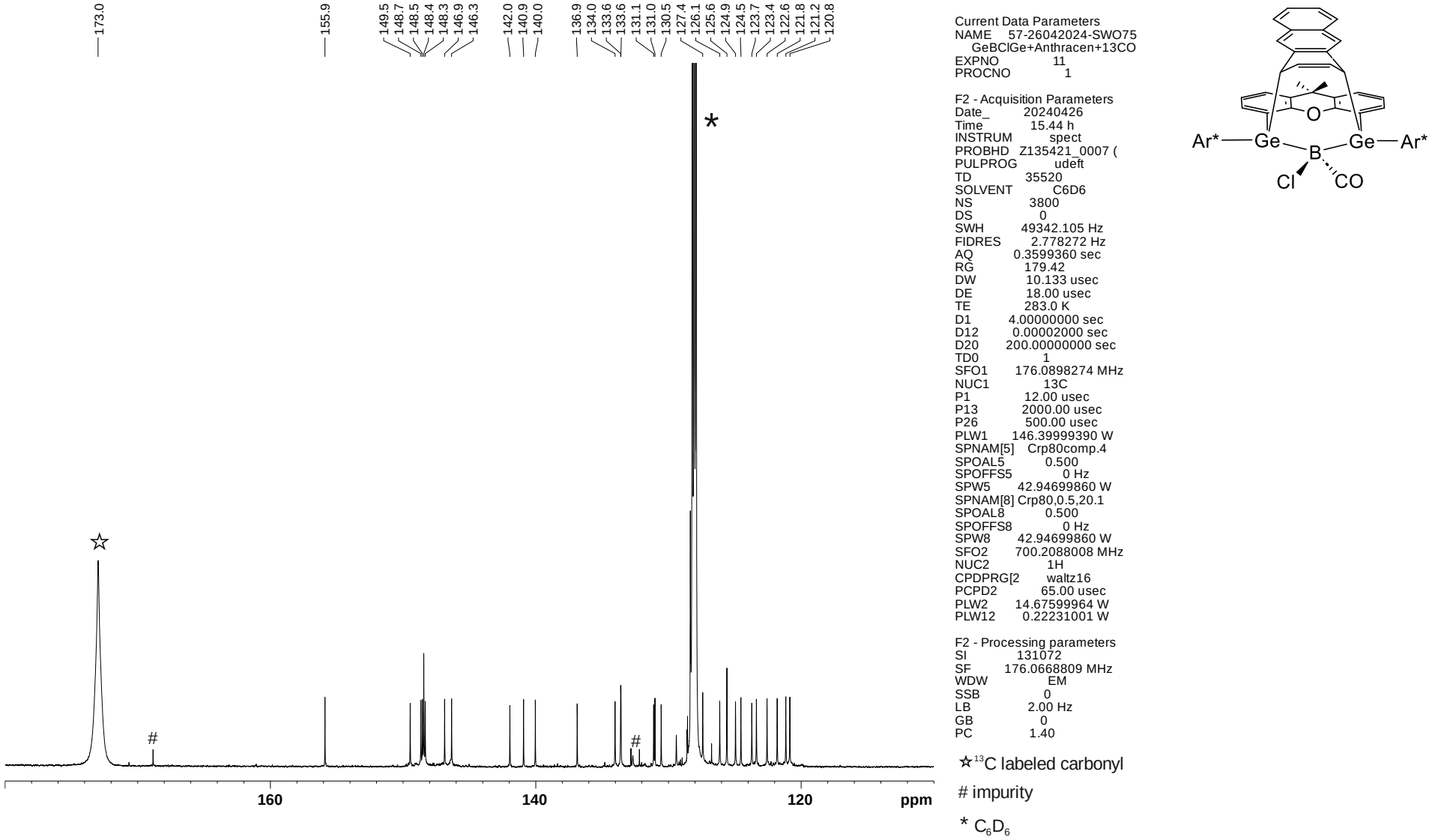
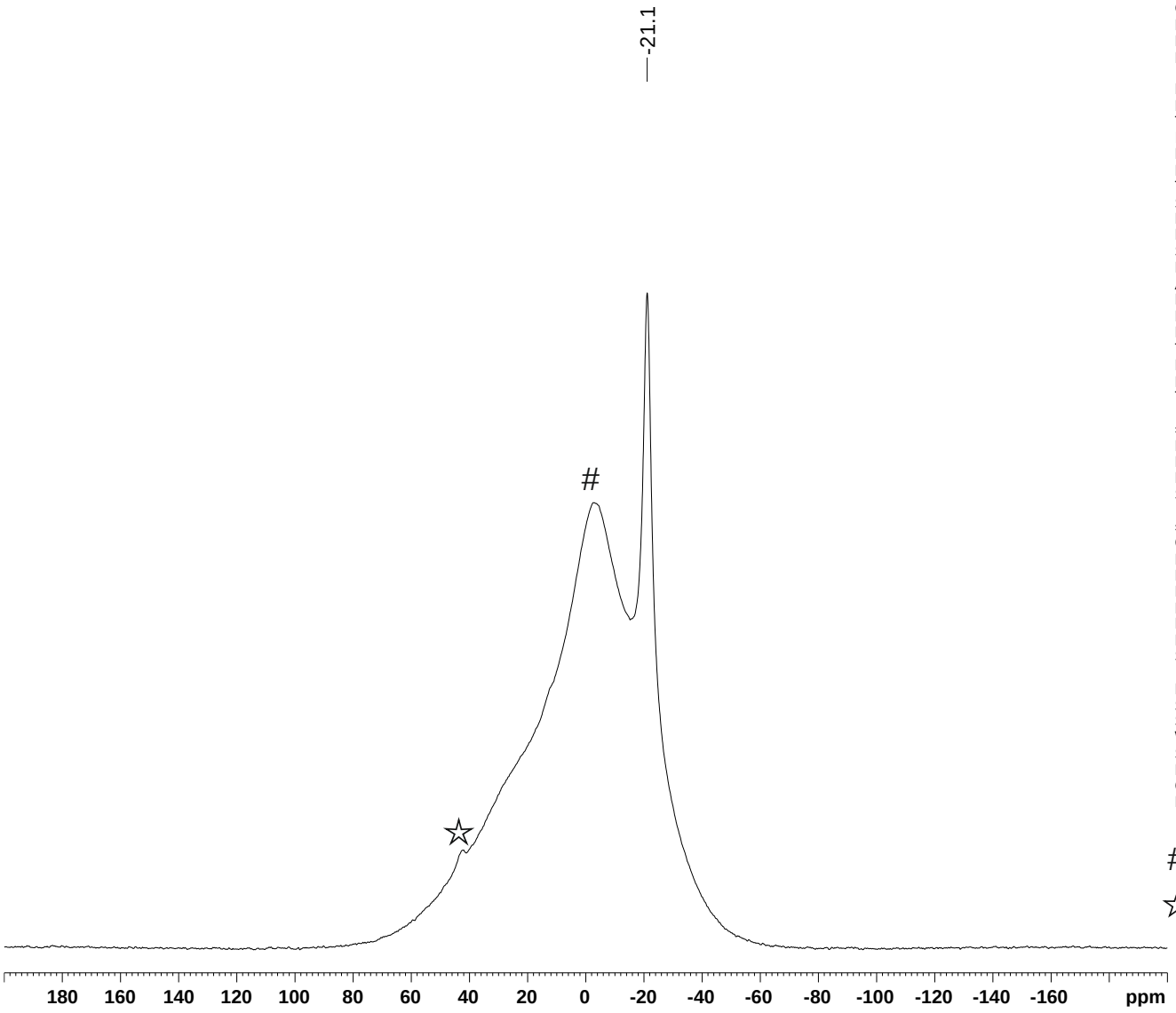


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8,** after the reaction with ^{13}C -labeled CO (110 – 180 ppm).



Current Data Parameters
NAME SW070
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 9.29
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PULPROG zgig30
TD 8192
SOLVENT C6D6
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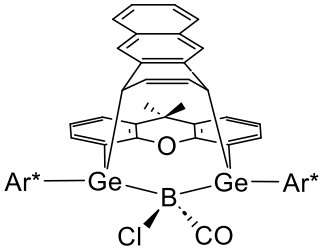
DS 0
SWH 64102.563 Hz
FIDRES 7.825020 Hz
AQ 0.0638976 sec
RG 1440
DW 7.800 usec
DE 6.00 usec
TE 299.2 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 15.00 usec
PL1 -3.00 dB
SFO1 128.3711880 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 15.65 dB
PL2W 11.35402870 W
PL12W 0.21885175 W
SFO2 400.1108002 MHz

F2 - Processing parameters
SI 8192
SF 128.3711880 MHz
WDW EM
SSB 0
LB 50.00 Hz
GB 0
PC 1.40



glass

☆unreacted Boradigermaallyl

Figure S43. $^{11}B\{^{1}H\}$ NMR spectrum of compound **8**.

NMR spectra of compound **9**.

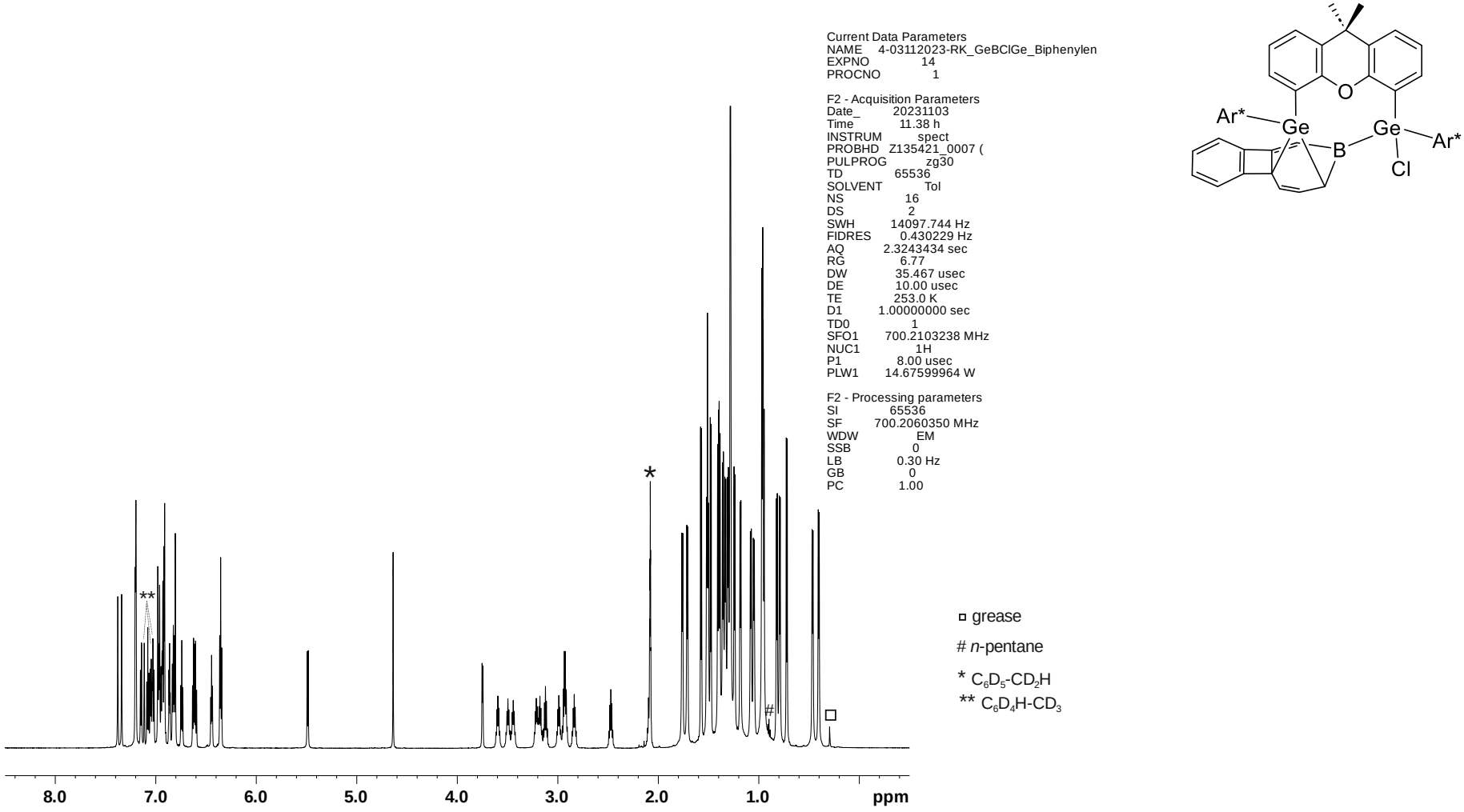


Figure S44. ^{1}H NMR spectrum of compound **9**.

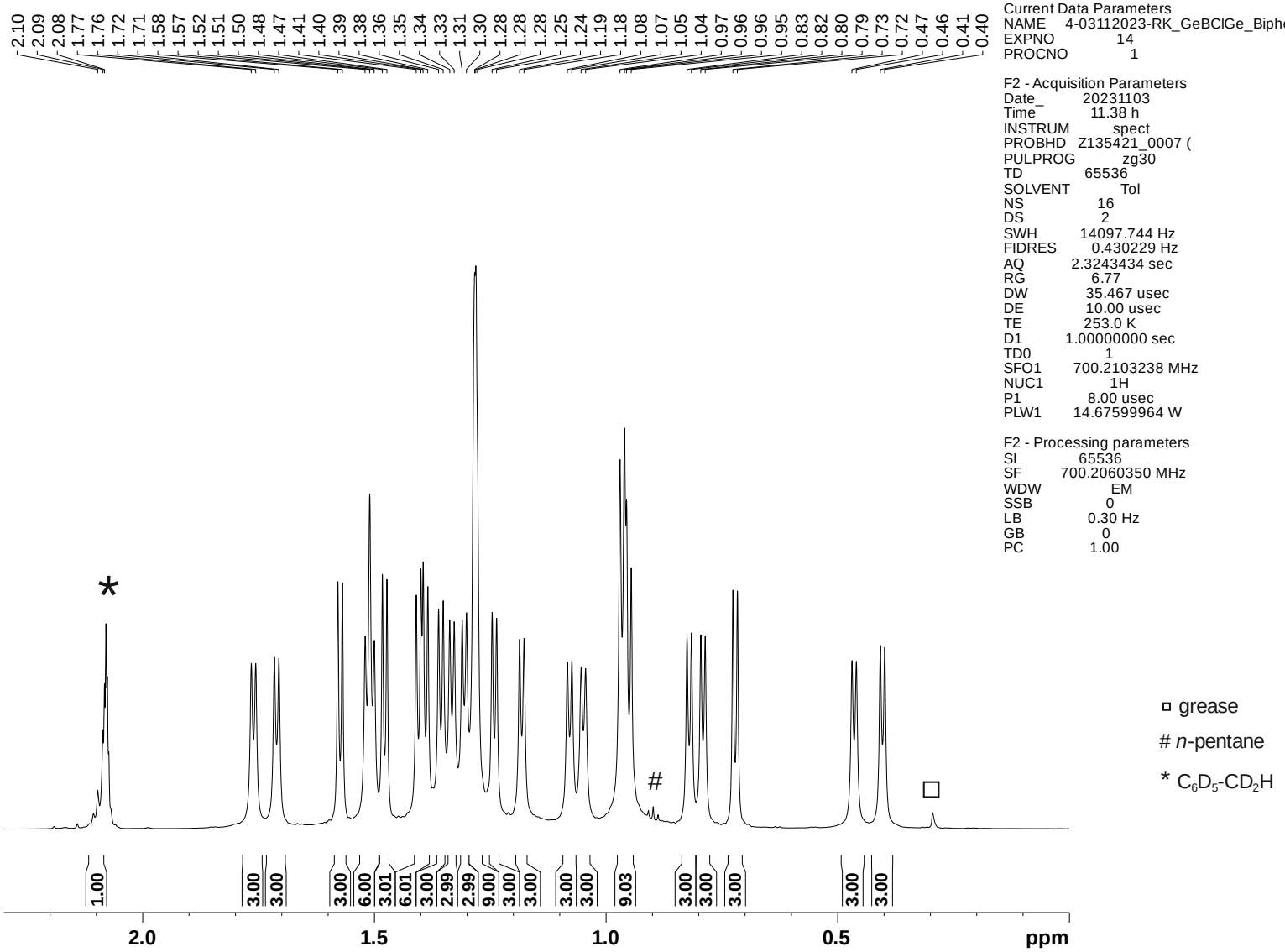


Figure S45. ^{1}H NMR spectrum of compound **9** (0 – 2.3 ppm).

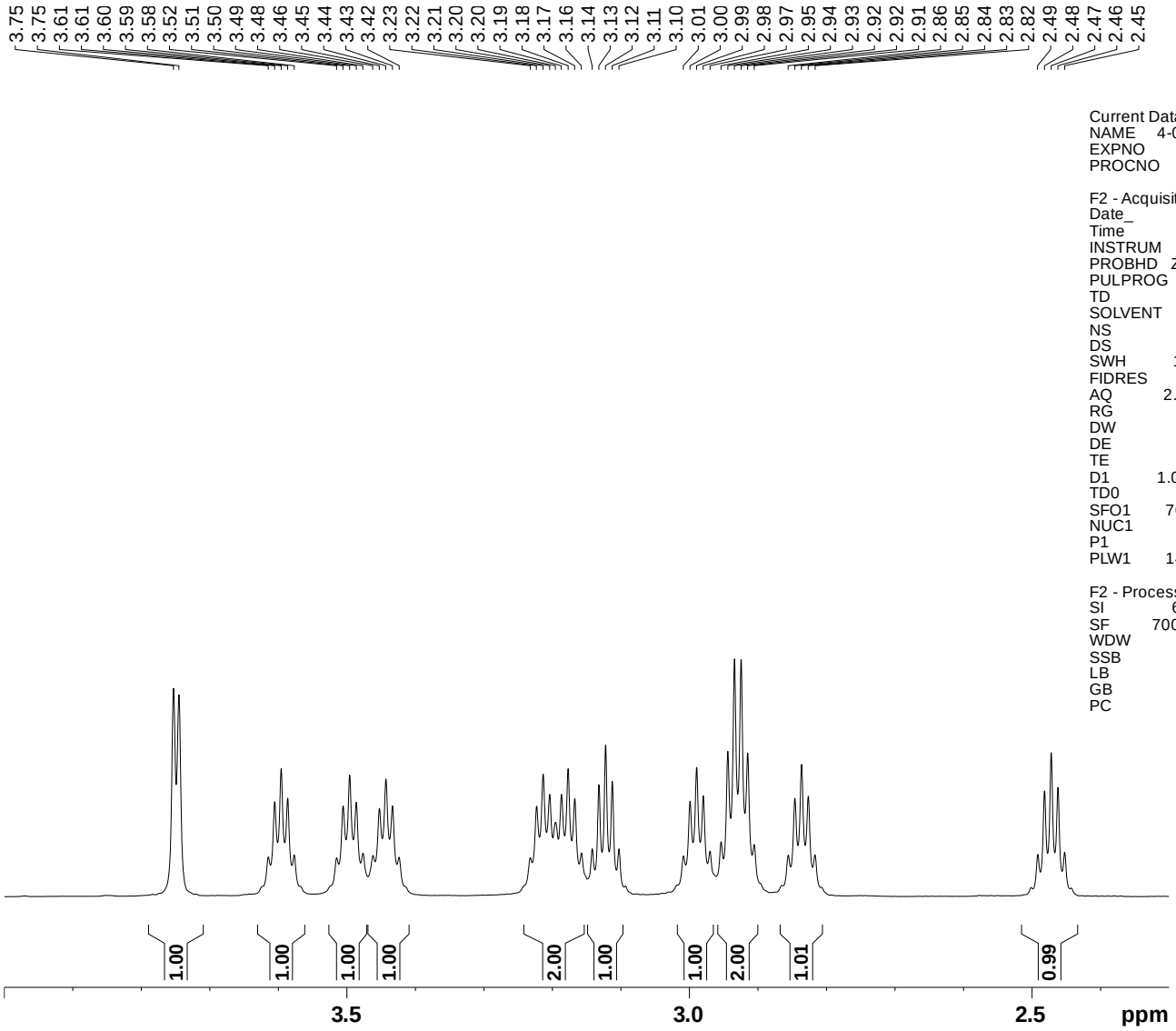
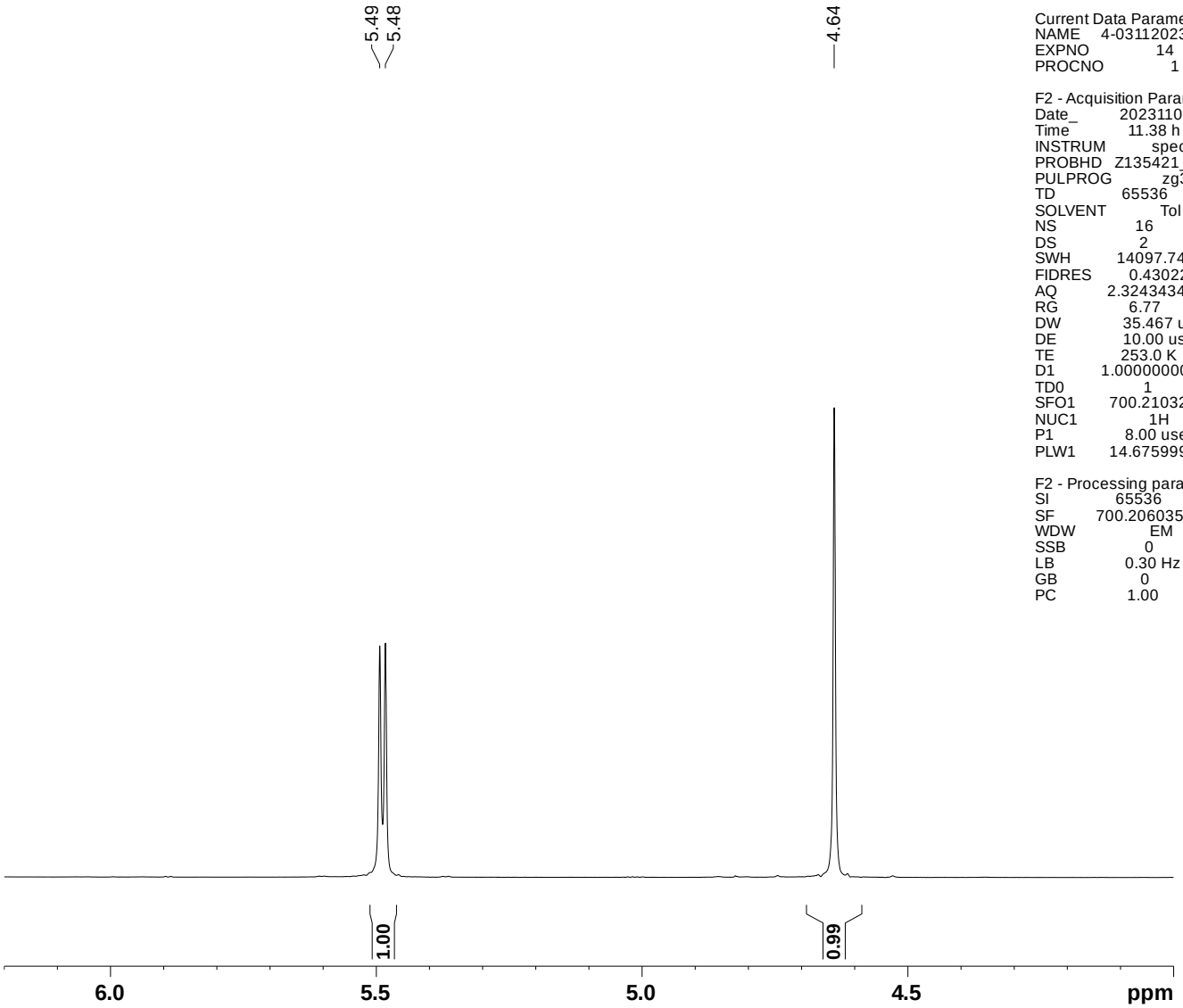


Figure S46. ^{1}H NMR spectrum of compound **9** (2.3 – 4.0 ppm).



Current Data Parameters
NAME 4-03112023-RK_GeBClGe_Biphenyler
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT Tol
NS 16
DS 2
SWH 14097.744 Hz
FIDRES 0.430229 Hz
AQ 2.3243434 sec
RG 6.77
DW 35.467 usec
DE 10.00 usec
TE 253.0 K
D1 1.00000000 sec
TD0 1
SFO1 700.2103238 MHz
NUC1 1H
P1 8.00 usec
PLW1 14.67599964 W

F2 - Processing parameters
SI 65536
SF 700.2060350 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

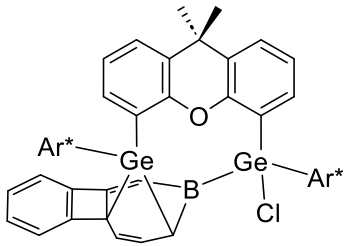


Figure S47. ^{1}H NMR spectrum of compound **9** (4.0 – 6.2 ppm).

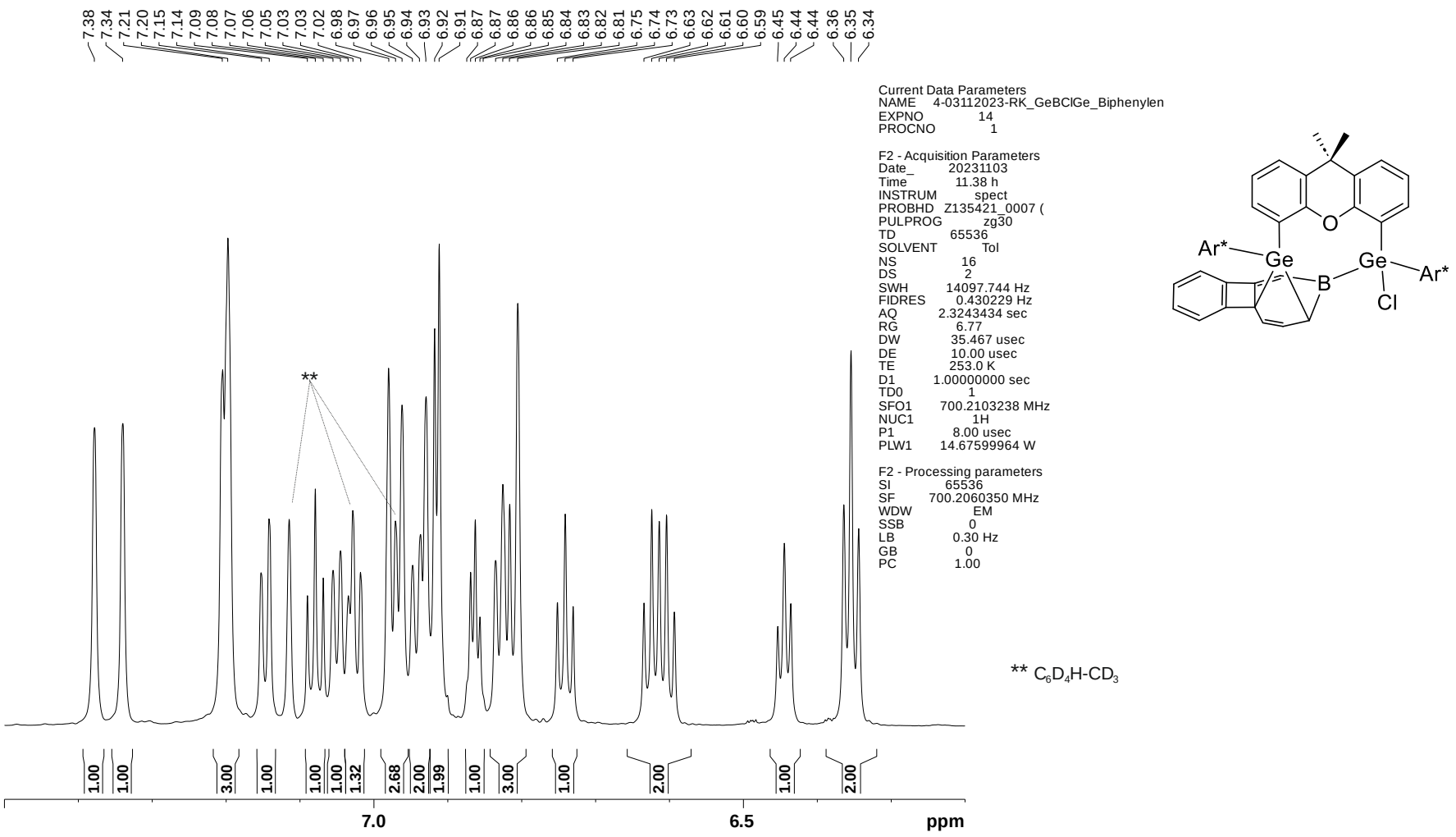


Figure S48. ^{1}H NMR spectrum of compound **9** (6.2 – 7.5 ppm).

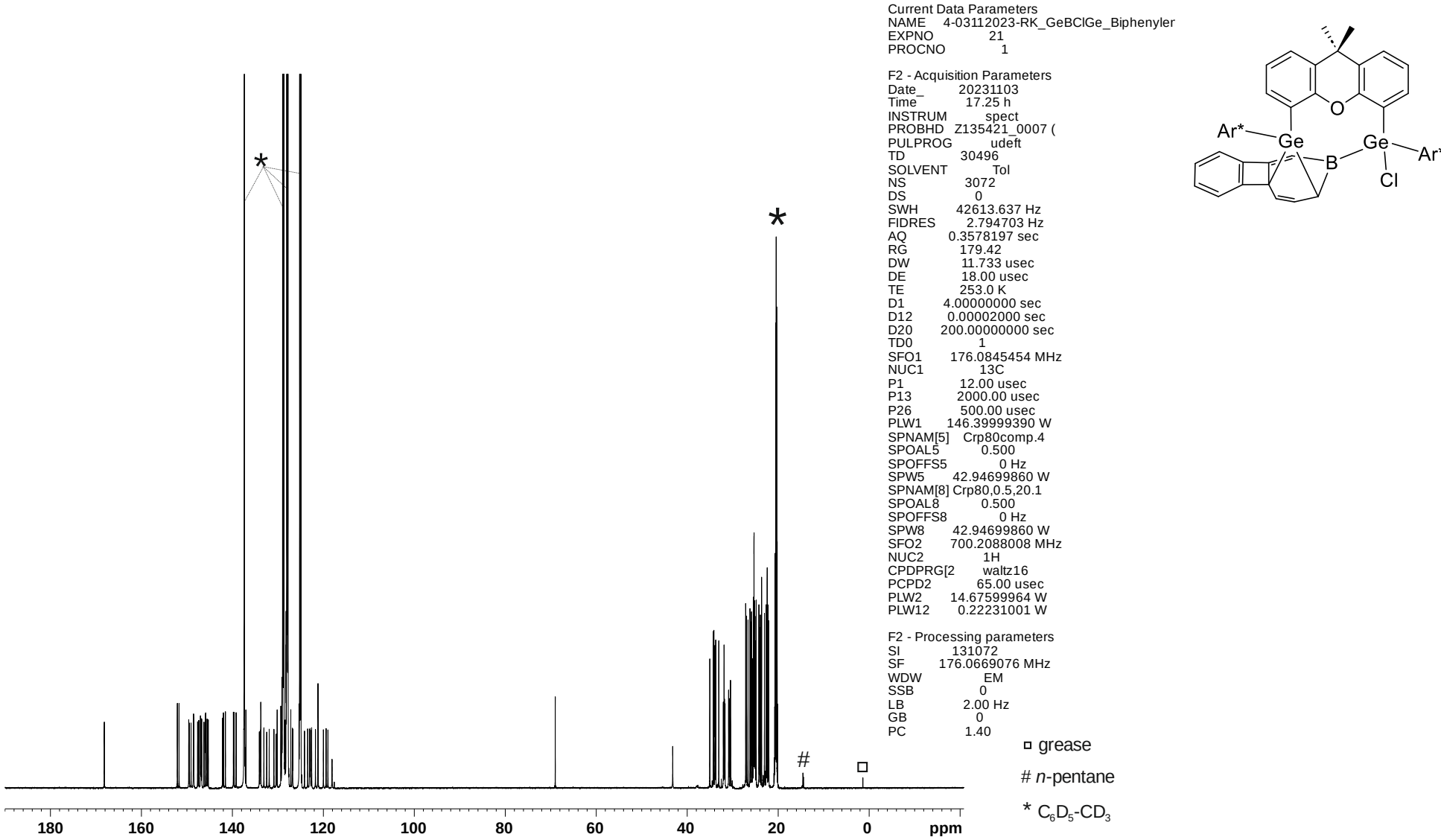
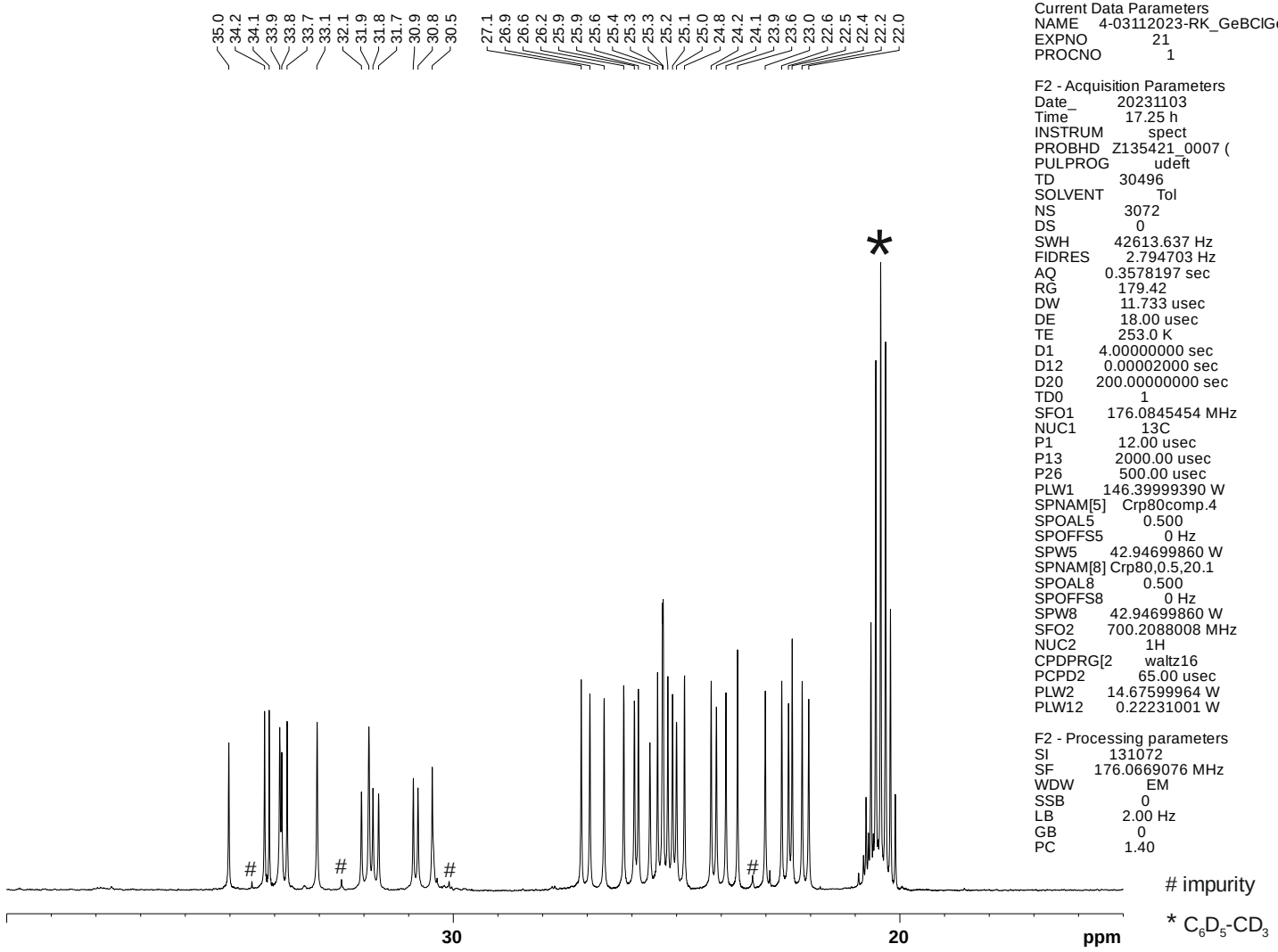


Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9**.



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EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
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Time 17.25 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 30496
SOLVENT Tol
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.794703 Hz
AQ 0.3578197 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 253.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0845454 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
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SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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SF 176.0669076 MHz
WDW EM
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GB 0
PC 1.40

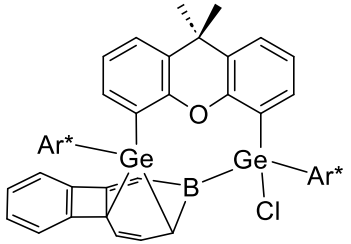
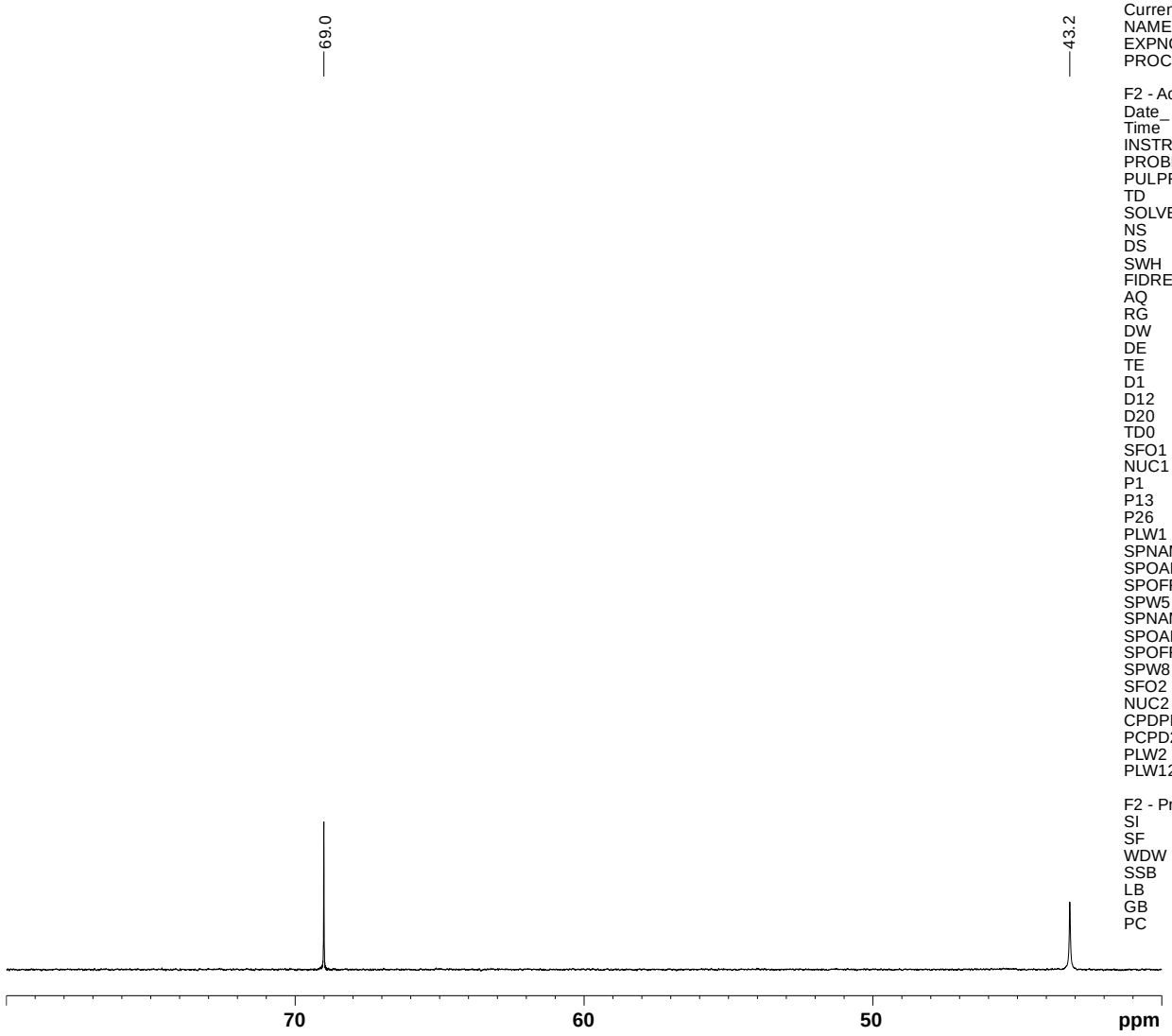


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** (15 – 40 ppm).



Current Data Parameters
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EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 17.25 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 30496
SOLVENT Tol
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.794703 Hz
AQ 0.3578197 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 253.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0845454 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
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SF 176.0669076 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

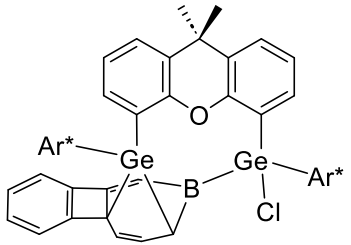


Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** (40 – 80 ppm).

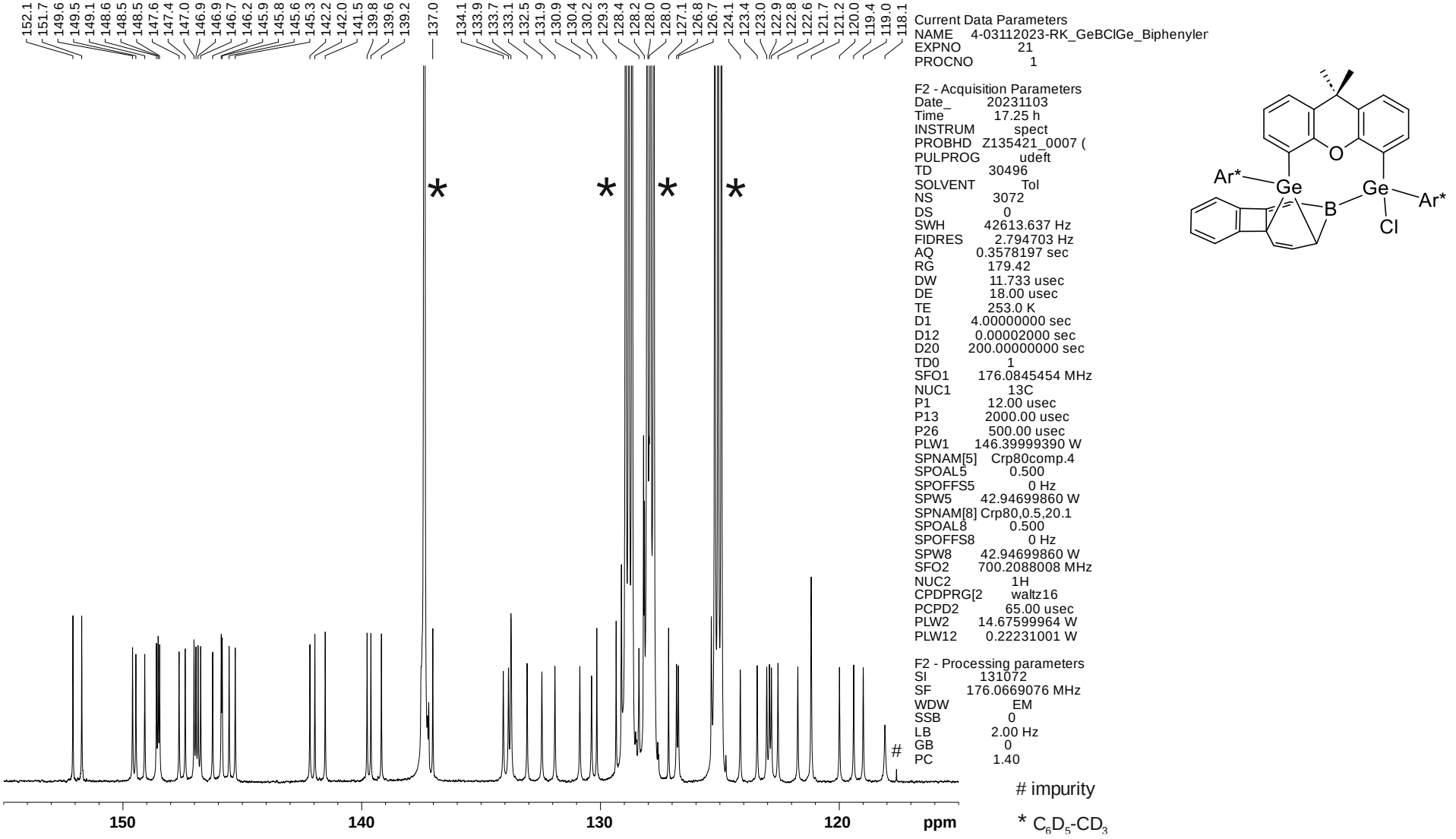
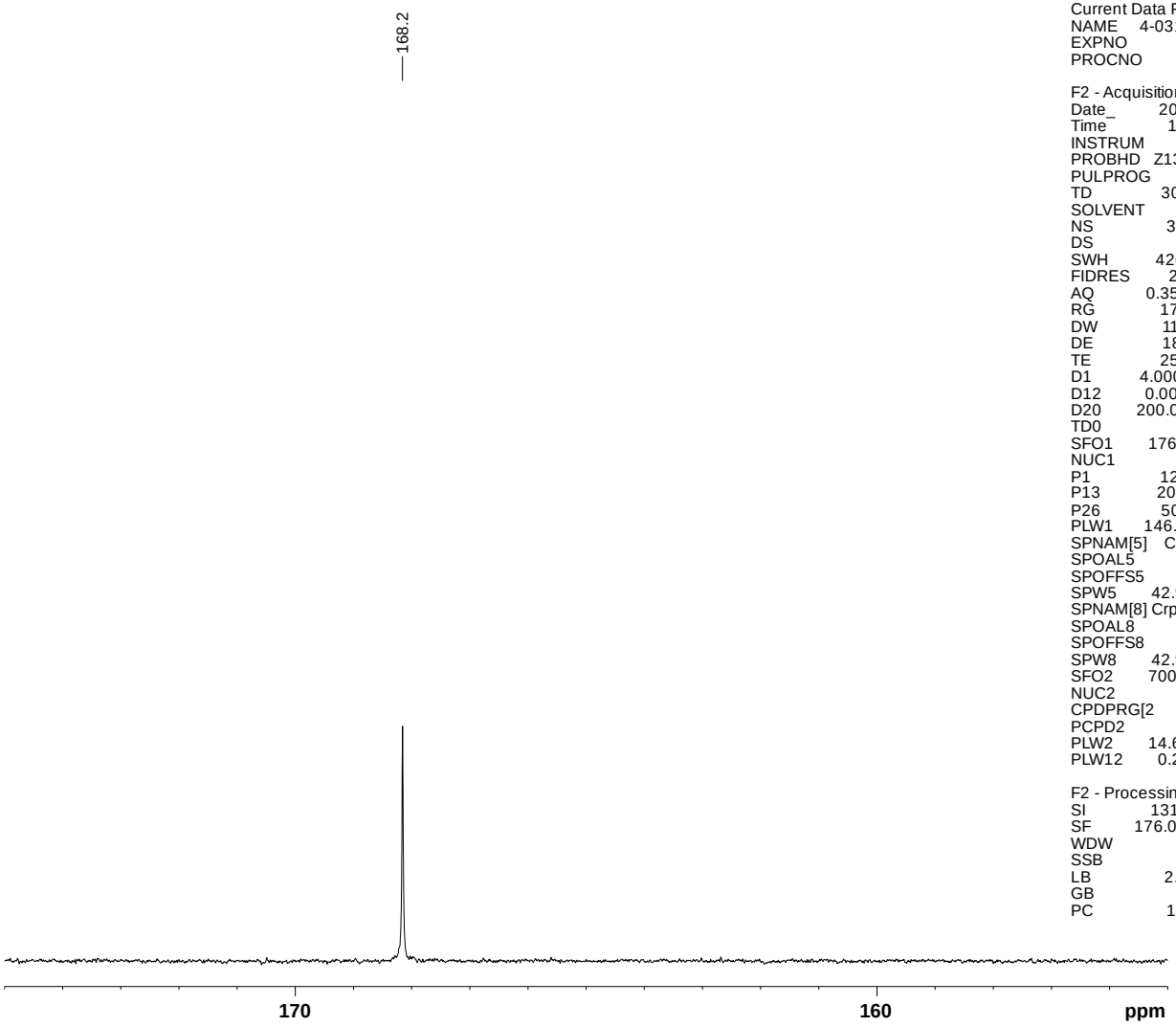


Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** (115 – 155 ppm).



Current Data Parameters
NAME 4-03112023-RK_GeBClGe_Biphenylen
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 17.25 h
INSTRUM spect
PROBHD Z135421_0007 (
PULPROG udeft
TD 30496
SOLVENT Tol
NS 3072
DS 0
SWH 42613.637 Hz
FIDRES 2.794703 Hz
AQ 0.3578197 sec
RG 179.42
DW 11.733 usec
DE 18.00 usec
TE 253.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 200.00000000 sec
TD0 1
SFO1 176.0845454 MHz
NUC1 13C
P1 12.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 146.39999390 W
SPNAM[5] Crp80comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 42.94699860 W
SPNAM[8] Crp80,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 42.94699860 W
SFO2 700.2088008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 14.67599964 W
PLW12 0.22231001 W

F2 - Processing parameters
SI 131072
SF 176.0669076 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

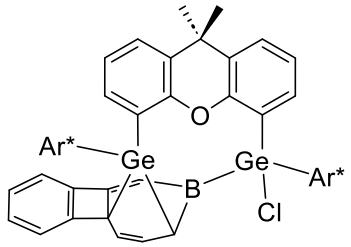


Figure S53. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** (155 – 175 ppm).

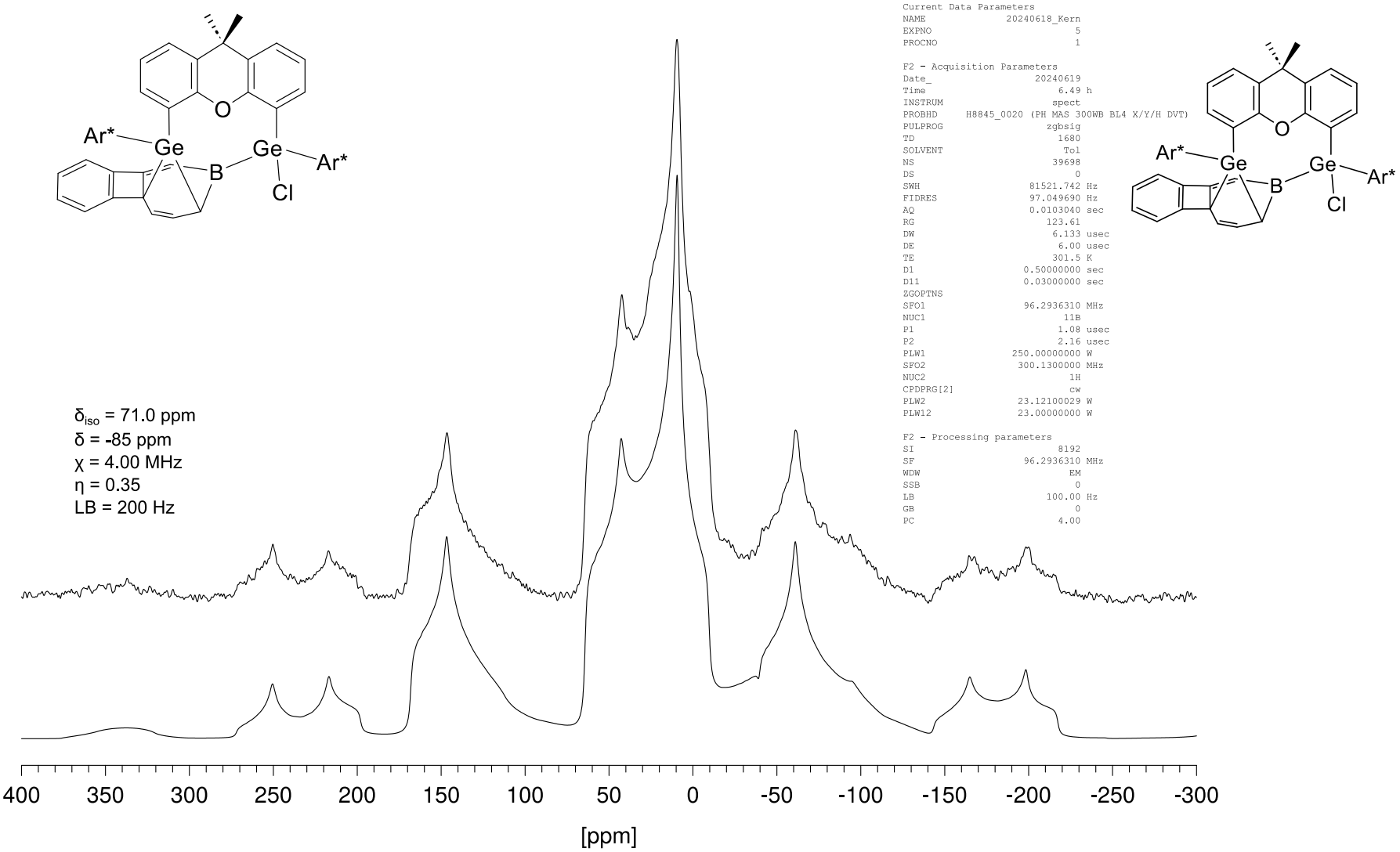


Figure S54. Experimental (top) and (bottom) calculated 96.29 MHz ^{11}B MAS NMR spectra of the central transition of **9**, spinning at 10 kHz.

IR-spectroscopy

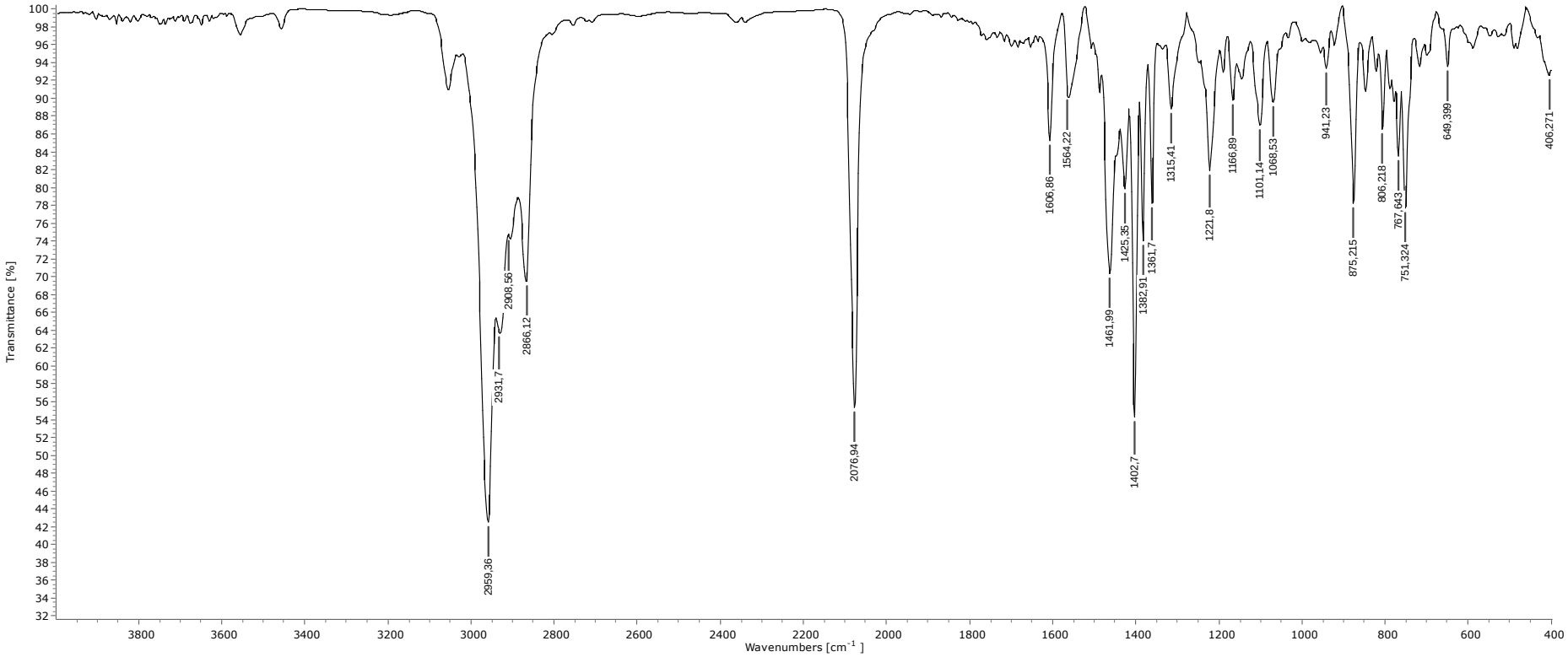
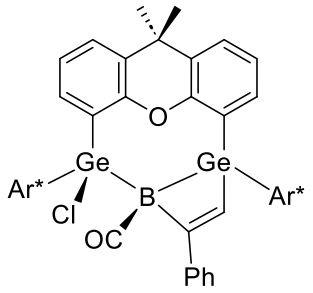


Figure S55. IR (KBr) spectrum of compound **6**.



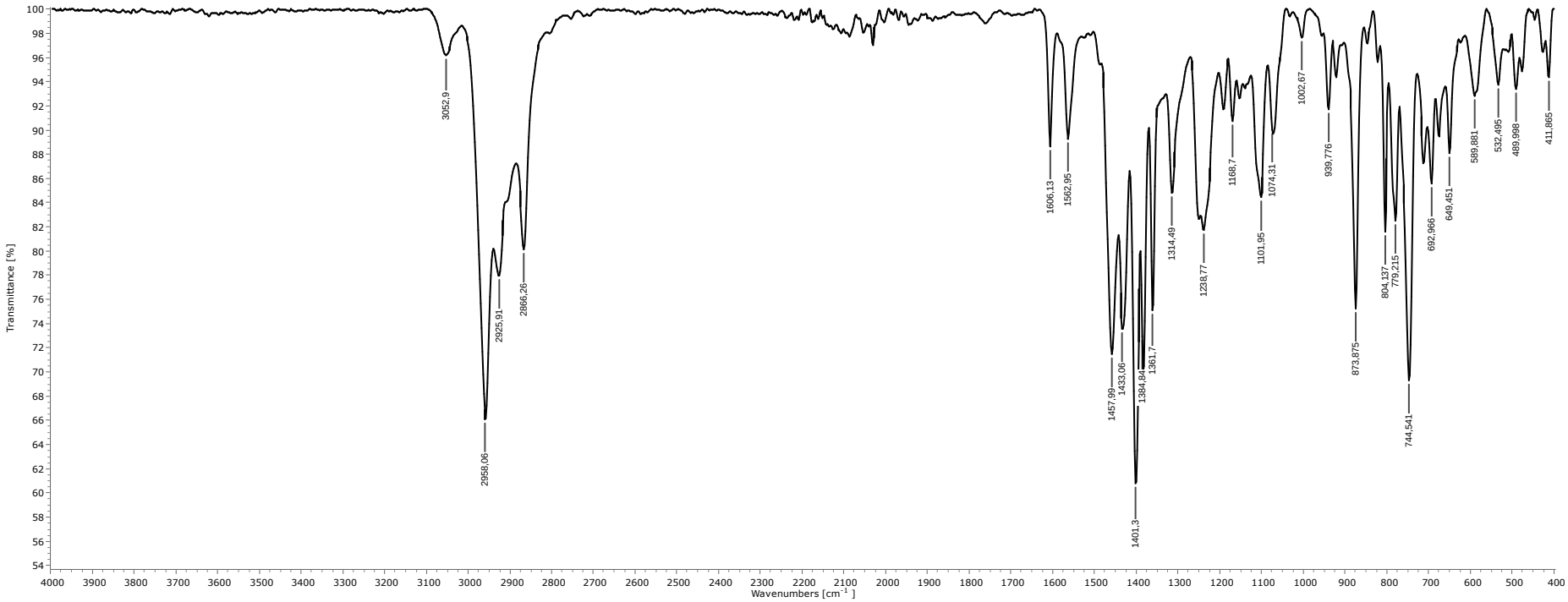
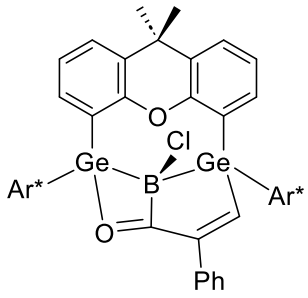


Figure S56. IR (ATR) spectrum of compound **7**.



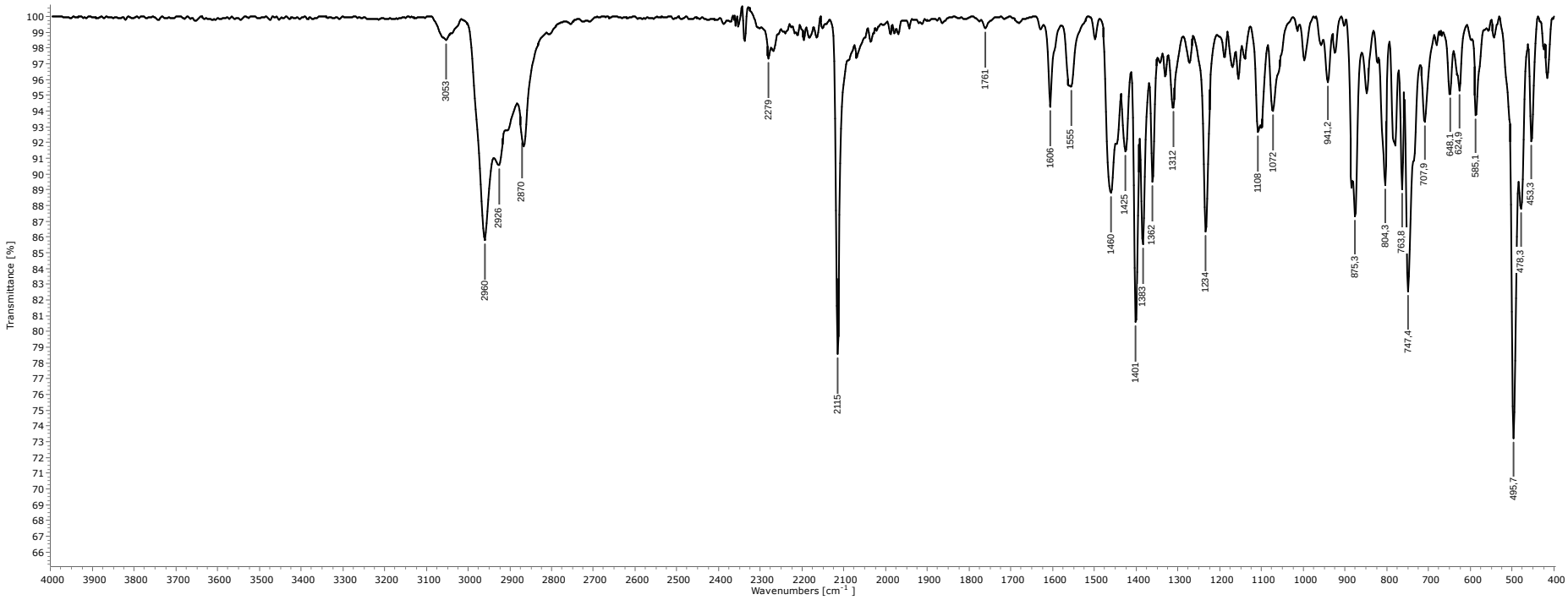
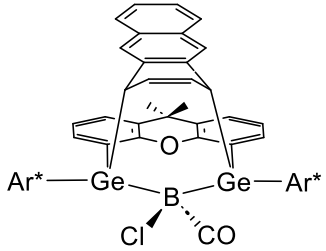


Figure S57. IR (ATR) spectrum of compound **8**.



UV-Vis spectroscopy

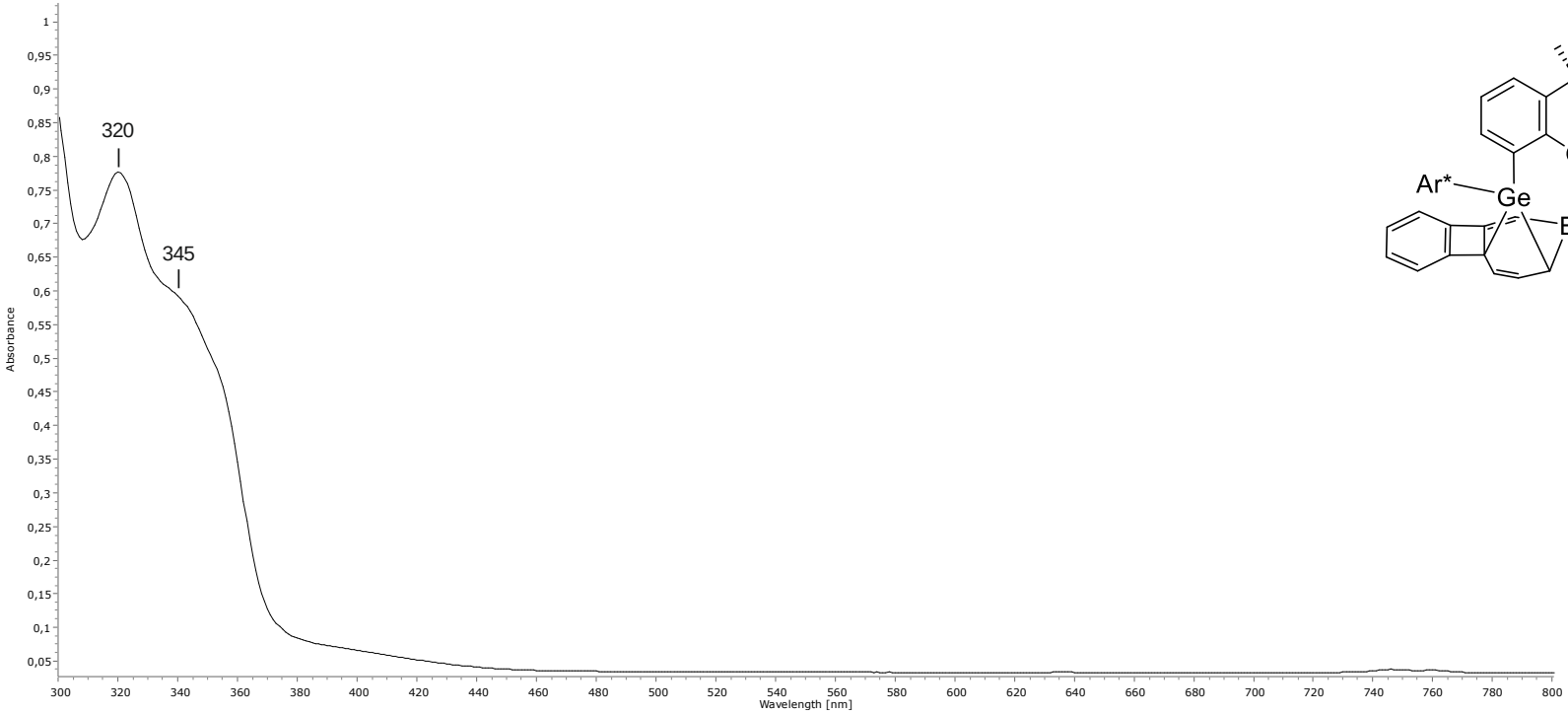


Figure S58. UV-Vis spectrum of compound **9.**

Computational Methods

The computations of the relative energies of structural isomers **6** and **7** used the experimental X-ray single crystal structures as models and starting point for geometry optimizations. The obtained structures were subsequently used for structural optimization of smaller model systems by removing groups and adding hydrogen atoms as appropriate. All geometry optimizations were performed using the "Swiss army knife" method r^2-SCAN-3c[10] that employs the r^{2}SCAN[11, 12] meta-GGA functional along with a triple-ζ Gaussian basis set (def2-mTZVPP) and a fitting basis set for the resolution of the identity approximation,[10] the D4 correction for London dispersion,[13, 14] and a geometrical counterpoise correction for the basis set superposition error.[15] All geometry optimizations were followed by computations of harmonic vibrational frequencies to confirm the nature of the stationary points as minima. The Gibbs free energy correction obtained from harmonic vibrational frequencies computed at the r^{2}SCAN-3c level give the final Gibbs energies at T = 298.15 K reported in the manuscript.[16] In addition, the structures were also optimized under the consideration of cyclohexane solvent using the conductor-like polarizable continuum model (CPCM).[17]

Single point energy evaluations were conducted using a range of different computational methods: RI-MP2, DLPNO-CCSD(T),[18-20] for the smallest model system, the double hybrid functionals the revDSD-PBEP86-D4[21] and B2-PLYP,[22] the hybrid B3LYP[23-25] functional, the hybrid meta-GGA functional M06-2X,[26] the range-separated hybrid functional ωB97X,[27] and ωB97X-V,[28] a range separated hybrid with non-local correction. The B3LYP and ωB97X functionals were either used without any correction for London dispersion interactions, with the atom-pairwise correction including Becke-Johnson damping D3(BJ)[29] and charge dependent atom-pairwise correction D4.[13, 14] For B3LYP, the non-local density dependent dispersion correction (NL)[30] that uses the nonlocal part of the VV10 functional was also used.[31] The single points were also computed using the geometries obtained from the CPCM computations and employed in these cases also the CPMC model. All single point runs were conducted with tight SCF convergence criteria and with the def2-TZVP and appropriate fitting basis sets (def2-TZVP/C, def2/J and def2/JK) for the RI approximation.[32-35] For the DFT computations the RIJK approximation was used except for the ωB97X family of functionals that were run with the RIJCOSX approximation. No approximations were employed for the Hartree-Fock part of the RI-MP2 and DLPNO-CCSD(T) computations. All these computations were performed with ORCA 5.0.4.[36-38]

We draw the following conclusions from this data (Table S3):

1. With the smaller substituents (R = Ph, Me, H) **6** is more stable than **7** at all computational models. This suggests that the observation of the fast reaction of **6** to **7** is not reflecting inherent properties of the chemical cores of these isomers. Rather the reaction is driven by steric effects. It turns out that the description of these steric effects vs. London dispersion is quite challenging in these systems.

2. Methods that correct for London dispersion interactions using D3(BJ) or D4 incorrectly place the energy of **7** above that of **6**. A case in point is the data obtained for the hybrid functional B3LYP. Without any consideration of London dispersion B3LYP is qualitatively correct (**7** more stable than **6** by 7 kcal/mol), but this is reversed using D3(BJ) or D4. The NL correction performs somewhat better as both isomers are essentially isoenergetic.

3. MP2 is known to overestimate London dispersion interactions, and this method indeed favors **6** most strongly. The double hybrid functionals that include MP2 correlation to some extent, reduce the energy difference between isomers. B2PLYP has **7** lower in energy than **6**, but explicit inclusion of London dispersion using D3(BJ) overcorrects. Also, revDSD-PBEP86-D4 overbinds **6**.

4. The composite DFT method using the meta-GGA functional r^2SCAN (r^2SCAN-3c) that is including D4 correction and the hybrid meta-GGA functional M06-2X that takes London dispersion into account by its construction also incorrectly favor **6** over **7**.

5. The range-separated hybrid functional ωB97X appears qualitatively correct, but with D3(BJ) correction both isomers become isoenergetic. The ωB97X-V, a range separated hybrid with non-local correction, seems to be able to provide a balanced description of steric strain and attractive London dispersion interactions.

Table S3. Computed relative electronic energies ΔE and relative Gibbs free energies ΔG (all in kcal/mol) of isomer **7** relative to that of isomer **6** depending on the substituent R bound to the Ge atoms (Ar* = C_6H_3-2,6-(Trip)$_2$ (Trip = 2,4,6-C_6H_2*i*Pr$_3$); terphenyl = [1,1':3',1''-terphenyl]-2'-yl). Geometries were optimized with the r^{2}SCAN-3c method, all other data are single point energies with the def2-TZVP basis set.

method	Ar*		terphenyl		C_6H_5		CH_3		H	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
r^{2}SCAN-3c	0.2	0.2	-0.4	1.3	9.8	11.5	8.8	9.8	8.1	9.7
DLPNO-CCSD(T)									7.3	8.9
M06-2X	2.1	2.1	0.9	2.7	9.7	11.4	8.8	9.8	8.7	10.3
B3LYP	-7.6	-7.6	3.3	5.1	6.1	7.8	7.1	8	8.3	9.9
B3LYP-D3(BJ)	3.3	3.2	1.5	3.2	11.6	13.3	9.8	10.8	9.1	10.6
B3LYP-D4	1.4	1.6	-0.2	1.5	10.3	12	8.3	9.2	7.6	9.2
B3LYP-NL	0.1	0	-0.9	0.9	8.0	9.7	6.5	7.5	6.0	7.6
RI-MP2	11.9	11.8	3.8	5.6	15.8	17.5	12.3	13.3	10.7	12.3
B2-PLYP	-1.1	-1.2	2.9	4.7	8.8	10.5	8.3	9.3	8.6	10.1
B2-PLYP-D3(BJ)	4.5	4.4	2.0	3.8	11.8	13.5	9.8	10.8	9.0	10.6
revDSD-PBEP86-D4	2.1	2.0	1.0	1	9.4	11.1	7.9	8.9	7.6	9.2
ωB97X	-4.3	-4.4	-1.4	0.3	5.4	7.1	4.5	5.4	5.3	6.8
ωB97X-D3(BJ)	0.3	0.2	-1.5	0.3	7.8	9.5	5.9	6.8	5.8	7.4
ωB97X-V	-1.7	-1.8	-3.3	-1.5	5.5	7.2	3.4	4.3	3.3	4.9
	CPCM(cyclohexane)									
r^{2}SCAN-3c	0.5	0.7	0.7	2.5	9.5	10.9	8.3	9.3	7.7	9.3
DLPNO-CCSD(T)									6.9	8.4
M06-2X	2.4	2.6	2.1	3.8	9.3	10.7	8.4	9.3	8.3	9.8
B3LYP	-7.0	-6.8	3.8	5.6	6.2	7.6	6.8	7.8	8.0	9.6
B3LYP-D3(BJ)	3.4	3.6	2.3	4.1	11.3	12.7	9.4	10.4	8.7	10.3
B3LYP-D4	1.7	1.8	0.6	2.4	10.0	11.4	7.9	8.9	7.3	8.8
B3LYP-NL	0.3	0.5	0.0	1.8	7.8	9.1	6.1	7.1	5.7	7.2
RI-MP2	11.7	11.9	4.9	6.7	15.2	16.7	11.8	12.8	10.3	11.8
B2-PLYP	-0.8	-0.7	3.7	5.5	8.6	10.0	7.9	8.9	8.2	9.8
B2-PLYP-D3(BJ)	4.6	4.8	2.9	4.7	11.4	12.8	9.4	10.4	8.6	10.2
revDSD-PBEP86-D4	2.2	2.3	1.8	3.6	9.0	10.4	7.4	8.4	7.2	8.7
ωB97X	-4.1	-4.0	-0.8	1.0	5.1	6.5	4.0	5.0	4.8	6.4
ωB97X-D3(BJ)	0.3	0.5	-0.7	1.1	7.4	8.8	5.4	6.4	5.3	1.6
ωB97X-V	-1.7	-1.5	-2.4	-0.7	5.1	6.5	2.8	3.8	2.8	4.4

Cartesian Coordinates

All structures were computed using r²-SCAN-3c without or with CPCM(cyclohexane) as implemented in Orca 5.0.4 and are given in Å.
In addition to **6** and **7** variants with smaller substituents on the Ge atoms were studied computationally. They are named as **6-X and 7-X**, where X denotes the substituent on the two Ge atoms (-H, -Me, -Ph, and -Terph for -terphenyl).

A. r²-SCAN-3c
Coordinates of compound **6**

Ge	4.568837000	4.286617000	4.700326000
Ge	7.538984000	4.502740000	7.153271000
Cl	7.597201000	6.727029000	7.113596000
O	4.677253000	3.375122000	7.583052000
O	7.543513000	6.197291000	3.802259000
C	11.675043000	3.363935000	6.728779000
H	12.561856000	3.766819000	6.247210000
C	3.373864000	3.748594000	7.314510000
C	2.400425000	7.319402000	2.661890000
H	2.232735000	8.388092000	2.763155000
C	0.822830000	4.558834000	6.731216000
H	-0.188533000	4.879337000	6.498506000
C	5.252988000	2.555888000	4.163395000
H	4.785706000	1.689617000	3.699784000
C	3.112336000	4.197240000	6.028725000
C	5.249511000	9.121898000	5.753607000
H	5.179104000	9.441245000	6.790331000
C	11.704331000	2.101413000	7.295578000
H	12.598193000	1.486921000	7.230645000
C	2.430068000	3.735030000	8.342625000
C	1.889309000	5.222894000	1.624116000
H	1.326981000	4.636517000	0.901596000
C	1.582818000	6.558973000	1.836964000
H	0.747333000	7.019766000	1.317472000
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H	10.950318000	8.784024000	7.058306000
C	1.803419000	4.598216000	5.746408000
H	1.557246000	4.982119000	4.759989000
C	6.194836000	9.710384000	4.919833000
C	6.240619000	9.298431000	3.592260000
H	6.950611000	9.778002000	2.922596000
C	5.394613000	8.310641000	3.088643000
C	7.610030000	1.736047000	4.042828000
C	2.930605000	4.606729000	2.326435000
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H	7.790554000	11.066631000	4.599991000
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C	6.450378000	4.357433000	8.787696000
C	4.455481000	7.710836000	3.958560000
C	1.137850000	4.145579000	8.024431000
H	0.368283000	4.160961000	8.789428000
C	3.681871000	5.350807000	3.266018000
C	10.739904000	6.649679000	6.994613000
C	11.072241000	4.498502000	3.808492000

H	10.936952000	3.569676000	4.365665000
C	3.478239000	6.747497000	3.345821000
C	5.155795000	3.867128000	8.784078000
C	5.767229000	0.247812000	6.886682000
H	5.445262000	-0.674131000	7.384256000
H	5.716301000	0.066980000	5.807787000
H	5.063695000	1.048371000	7.125213000
C	4.367027000	8.146624000	5.293204000
C	6.564802000	0.512948000	9.706157000
H	5.750842000	-0.150276000	9.426365000
C	4.718636000	1.646982000	0.790810000
H	5.620407000	1.451913000	0.216712000
C	9.357560000	3.681012000	7.421558000
C	10.660324000	5.516409000	6.149820000
C	6.316432000	12.064153000	5.795374000
H	5.710321000	12.409694000	4.951668000
H	6.990539000	12.874958000	6.094270000
H	5.640831000	11.862755000	6.634409000
C	4.298829000	3.915779000	9.887067000
C	4.781446000	4.530215000	11.038049000
H	4.148325000	4.621978000	11.914705000
C	7.309744000	0.672784000	3.172654000
H	6.308119000	0.581499000	2.764591000
C	7.390696000	1.039627000	8.712294000
C	10.594685000	1.659395000	7.994678000
H	10.615910000	0.701324000	8.505113000
C	12.104101000	6.043976000	9.013735000
H	12.865871000	6.791544000	8.763577000
H	12.399986000	5.091403000	8.565964000
H	12.090359000	5.920170000	10.103246000
C	10.860674000	5.668520000	4.761352000
C	3.267380000	3.194375000	1.953852000
C	2.738821000	0.836494000	1.845966000
H	2.075476000	0.016074000	2.109591000
C	6.073929000	5.050672000	11.074860000
H	6.428135000	5.541358000	11.976716000
C	5.327442000	1.211584000	13.108463000
H	6.132909000	1.605639000	13.737830000
H	4.584258000	0.755295000	13.771818000
H	4.866220000	2.060180000	12.593016000
C	6.752981000	0.801228000	11.053742000
C	6.571205000	2.706960000	4.433011000
C	7.813599000	1.630322000	11.406728000
H	7.987949000	1.851268000	12.456014000
C	2.408133000	2.125776000	2.268096000
C	5.382833000	4.076682000	0.807026000
H	5.369180000	4.816801000	1.615427000
C	3.261676000	7.660826000	6.206700000
H	2.797842000	6.793315000	5.731916000
C	10.982432000	6.955205000	4.234368000
H	11.099854000	7.067962000	3.159673000
C	2.909115000	3.306808000	9.724186000
C	7.969701000	10.331814000	6.604550000
H	7.344661000	10.080385000	7.468998000
H	8.666917000	11.119596000	6.913909000
H	8.544349000	9.438613000	6.341427000
C	7.202735000	0.618412000	7.264977000
H	7.501118000	1.465230000	6.635092000
C	4.445204000	2.948452000	1.208088000
C	5.441769000	7.999228000	1.596900000

H	4.879296000	7.075440000	1.421266000
C	4.222055000	-0.826644000	0.638622000
H	5.209059000	-0.777866000	0.156573000
C	9.437435000	2.438645000	8.102523000
C	6.900536000	4.960434000	9.962906000
H	7.893594000	5.402632000	9.991855000
C	9.588735000	-0.116330000	3.275749000
H	10.350829000	-0.831790000	2.980633000
C	5.859043000	0.179473000	12.107229000
H	4.997748000	-0.257273000	11.581582000
C	9.549361000	3.937817000	12.105250000
H	8.647810000	4.529389000	11.938853000
H	10.390445000	4.621453000	12.265042000
H	9.413600000	3.375087000	13.035554000
C	11.126027000	9.473390000	4.453455000
H	10.805453000	10.184669000	5.227925000
C	7.239881000	5.272338000	4.405845000
C	10.298191000	7.763167000	9.267420000
H	11.062158000	8.547122000	9.210087000
H	10.166406000	7.522645000	10.328330000
H	9.354523000	8.166700000	8.889733000
C	10.102775000	4.460438000	2.622376000
H	9.080941000	4.254496000	2.945648000
H	10.388188000	3.657515000	1.933355000
H	10.099806000	5.403244000	2.064320000
C	8.665206000	2.182787000	10.453677000
C	9.858481000	3.008055000	10.923610000
H	10.193018000	3.630890000	10.084821000
C	8.284299000	-0.240401000	2.798011000
H	8.026922000	-1.050987000	2.121099000
C	1.172751000	1.470896000	4.370260000
H	1.132331000	0.398394000	4.149173000
H	0.313898000	1.716701000	5.004588000
H	2.082114000	1.666501000	4.947219000
C	1.141110000	2.308594000	3.084222000
H	1.078128000	3.360444000	3.377067000
C	8.924941000	1.848958000	4.502613000
H	9.177606000	2.657680000	5.178384000
C	10.984705000	8.084459000	5.040737000
C	8.433229000	1.907732000	9.087208000
C	10.724500000	6.503302000	8.510424000
H	10.005237000	5.713522000	8.757500000
C	6.838989000	3.644023000	0.619926000
H	7.206321000	3.073950000	1.479759000
H	7.470190000	4.531583000	0.501980000
H	6.974452000	3.032581000	-0.279379000
C	1.952118000	3.746533000	10.831114000
H	2.325354000	3.421515000	11.807019000
H	0.971545000	3.280299000	10.697423000
H	1.823991000	4.833989000	10.849264000
C	4.750534000	9.121236000	0.804129000
H	3.722304000	9.278694000	1.141030000
H	4.728057000	8.877634000	-0.264437000
H	5.292840000	10.065715000	0.928396000
C	9.903631000	0.935166000	4.129094000
H	10.913276000	1.047331000	4.515212000
C	4.858145000	4.763455000	-0.463845000
H	5.516448000	5.589119000	-0.756613000
H	3.851138000	5.164390000	-0.312867000
H	4.819363000	4.045626000	-1.291707000

C	3.029381000	1.764252000	9.756102000
H	3.712541000	1.404700000	8.983103000
H	2.046178000	1.309470000	9.592443000
H	3.414754000	1.440131000	10.728606000
C	12.523106000	4.510677000	3.296053000
H	12.702435000	5.374899000	2.646809000
H	12.728960000	3.603916000	2.715877000
H	13.240657000	4.566273000	4.121159000
C	8.126625000	-0.561423000	6.918886000
H	9.181338000	-0.302570000	7.033768000
H	7.970318000	-0.869387000	5.878923000
H	7.905325000	-1.413757000	7.572521000
C	6.858632000	7.788952000	1.046686000
H	7.469701000	8.693486000	1.139261000
H	6.806281000	7.544785000	-0.020277000
H	7.380705000	6.978911000	1.559563000
C	6.590218000	-0.958080000	12.834743000
H	6.937329000	-1.717472000	12.126932000
H	5.932692000	-1.439608000	13.567603000
H	7.466467000	-0.570272000	13.366868000
C	4.318072000	-1.817157000	1.806018000
H	5.036377000	-1.479415000	2.560424000
H	4.634816000	-2.802948000	1.447835000
H	3.348285000	-1.940438000	2.300453000
C	10.226726000	9.678164000	3.229305000
H	10.589918000	9.108335000	2.366597000
H	10.207222000	10.734510000	2.938569000
H	9.204014000	9.350347000	3.439865000
C	3.757320000	7.224070000	7.588171000
H	4.579112000	6.505778000	7.515596000
H	2.938290000	6.757023000	8.146824000
H	4.119799000	8.074483000	8.176529000
C	3.210820000	-1.314664000	-0.407777000
H	3.491892000	-2.302763000	-0.788982000
H	3.152781000	-0.620658000	-1.252191000
H	2.209298000	-1.394333000	0.030066000
C	2.170836000	8.734159000	6.339126000
H	2.569489000	9.635756000	6.818720000
H	1.340687000	8.359044000	6.949233000
H	1.775944000	9.021500000	5.358861000
C	-0.109017000	1.987315000	2.253934000
H	-0.156409000	2.606046000	1.351784000
H	-1.016061000	2.165871000	2.842267000
H	-0.114453000	0.937878000	1.938285000
C	12.592582000	9.774127000	4.113207000
H	13.231672000	9.668843000	4.995779000
H	12.702805000	10.792944000	3.724154000
H	12.957113000	9.076502000	3.350117000
C	11.026235000	2.089453000	11.322864000
H	10.719432000	1.428466000	12.142069000
H	11.879785000	2.685927000	11.665669000
H	11.360876000	1.465100000	10.491871000
B	6.748989000	4.124472000	5.209409000

Coordinates of compound **7**

Ge	-4.827875000	-4.798486000	-17.076919000
Ge	-1.238664000	-5.360893000	-15.432188000
Cl	-4.082100000	-5.144591000	-13.834366000
O	-2.098814000	-4.867983000	-18.241498000
O	-4.050011000	-2.959958000	-16.765750000
C	-5.716945000	0.443270000	-16.332257000
C	-6.906908000	-9.848739000	-16.179210000
C	-0.086968000	-1.850281000	-11.869917000
H	-0.678855000	-1.072255000	-11.391206000
C	-0.623926000	-3.132323000	-11.993293000
C	-7.019294000	-8.185342000	-17.950046000
C	-2.010770000	-3.390539000	-11.434552000
H	-2.323905000	-4.388749000	-11.757953000
C	-0.297924000	-5.572670000	-12.635724000
C	-6.869986000	-9.505974000	-17.521559000
H	-6.713572000	-10.279735000	-18.267484000
C	-4.319148000	-4.941510000	-18.978318000
C	-6.811391000	-1.652823000	-15.752943000
C	-6.809623000	-4.616028000	-17.250452000
C	-8.693463000	-3.279352000	-18.007708000
H	-9.124234000	-2.297035000	-18.183517000
C	-6.280246000	-0.417098000	-15.393987000
H	-6.318013000	-0.113890000	-14.352096000
C	-5.181875000	1.802466000	-15.932811000
H	-4.507572000	2.130149000	-16.736312000
C	0.298334000	-11.015578000	-18.459320000
H	1.372889000	-11.245753000	-18.491037000
C	-2.003201000	-3.363365000	-9.898402000
H	-1.713496000	-2.373430000	-9.526816000
H	-3.002560000	-3.589868000	-9.510084000
H	-1.302710000	-4.093271000	-9.481847000
C	-5.226637000	-4.983992000	-20.036811000
H	-6.289789000	-4.889589000	-19.836244000
C	-1.777231000	-1.163681000	-15.958282000
C	-3.421074000	-5.280931000	-21.611132000
H	-3.099132000	-5.421112000	-22.638100000
C	-0.388865000	-8.598916000	-14.931342000
C	-0.233462000	-6.232123000	-11.403446000
H	-0.003291000	-5.652277000	-10.514124000
C	-0.565958000	-6.307983000	-13.815674000
C	-0.426203000	-7.602214000	-11.312181000
H	-0.412972000	-8.096111000	-10.344671000
C	-1.017573000	-0.385462000	-15.075873000
H	-0.623729000	-0.844310000	-14.173428000
C	-1.456618000	-8.933040000	-15.779977000
C	-7.087844000	-8.825157000	-15.249289000
H	-7.113279000	-9.090742000	-14.196169000
C	1.174786000	-1.522066000	-12.352593000
C	1.431588000	-3.825173000	-13.106799000
C	-7.590707000	-5.778293000	-17.429464000
C	0.955717000	-6.378673000	-19.548480000
H	1.458523000	-6.602059000	-20.484025000
C	-7.399776000	-3.352458000	-17.484136000
C	-4.781689000	-5.152383000	-21.343401000

H	-5.496947000	-5.189885000	-22.160049000
C	-5.704288000	0.040973000	-17.663032000
H	-5.270984000	0.709838000	-18.404927000
C	0.899318000	-9.114516000	-15.194371000
C	-8.883678000	-5.662548000	-17.957841000
H	-9.474524000	-6.566638000	-18.078816000
C	-7.202100000	-7.161772000	-16.999365000
C	-2.473806000	-5.205326000	-20.589352000
C	-0.548746000	-8.343160000	-12.478397000
H	-0.594308000	-9.427745000	-12.435972000
C	0.960394000	-6.434639000	-17.135254000
H	1.442911000	-6.709853000	-16.204502000
C	1.574423000	-6.722596000	-18.349601000
H	2.540427000	-7.219633000	-18.363779000
C	-0.285439000	-5.740212000	-19.557832000
C	0.053745000	-10.194646000	-17.210230000
C	-1.216855000	-9.714504000	-16.907755000
H	-2.045065000	-9.955260000	-17.567927000
C	-0.872145000	-5.496136000	-18.317812000
C	-7.472449000	-6.440016000	-14.543072000
H	-6.896956000	-5.548440000	-14.820498000
C	1.089536000	-9.902010000	-16.331075000
H	2.081401000	-10.291304000	-16.549292000
C	-0.964481000	-5.188752000	-20.808569000
C	-9.422045000	-4.427924000	-18.281792000
H	-10.422740000	-4.358404000	-18.698865000
C	-2.305831000	-0.561201000	-17.106395000
H	-2.906922000	-1.142447000	-17.794182000
C	-6.794886000	-11.281736000	-15.699158000
H	-6.306628000	-11.249923000	-14.714075000
C	-2.962984000	-5.019764000	-19.297166000
C	2.360296000	-4.880815000	-13.687820000
H	1.749981000	-5.721647000	-14.030184000
C	-1.925243000	-2.614560000	-15.701668000
C	-6.964565000	-7.921684000	-19.444630000
H	-7.068426000	-6.844599000	-19.599569000
C	2.085996000	-8.875707000	-14.268576000
H	1.833896000	-8.048160000	-13.595498000
C	-4.733918000	-1.523170000	-20.101419000
H	-4.069843000	-2.169362000	-19.520133000
H	-4.722697000	-1.879562000	-21.137642000
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C	-0.569388000	-7.721519000	-13.729405000
C	-6.162544000	-1.559740000	-19.543159000
H	-6.525640000	-2.587941000	-19.645862000
C	-0.291768000	-5.829310000	-17.096770000
C	-6.761218000	-2.052824000	-17.104692000
C	-3.136148000	-3.375149000	-15.967911000
C	-0.881891000	-3.408262000	-15.330917000
H	0.101249000	-2.959017000	-15.199753000
C	-3.039621000	-2.384221000	-11.968106000
H	-2.851053000	-1.374089000	-11.587140000
H	-3.030228000	-2.344185000	-13.061183000
H	-4.045837000	-2.675983000	-11.650139000
C	0.137289000	-4.137379000	-12.625191000
C	1.917509000	-2.526290000	-12.966131000
H	2.910892000	-2.297546000	-13.338545000
C	-7.233148000	-7.491258000	-15.618796000
C	-6.994530000	-6.864766000	-13.151782000

H	-7.658212000	-7.617402000	-12.709598000
H	-5.975732000	-7.261306000	-13.173614000
H	-6.998168000	-5.995492000	-12.486319000
C	-1.284723000	1.543270000	-16.497960000
H	-1.092706000	2.591327000	-16.710073000
C	-0.777576000	0.957002000	-15.341384000
H	-0.194602000	1.548297000	-14.640355000
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C	-3.521986000	-9.614300000	-14.562201000
H	-4.543217000	-9.322667000	-14.295344000
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C	-7.517662000	-2.491697000	-14.700936000
H	-7.548548000	-3.525435000	-15.058752000
C	-2.871266000	-8.527014000	-15.431409000
H	-2.831035000	-7.617983000	-14.819022000
C	-4.371034000	1.761848000	-14.634144000
H	-3.613840000	0.973216000	-14.667090000
H	-3.862987000	2.718958000	-14.473010000
H	-5.015626000	1.583136000	-13.766003000
C	-0.533159000	-3.708178000	-20.961536000
H	0.553197000	-3.644021000	-21.087721000
H	-1.022263000	-3.259988000	-21.833734000
H	-0.810772000	-3.129178000	-20.074852000
C	-0.050014000	-10.220148000	-19.724585000
H	0.494092000	-9.270707000	-19.751097000
H	0.198225000	-10.795298000	-20.623937000
H	-1.120616000	-9.987804000	-19.758927000
C	-0.561828000	-5.962824000	-22.066308000
H	-0.847346000	-7.017490000	-21.993596000
H	-1.030657000	-5.532038000	-22.955011000
H	0.517716000	-5.902211000	-22.227364000
C	2.342930000	-10.120834000	-13.404196000
H	1.455898000	-10.402262000	-12.830884000
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H	3.164219000	-9.939652000	-12.701294000
C	-8.957081000	-6.045290000	-14.469269000
H	-9.115373000	-5.329527000	-13.654181000
H	-9.309941000	-5.586384000	-15.396236000
H	-9.572480000	-6.930340000	-14.269119000
C	-8.122303000	-8.607739000	-20.183210000
H	-9.092687000	-8.296509000	-19.783708000
H	-8.094335000	-8.358671000	-21.250033000
H	-8.058940000	-9.697872000	-20.092720000
C	-5.616353000	-8.353321000	-20.039126000
H	-5.476442000	-9.437311000	-19.959416000
H	-5.564150000	-8.084470000	-21.099734000
H	-4.782652000	-7.863674000	-19.527266000
C	1.715138000	-0.117957000	-12.170539000
H	0.844135000	0.548625000	-12.081955000
C	3.378643000	-8.500542000	-15.006720000
H	4.161837000	-8.258001000	-14.280345000
H	3.752593000	-9.327449000	-15.619351000
H	3.245667000	-7.633372000	-15.660166000
C	3.286447000	-5.404870000	-12.579352000
H	2.705853000	-5.828860000	-11.753373000
H	3.955222000	-6.181608000	-12.967039000
H	3.901848000	-4.590312000	-12.179433000
C	-7.090379000	-0.658229000	-20.369819000

H	-6.764440000	0.387065000	-20.322960000
H	-7.089098000	-0.965407000	-21.421946000
H	-8.119611000	-0.702169000	-19.998981000
C	-6.328978000	2.819001000	-15.830143000
H	-5.945757000	3.815417000	-15.581319000
H	-6.884493000	2.885439000	-16.771371000
H	-7.033542000	2.519284000	-15.045503000
C	-3.721210000	-8.230044000	-16.663948000
H	-4.668686000	-7.776407000	-16.362854000
H	-3.201621000	-7.546641000	-17.345451000
H	-3.971898000	-9.140537000	-17.218147000
C	2.509855000	-0.021587000	-10.858872000
H	1.896710000	-0.321378000	-10.003107000
H	3.382775000	-0.683826000	-10.894798000
H	2.864117000	1.001918000	-10.691105000
C	-8.197138000	-11.881763000	-15.508523000
H	-8.793983000	-11.280339000	-14.815560000
H	-8.727683000	-11.914463000	-16.467276000
H	-8.134838000	-12.903041000	-15.115830000
C	-5.948730000	-12.173267000	-16.610057000
H	-5.779574000	-13.145184000	-16.135055000
H	-6.450016000	-12.362910000	-17.565972000
H	-4.973592000	-11.721517000	-16.820671000
C	3.173368000	-4.391242000	-14.890758000
H	3.913977000	-3.635325000	-14.608649000
H	3.724651000	-5.229480000	-15.330628000
H	2.529658000	-3.967212000	-15.668892000
C	-0.465732000	-12.345604000	-18.418240000
H	-1.548263000	-12.174406000	-18.408640000
H	-0.231458000	-12.954779000	-19.298594000
H	-0.209949000	-12.919535000	-17.521768000
C	-6.806201000	-2.498519000	-13.345571000
H	-7.270797000	-3.240014000	-12.685619000
H	-5.749463000	-2.757335000	-13.453647000
H	-6.876037000	-1.528164000	-12.841109000
C	2.560806000	0.365527000	-13.352342000
H	3.517126000	-0.166540000	-13.403291000
H	2.040772000	0.218183000	-14.304477000
H	2.789446000	1.431195000	-13.243587000
B	-3.319214000	-4.903323000	-15.509224000
C	-8.971827000	-2.017938000	-14.548506000
H	-8.999859000	-0.974421000	-14.213486000
H	-9.510542000	-2.084084000	-15.499210000
H	-9.502082000	-2.631047000	-13.810652000

Coordinates of compound **6-Terph**

Ge	4.444433000	4.167223000	4.776626000
Ge	7.572669000	4.611932000	6.940083000
Cl	7.728142000	6.822851000	6.862528000
O	4.753805000	3.518453000	7.644880000
O	7.295368000	5.821124000	3.197074000
C	11.827268000	4.167562000	7.480503000
H	12.724620000	4.708374000	7.192051000
C	3.445607000	3.909020000	7.474583000
C	3.860289000	7.181291000	1.797018000
H	4.005259000	8.255126000	1.719340000
C	0.869937000	4.733459000	7.042395000
H	-0.151250000	5.062618000	6.874881000
C	5.154108000	2.415251000	4.320240000
H	4.701818000	1.495863000	3.951438000
C	3.075848000	4.243204000	6.180406000
C	4.240761000	8.305374000	6.399767000
H	3.715749000	8.284964000	7.350487000
C	11.911857000	3.069424000	8.321387000
H	12.875602000	2.746141000	8.704558000
C	2.595149000	3.993846000	8.577735000
C	3.231984000	5.090157000	0.807828000
H	2.885882000	4.511890000	-0.044787000
C	3.451804000	6.454208000	0.689948000
H	3.288039000	6.954030000	-0.260548000
C	11.277272000	8.080420000	5.688689000
H	11.676606000	9.015020000	6.072372000
C	1.756258000	4.652141000	5.972846000
H	1.430183000	4.952927000	4.978921000
C	5.281013000	9.202852000	6.192985000
C	5.940283000	9.218695000	4.967306000
H	6.768527000	9.901923000	4.803064000
C	5.561559000	8.344291000	3.957944000
C	7.565733000	1.790218000	3.966776000
C	3.422112000	4.444182000	2.033555000
C	2.657599000	0.226170000	2.161203000
C	10.596224000	4.593206000	6.964864000
C	6.652786000	4.455959000	8.674917000
C	4.515710000	7.431701000	4.153679000
C	1.290117000	4.417348000	8.334617000
H	0.586635000	4.509447000	9.155879000
C	3.857350000	5.169008000	3.164568000
C	11.186143000	6.975859000	6.524366000
C	4.070164000	6.561050000	3.035902000
C	5.348815000	4.005263000	8.793547000
C	3.858151000	7.431152000	5.388089000
C	6.418434000	0.607988000	7.894482000
H	5.764243000	0.227380000	7.115061000
C	3.576501000	0.747429000	1.253741000
H	4.112944000	0.084745000	0.580132000
C	9.410396000	3.911806000	7.317455000
C	10.648576000	5.770914000	6.059681000
C	4.606509000	4.065351000	9.974942000
C	5.254248000	4.564397000	11.102040000
H	4.725497000	4.637980000	12.046827000
C	7.299801000	0.693643000	3.129388000
H	6.279215000	0.497008000	2.812859000
C	7.488982000	1.424755000	7.546488000

C	10.760318000	2.369864000	8.644453000
H	10.814346000	1.480933000	9.266990000
C	10.240560000	5.689226000	4.727740000
C	3.151982000	2.985307000	2.082679000
C	1.975738000	1.084941000	3.019253000
H	1.249027000	0.689713000	3.723201000
C	6.582672000	4.983568000	11.032658000
H	7.071269000	5.368571000	11.922908000
C	6.195939000	0.283426000	9.227057000
C	6.478748000	2.666847000	4.436470000
C	7.045745000	0.787353000	10.210570000
H	6.868471000	0.550333000	11.255924000
C	2.217089000	2.453548000	2.975673000
C	10.339854000	6.793045000	3.886806000
H	10.016051000	6.710902000	2.853581000
C	3.159764000	3.576983000	9.932403000
C	3.820289000	2.115842000	1.213241000
C	9.514639000	2.769926000	8.148299000
C	7.272453000	4.942550000	9.827393000
H	8.294223000	5.311640000	9.774642000
C	9.647634000	0.133315000	3.051725000
H	10.449179000	-0.508058000	2.697042000
C	7.058574000	5.114303000	4.068154000
C	8.116173000	1.598564000	9.861989000
C	8.327619000	-0.123113000	2.681511000
H	8.101040000	-0.963378000	2.030924000
C	8.898566000	2.039783000	4.317548000
H	9.128164000	2.868493000	4.979964000
C	10.849996000	7.993863000	4.365987000
C	8.348940000	1.932678000	8.522063000
C	2.332052000	4.122491000	11.095859000
H	2.745579000	3.786003000	12.050784000
H	1.306942000	3.743763000	11.048092000
H	2.303695000	5.217091000	11.092923000
C	9.928863000	1.219970000	3.872452000
H	10.950983000	1.433190000	4.172521000
C	3.154774000	2.030276000	9.992600000
H	3.724866000	1.608803000	9.161139000
H	2.126060000	1.656650000	9.940261000
H	3.613368000	1.691007000	10.928074000
B	6.641213000	4.145425000	5.108809000
H	6.095238000	8.346585000	3.011680000
H	4.557475000	2.519173000	0.523821000
H	2.470326000	-0.843121000	2.195908000
H	1.673804000	3.118136000	3.640528000
H	5.364746000	-0.358813000	9.503539000
H	7.680575000	1.634753000	6.500723000
H	8.761144000	2.010773000	10.633298000
H	11.499299000	7.049104000	7.562502000
H	10.921188000	8.857258000	3.710791000
H	5.587527000	9.877698000	6.986629000
H	3.013634000	6.771556000	5.546743000
H	9.863775000	4.749200000	4.335012000

Coordinates of compound **7-Terph**

Ge	4.593584000	4.798202000	17.198687000
Ge	1.237287000	5.044678000	15.309050000
Cl	4.148233000	4.738238000	13.880898000
O	1.922203000	5.059333000	18.242911000
O	3.700580000	2.963850000	17.233078000
C	5.313456000	-0.308809000	15.958413000
C	5.993993000	9.578468000	16.311653000
C	1.143254000	2.375878000	11.666644000
H	2.090105000	1.877865000	11.476446000
C	1.139564000	3.706505000	12.071895000
C	6.939834000	8.132237000	17.997094000
C	-0.078401000	5.799514000	12.720434000
C	6.536942000	9.395398000	17.581932000
H	6.645293000	10.242579000	18.253167000
C	4.094573000	5.465737000	18.976879000
C	6.038351000	1.963918000	15.617632000
C	6.554050000	4.526104000	17.285274000
C	8.478535000	3.182293000	17.889516000
H	8.943612000	2.203716000	17.974765000
C	5.440879000	0.806044000	15.135542000
H	5.067783000	0.777600000	14.115527000
C	4.967347000	5.916371000	19.965462000
H	6.041127000	5.842248000	19.815142000
C	1.856996000	0.904787000	15.905294000
C	3.089611000	6.553397000	21.349388000
H	2.728148000	6.979647000	22.279990000
C	1.027169000	8.163475000	15.483229000
C	-0.749648000	6.700556000	11.884971000
H	-1.212296000	6.327878000	10.974734000
C	0.533911000	6.254136000	13.902991000
C	-0.807319000	8.050407000	12.199375000
H	-1.317289000	8.743503000	11.536207000
C	1.443478000	0.075537000	14.855962000
H	1.196391000	0.521684000	13.895834000
C	2.357695000	7.935465000	15.847751000
C	5.840645000	8.486863000	15.464375000
H	5.419383000	8.618510000	14.472021000
C	-0.056329000	1.687574000	11.507284000
C	-1.266879000	3.674831000	12.144174000
C	7.321514000	5.687292000	17.509277000
C	-1.351360000	6.435167000	19.070472000
H	-1.929058000	6.814001000	19.907577000
C	7.168234000	3.265508000	17.403765000
C	4.465154000	6.467883000	21.140782000
H	5.146546000	6.826614000	21.906464000
C	5.793673000	-0.260759000	17.263900000
H	5.687043000	-1.125848000	17.912463000
C	0.197364000	8.859923000	16.370344000
C	8.632356000	5.578246000	17.983809000
H	9.219283000	6.480086000	18.136692000
C	6.797401000	7.026037000	17.149872000
C	2.180073000	6.080096000	20.402339000
C	-0.201552000	8.512484000	13.359607000
H	-0.232105000	9.569281000	13.611945000
C	-1.233345000	5.896465000	16.718276000
H	-1.697448000	5.887251000	15.734175000
C	-1.954498000	6.352067000	17.818327000

H	-2.988486000	6.662490000	17.698628000
C	-0.030273000	6.027980000	19.261645000
C	1.981991000	8.990425000	17.984773000
C	2.827093000	8.336774000	17.095073000
H	3.857046000	8.138487000	17.373154000
C	0.637883000	5.542645000	18.139728000
C	0.668990000	9.266804000	17.611521000
H	0.000856000	9.778230000	18.298925000
C	0.670119000	6.005059000	20.618638000
C	9.193951000	4.328275000	18.208610000
H	10.212675000	4.248216000	18.577080000
C	2.191516000	0.328564000	17.135971000
H	2.524804000	0.960216000	17.951665000
C	2.725573000	5.552476000	19.234274000
C	1.920039000	2.366100000	15.692773000
C	6.392339000	0.896862000	17.748673000
C	0.466183000	7.631452000	14.215358000
C	0.095235000	5.500576000	16.860987000
C	6.508450000	2.025815000	16.933486000
C	3.028096000	3.197446000	16.163287000
C	0.944316000	3.095441000	15.082889000
H	0.047307000	2.600486000	14.711667000
C	-0.065716000	4.370348000	12.316245000
C	-1.262181000	2.340693000	11.749694000
H	-2.202516000	1.809791000	11.631246000
C	6.233473000	7.218456000	15.879941000
C	1.687203000	-1.866900000	16.263137000
H	1.620567000	-2.942047000	16.403870000
C	1.363750000	-1.300277000	15.032490000
H	1.048731000	-1.932410000	14.206852000
C	2.095456000	-1.047117000	17.311029000
H	2.348414000	-1.482023000	18.274089000
C	0.358785000	4.646700000	21.294801000
H	-0.721173000	4.539773000	21.445373000
H	0.863492000	4.582886000	22.265346000
H	0.702932000	3.815795000	20.671110000
C	0.177084000	7.142072000	21.520495000
H	0.383827000	8.118635000	21.070551000
H	0.656160000	7.097856000	22.502204000
H	-0.898151000	7.059515000	21.697820000
B	3.303194000	4.636186000	15.542316000
H	5.681861000	10.567355000	15.989439000
H	6.153485000	6.377229000	15.195699000
H	7.360740000	7.994517000	18.989649000
H	6.749749000	0.940107000	18.774551000
H	6.139410000	2.833384000	14.973228000
H	4.823758000	-1.205548000	15.589837000
H	2.075659000	4.241612000	12.194991000
H	-0.053471000	0.647651000	11.192393000
H	-2.207971000	4.183491000	12.338342000
H	3.027478000	7.439707000	15.150490000
H	2.349406000	9.282698000	18.964704000
H	-0.841441000	9.030500000	16.101068000

Coordinates of compound **6-Ph**

Ge	-4.136387000	-4.207966000	-4.705085000
Ge	-7.330243000	-4.573808000	-6.850495000
Cl	-7.686202000	-6.760427000	-6.943356000
O	-4.562709000	-3.411611000	-7.516565000
O	-6.976744000	-6.102620000	-3.360269000
C	-11.450209000	-3.770581000	-6.208993000
H	-12.300646000	-4.277505000	-5.761006000
C	-3.256986000	-3.841729000	-7.427097000
C	-2.585736000	-7.369365000	-2.351847000
H	-2.210931000	-8.373853000	-2.527717000
C	-0.691512000	-4.748658000	-7.158847000
H	0.328187000	-5.107984000	-7.058198000
C	-4.861980000	-2.471850000	-4.214267000
H	-4.460327000	-1.543834000	-3.807677000
C	-2.850000000	-4.288383000	-6.176638000
C	-11.596322000	-2.484684000	-6.722953000
H	-12.559287000	-1.984004000	-6.670879000
C	-2.445703000	-3.829728000	-8.559609000
C	-3.148025000	-5.585307000	-0.832417000
H	-3.209608000	-5.193747000	0.179178000
C	-2.656941000	-6.868434000	-1.054560000
H	-2.334634000	-7.480372000	-0.216836000
C	-1.533076000	-4.736387000	-6.049639000
H	-1.169125000	-5.088670000	-5.087885000
C	-7.278072000	-1.759737000	-4.340209000
C	-3.563709000	-4.802941000	-1.906301000
C	-10.216212000	-4.411406000	-6.272459000
C	-6.518624000	-4.161698000	-8.587707000
C	-1.144942000	-4.306033000	-8.401183000
H	-0.468257000	-4.332829000	-9.249334000
C	-3.485811000	-5.289928000	-3.214951000
C	-2.999392000	-6.585661000	-3.424654000
C	-5.200707000	-3.742634000	-8.694455000
C	-9.117794000	-3.774206000	-6.854868000
C	-4.497085000	-3.678106000	-9.897806000
C	-5.202457000	-4.000234000	-11.055110000
H	-4.705939000	-3.971892000	-12.019728000
C	-7.090512000	-0.390009000	-4.572774000
H	-6.114120000	-0.035295000	-4.891635000
C	-10.508528000	-1.843293000	-7.307842000
H	-10.618038000	-0.839797000	-7.709340000
C	-6.548439000	-4.361696000	-10.995771000
H	-7.081274000	-4.598196000	-11.911725000
C	-6.165900000	-2.710055000	-4.489020000
C	-3.034808000	-3.243415000	-9.840590000
C	-9.276297000	-2.485943000	-7.374632000
C	-7.201320000	-4.452743000	-9.771701000
H	-8.236457000	-4.783249000	-9.730926000
C	-9.404792000	0.043614000	-4.048032000
H	-10.230189000	0.741758000	-3.942671000
C	-6.730796000	-5.253279000	-4.092010000
C	-8.145643000	0.501811000	-4.429408000
H	-7.988277000	1.558938000	-4.624544000
C	-8.553130000	-2.207823000	-3.974414000
H	-8.721225000	-3.269609000	-3.814603000
C	-2.255348000	-3.672712000	-11.083149000
H	-2.680529000	-3.215012000	-11.980845000

H	-1.217864000	-3.332161000	-11.020371000
H	-2.261476000	-4.760520000	-11.207328000
C	-9.604122000	-1.314603000	-3.817631000
H	-10.585735000	-1.683098000	-3.535379000
C	-2.987762000	-1.698858000	-9.725369000
H	-3.540461000	-1.353539000	-8.847075000
H	-1.949309000	-1.362350000	-9.635114000
H	-3.433813000	-1.243482000	-10.616147000
B	-6.307107000	-4.221425000	-5.059640000
H	-3.953910000	-3.803430000	-1.724461000
H	-2.943942000	-6.990689000	-4.433364000
H	-10.111426000	-5.419203000	-5.876909000
H	-8.431578000	-1.974830000	-7.832566000

Coordinates of compound **7-Ph**

Ge	4.648007000	4.779335000	17.504708000
Ge	1.359365000	5.291543000	15.617604000
Cl	4.251060000	5.102586000	14.168659000
O	1.908759000	4.809488000	18.552260000
O	3.859308000	2.917714000	17.196415000
C	0.687037000	5.767824000	12.826741000
C	4.097549000	5.147149000	19.341597000
C	6.575763000	4.506605000	17.464936000
C	8.586720000	3.507149000	18.374585000
H	9.070510000	2.880374000	19.118599000
C	4.956684000	5.530357000	20.375390000
H	6.030920000	5.544517000	20.209540000
C	2.025661000	1.079099000	15.548524000
C	3.061798000	5.932287000	21.822739000
H	2.683487000	6.247667000	22.789800000
C	0.318157000	6.515308000	11.712073000
H	0.253522000	6.039451000	10.737374000
C	0.775032000	6.360978000	14.089702000
C	0.039732000	7.872338000	11.845317000
H	-0.246296000	8.457945000	10.976033000
C	1.467348000	0.466544000	14.418882000
H	1.095629000	1.086943000	13.607658000
C	7.342151000	5.095431000	16.452985000
C	-1.143233000	6.585143000	19.477713000
H	-1.695793000	6.914221000	20.351773000
C	7.211383000	3.708244000	18.424239000
C	4.439174000	5.920986000	21.606409000
H	5.109746000	6.227406000	22.403508000
C	8.720188000	4.902189000	16.411430000
H	9.307386000	5.364305000	15.622956000
C	2.172111000	5.547193000	20.820440000
C	0.137541000	8.479254000	13.094512000
H	-0.070328000	9.540455000	13.201786000
C	-0.956787000	6.463630000	17.069845000
H	-1.355799000	6.699499000	16.086585000
C	-1.649371000	6.861954000	18.209853000
H	-2.589352000	7.396908000	18.111871000
C	0.053374000	5.885757000	19.629946000
C	0.713381000	5.504055000	18.462461000
C	0.656800000	5.456854000	20.964554000
C	9.342012000	4.109027000	17.370859000

H	10.416751000	3.954209000	17.334063000
C	2.543923000	0.270926000	16.568640000
H	2.979205000	0.729489000	17.448659000
C	2.728657000	5.169190000	19.600085000
C	2.044403000	2.553818000	15.631180000
C	0.505956000	7.728818000	14.207245000
C	0.261057000	5.787383000	17.178132000
C	3.157302000	3.322407000	16.203040000
C	1.027899000	3.368590000	15.243393000
H	0.096225000	2.930727000	14.883626000
C	1.919565000	-1.713333000	15.340096000
H	1.880117000	-2.795775000	15.259925000
C	1.413819000	-0.916750000	14.315963000
H	0.985317000	-1.375004000	13.429287000
C	2.482468000	-1.114171000	16.462452000
H	2.878842000	-1.729464000	17.265164000
C	0.285268000	3.971656000	21.205129000
H	-0.802876000	3.866120000	21.271631000
H	0.735498000	3.618391000	22.139286000
H	0.643361000	3.339029000	20.387905000
C	0.135818000	6.292987000	22.133193000
H	0.371479000	7.354902000	22.007525000
H	0.568831000	5.946026000	23.075777000
H	-0.947946000	6.183433000	22.229230000
B	3.408515000	4.852200000	15.805644000
H	6.859859000	5.696034000	15.685917000
H	6.629022000	3.232167000	19.210292000
H	0.919529000	4.711101000	12.708561000
H	0.581849000	8.217471000	15.176659000

Coordinates of compound **6-Me**

Ge	4.429398000	3.998305000	4.719769000
Ge	7.399270000	3.806734000	7.059213000
Cl	9.355817000	4.854003000	7.141134000
O	4.630578000	3.341813000	7.714768000
O	7.215803000	6.510683000	4.314491000
C	3.327841000	3.698979000	7.421688000
C	0.752982000	4.395643000	6.790304000
H	-0.270378000	4.660681000	6.542045000
C	5.318507000	2.443298000	3.957148000
H	5.005459000	1.587387000	3.360495000
C	3.019871000	3.913886000	6.083627000
C	2.424669000	3.888620000	8.469420000
C	1.697977000	4.255343000	5.779526000
H	1.407343000	4.442778000	4.749140000
C	7.827049000	2.125503000	3.794826000
C	6.485458000	4.410152000	8.685694000
C	1.120363000	4.236921000	8.125036000
H	0.378422000	4.396375000	8.900752000
C	5.162116000	4.014327000	8.806557000
C	4.359265000	4.268667000	9.914470000
C	4.946550000	4.984873000	10.956852000
H	4.370165000	5.225880000	11.844350000
C	7.802068000	0.807136000	3.312578000
H	6.858479000	0.271187000	3.267798000
C	6.275781000	5.399197000	10.876362000
H	6.712255000	5.955637000	11.700457000

C	6.596732000	2.808378000	4.222485000
C	2.941395000	3.704213000	9.893990000
C	7.047466000	5.109476000	9.753302000
H	8.080730000	5.440469000	9.697251000
C	10.193103000	0.842761000	2.991689000
H	11.107497000	0.343288000	2.685111000
C	6.972508000	5.440485000	4.654084000
C	8.970722000	0.175423000	2.914956000
H	8.933146000	-0.847370000	2.550606000
C	9.063609000	2.778297000	3.876705000
H	9.111762000	3.789517000	4.272603000
C	2.038144000	4.374331000	10.928595000
H	2.433697000	4.218545000	11.936340000
H	1.038472000	3.930660000	10.911870000
H	1.948048000	5.450883000	10.750040000
C	10.234776000	2.146112000	3.474766000
H	11.182022000	2.672000000	3.549511000
C	3.016249000	2.187717000	10.200734000
H	3.657596000	1.670403000	9.481967000
H	2.015110000	1.745813000	10.151433000
H	3.425039000	2.029725000	11.204516000
B	6.551462000	4.128118000	5.167242000
C	7.806372000	1.902765000	7.278084000
H	6.879392000	1.332873000	7.160759000
H	8.526294000	1.574102000	6.525925000
H	8.212718000	1.736881000	8.279174000
C	3.787065000	5.235020000	3.328064000
H	4.582010000	5.409836000	2.597934000
H	2.929789000	4.806158000	2.799544000
H	3.486012000	6.191411000	3.765112000

Coordinates of compound **7-Me**

Ge	4.625572000	4.903121000	17.450743000
Ge	1.299501000	5.354401000	15.591114000
Cl	4.230439000	5.213014000	14.164325000
O	1.878239000	4.831656000	18.519882000
O	3.964592000	3.006580000	17.086671000
C	4.070579000	5.168517000	19.303953000
C	4.933664000	5.494437000	20.353507000
H	6.008821000	5.502917000	20.191216000
C	2.051912000	1.140620000	15.606710000
C	3.045872000	5.847494000	21.820792000
H	2.671454000	6.127068000	22.800294000
C	1.504733000	0.493620000	14.491371000
H	1.126794000	1.089961000	13.665012000
C	-1.145478000	6.627238000	19.500537000
H	-1.686699000	6.947054000	20.384983000
C	4.423032000	5.832437000	21.602781000
H	5.097101000	6.094166000	22.412768000
C	2.152038000	5.506179000	20.806433000
C	-0.969946000	6.559923000	17.090478000
H	-1.367849000	6.835541000	16.117006000
C	-1.646732000	6.952136000	18.242383000
H	-2.569794000	7.518674000	18.162240000
C	0.035859000	5.897411000	19.629486000
C	0.683385000	5.531868000	18.449952000

C	0.636342000	5.423459000	20.950315000
C	2.575013000	0.365223000	16.649430000
H	2.999961000	0.851769000	17.519488000
C	2.703031000	5.170069000	19.571126000
C	2.049752000	2.617762000	15.654882000
C	0.226616000	5.844194000	17.173758000
C	3.168166000	3.413460000	16.167255000
C	1.001432000	3.405274000	15.295272000
H	0.067450000	2.932975000	14.987320000
C	1.981311000	-1.656848000	15.468249000
H	1.955745000	-2.741394000	15.415225000
C	1.469469000	-0.892809000	14.422787000
H	1.049588000	-1.378654000	13.546719000
C	2.531169000	-1.022779000	16.578086000
H	2.930531000	-1.612871000	17.398090000
C	0.252281000	3.935036000	21.146657000
H	-0.836800000	3.836559000	21.208442000
H	0.697939000	3.550501000	22.070623000
H	0.606447000	3.324050000	20.311507000
C	0.123563000	6.228669000	22.144028000
H	0.369170000	7.291630000	22.050291000
H	0.553176000	5.849562000	23.075695000
H	-0.961223000	6.126267000	22.237145000
B	3.340875000	4.963772000	15.789060000
C	6.574723000	4.770948000	17.364749000
H	6.940012000	4.023956000	18.075461000
H	6.875060000	4.491576000	16.352396000
H	7.026910000	5.738418000	17.606103000
C	0.622427000	6.383933000	14.063032000
H	1.260395000	6.195580000	13.195849000
H	-0.403464000	6.094012000	13.815599000
H	0.642602000	7.455019000	14.283615000

Coordinates of compound **6-H**

Ge	-4.156894000	-3.829828000	-4.903341000
Ge	-7.226736000	-3.611463000	-7.104187000
Cl	-9.144625000	-4.715604000	-7.110353000
O	-4.453017000	-3.151770000	-7.865108000
O	-7.091240000	-6.147649000	-4.192926000
C	-3.157477000	-3.578283000	-7.636528000
C	-0.606375000	-4.442370000	-7.123684000
H	0.406468000	-4.778761000	-6.923780000
C	-4.944349000	-2.217831000	-4.155669000
H	-4.561076000	-1.354868000	-3.613996000
C	-2.809124000	-3.846183000	-6.319036000
C	-2.304732000	-3.780465000	-8.722339000
C	-1.502199000	-4.277187000	-6.072584000
H	-1.191040000	-4.512554000	-5.057671000
C	-7.428412000	-1.751330000	-3.957558000
C	-6.385818000	-4.112524000	-8.799127000
C	-1.011548000	-4.215120000	-8.437713000
H	-0.308398000	-4.389770000	-9.245560000
C	-5.053922000	-3.759976000	-8.956608000
C	-4.306031000	-4.006313000	-10.105115000
C	-4.962599000	-4.653974000	-11.150244000
H	-4.430323000	-4.883323000	-12.067828000

C	-7.314942000	-0.429604000	-3.497272000
H	-6.339076000	0.046041000	-3.467914000
C	-6.304351000	-5.016107000	-11.034252000
H	-6.795922000	-5.519097000	-11.861465000
C	-6.247184000	-2.520983000	-4.373090000
C	-2.861340000	-3.514271000	-10.118234000
C	-7.017642000	-4.745616000	-9.869526000
H	-8.058898000	-5.042862000	-9.783423000
C	-9.698829000	-0.309944000	-3.147879000
H	-10.575873000	0.250060000	-2.836853000
C	-6.777565000	-5.134825000	-4.629076000
C	-8.436049000	0.280025000	-3.095942000
H	-8.329177000	1.303091000	-2.746485000
C	-8.704647000	-2.325450000	-4.015646000
H	-8.824465000	-3.339935000	-4.388081000
C	-2.031386000	-4.188380000	-11.210079000
H	-2.450010000	-3.969485000	-12.196549000
H	-1.009009000	-3.799734000	-11.210038000
H	-1.994620000	-5.274760000	-11.078323000
C	-9.828654000	-1.614555000	-3.610609000
H	-10.807783000	-2.081036000	-3.665349000
C	-2.867808000	-1.984960000	-10.365649000
H	-3.451061000	-1.462654000	-9.602497000
H	-1.843211000	-1.598476000	-10.342737000
H	-3.307398000	-1.768037000	-11.345023000
B	-6.291291000	-3.888725000	-5.250131000
H	-3.612815000	-4.787535000	-3.823165000
H	-7.647667000	-2.135376000	-7.176217000

Coordinates of compound **7-H**

Ge	4.612506000	4.898574000	17.450773000
Ge	1.300068000	5.345627000	15.600722000
Cl	4.225954000	5.211749000	14.150501000
O	1.873633000	4.826742000	18.519005000
O	3.977156000	3.010287000	17.068432000
C	4.066766000	5.156530000	19.300868000
C	4.935151000	5.480141000	20.347178000
H	6.009560000	5.480616000	20.180642000
C	2.063156000	1.136502000	15.587363000
C	3.049848000	5.846177000	21.815422000
H	2.678591000	6.130041000	22.794877000
C	1.504032000	0.493731000	14.475545000
H	1.114452000	1.092521000	13.656451000
C	-1.141986000	6.638710000	19.494889000
H	-1.682224000	6.963909000	20.377958000
C	4.426813000	5.823740000	21.595651000
H	5.103042000	6.083426000	22.404377000
C	2.151790000	5.506425000	20.804038000
C	-0.965711000	6.566338000	17.084445000
H	-1.358443000	6.840561000	16.108328000
C	-1.641264000	6.962834000	18.235449000
H	-2.561174000	7.534065000	18.153667000
C	0.035971000	5.904026000	19.627580000
C	0.681518000	5.531952000	18.449387000
C	0.635520000	5.432726000	20.950004000
C	2.602834000	0.358342000	16.619414000

H	3.037413000	0.841273000	17.486750000
C	2.699513000	5.164118000	19.569517000
C	2.057935000	2.612979000	15.642423000
C	0.226230000	5.844139000	17.173296000
C	3.174682000	3.410403000	16.150724000
C	1.006508000	3.400751000	15.290898000
H	0.070819000	2.931313000	14.986639000
C	2.001577000	-1.659533000	15.435347000
H	1.979947000	-2.743844000	15.376797000
C	1.473352000	-0.892341000	14.400385000
H	1.044645000	-1.375297000	13.527079000
C	2.563392000	-1.029361000	16.541325000
H	2.976165000	-1.622050000	17.352685000
C	0.243634000	3.947380000	21.153824000
H	-0.845834000	3.855184000	21.217912000
H	0.688609000	3.564715000	22.078844000
H	0.592893000	3.330220000	20.321118000
C	0.128898000	6.246791000	22.140312000
H	0.380693000	7.307799000	22.041311000
H	0.557095000	5.869474000	23.073321000
H	-0.956345000	6.151242000	22.235016000
B	3.344444000	4.960187000	15.766736000
H	6.150356000	4.789272000	17.438562000
H	0.728518000	6.152669000	14.424646000

B. r²-SCAN-3c(CPCM: cyclohexane)
Coordinates of compound **6** (CPCM(cyclohexane))

Ge	4.555948000	4.279594000	4.691283000
Ge	7.542981000	4.489470000	7.145749000
Cl	7.606305000	6.721559000	7.098373000
O	4.672961000	3.385038000	7.579044000
O	7.526081000	6.182418000	3.795877000
C	11.682319000	3.359206000	6.728719000
H	12.570244000	3.761983000	6.249118000
C	3.367847000	3.755320000	7.312427000
C	2.393644000	7.316715000	2.649991000
H	2.223497000	8.385126000	2.751045000
C	0.812782000	4.551503000	6.727002000
H	-0.200854000	4.864304000	6.493155000
C	5.238769000	2.546377000	4.159550000
H	4.771097000	1.683604000	3.689963000
C	3.103185000	4.194653000	6.023859000
C	5.203014000	9.147195000	5.746864000
H	5.118184000	9.476631000	6.779536000
C	11.713338000	2.097439000	7.297734000
H	12.608048000	1.484106000	7.234128000
C	2.426340000	3.746211000	8.342678000
C	1.889735000	5.221211000	1.605724000
H	1.330023000	4.636230000	0.879959000
C	1.580559000	6.556716000	1.819596000
H	0.746840000	7.017651000	1.297166000
C	10.933131000	7.899619000	6.437262000
H	10.981254000	8.774399000	7.079959000
C	1.792108000	4.588023000	5.740110000
H	1.541821000	4.961869000	4.750938000
C	6.147898000	9.741736000	4.915685000
C	6.211812000	9.318026000	3.591765000
H	6.921650000	9.800959000	2.924273000
C	5.380567000	8.316323000	3.088753000
C	7.595042000	1.718999000	4.048171000
C	2.928270000	4.604802000	2.312376000
C	3.883508000	0.572591000	1.091473000
C	7.053954000	10.845965000	5.423303000
H	7.690284000	11.155206000	4.582312000
C	10.528507000	4.151053000	6.762000000
C	6.453148000	4.358011000	8.780147000
C	4.439757000	7.712528000	3.954851000
C	1.131564000	4.149621000	8.023419000
H	0.362732000	4.166562000	8.789185000
C	3.674754000	5.347981000	3.256743000
C	10.753957000	6.640985000	7.003793000
C	11.088355000	4.502882000	3.808865000
H	10.943450000	3.573057000	4.362018000
C	3.468992000	6.744501000	3.338007000
C	5.154307000	3.877208000	8.778045000
C	5.760360000	0.242507000	6.914527000
H	5.449184000	-0.682485000	7.413144000
H	5.700498000	0.066520000	5.835102000
H	5.053955000	1.037033000	7.165214000
C	4.336346000	8.157048000	5.286056000
C	6.572602000	0.519272000	9.726753000
H	5.750800000	-0.136876000	9.453189000
C	4.723269000	1.642254000	0.787396000

H	5.628817000	1.444685000	0.220012000
C	9.362528000	3.672384000	7.416614000
C	10.670574000	5.512332000	6.152856000
C	6.244658000	12.069596000	5.873769000
H	5.595265000	12.430748000	5.069392000
H	6.913942000	12.884789000	6.171390000
H	5.612219000	11.823691000	6.734368000
C	4.299721000	3.930930000	9.883204000
C	4.789961000	4.539972000	11.034678000
H	4.160648000	4.631321000	11.914049000
C	7.291029000	0.638855000	3.199882000
H	6.283975000	0.528864000	2.810176000
C	7.394528000	1.042796000	8.727091000
C	10.604184000	1.655521000	7.997923000
H	10.630265000	0.699880000	8.512636000
C	12.111872000	6.031701000	9.024932000
H	12.869741000	6.788585000	8.790440000
H	12.417123000	5.087680000	8.564978000
H	12.090815000	5.892390000	10.112450000
C	10.880413000	5.670206000	4.765765000
C	3.265868000	3.192332000	1.940947000
C	2.730226000	0.835511000	1.822980000
H	2.061078000	0.016591000	2.076557000
C	6.087527000	5.049756000	11.070192000
H	6.449933000	5.531783000	11.973613000
C	5.351836000	1.225443000	13.126718000
H	6.160015000	1.640355000	13.739253000
H	4.623659000	0.766929000	13.805073000
H	4.868085000	2.057725000	12.604944000
C	6.775826000	0.802133000	11.074207000
C	6.556505000	2.691611000	4.434697000
C	7.846935000	1.622010000	11.419706000
H	8.036935000	1.833082000	12.468603000
C	2.400768000	2.125352000	2.246025000
C	5.391723000	4.071140000	0.809736000
H	5.374398000	4.812136000	1.617216000
C	3.230957000	7.663953000	6.195857000
H	2.777472000	6.790840000	5.721305000
C	11.017217000	6.958831000	4.245856000
H	11.148337000	7.076365000	3.173002000
C	2.906574000	3.327444000	9.726979000
C	7.968432000	10.350463000	6.550042000
H	7.381556000	10.043114000	7.423420000
H	8.654437000	11.145349000	6.866047000
H	8.560129000	9.487188000	6.229000000
C	7.197048000	0.620078000	7.281396000
H	7.489581000	1.466115000	6.647169000
C	4.449334000	2.944215000	1.204151000
C	5.439922000	7.999087000	1.598552000
H	4.886243000	7.069891000	1.423741000
C	4.218747000	-0.829258000	0.623404000
H	5.215384000	-0.785330000	0.161688000
C	9.444687000	2.432491000	8.102270000
C	6.911503000	4.954252000	9.955928000
H	7.910205000	5.383018000	9.985461000
C	9.579859000	-0.126958000	3.279012000
H	10.344524000	-0.839063000	2.981896000
C	5.886368000	0.185524000	12.134797000
H	5.026775000	-0.260680000	11.614834000
C	9.599802000	3.947156000	12.081868000

H	8.738015000	4.584382000	11.876924000
H	10.470633000	4.588767000	12.256398000
H	9.404837000	3.406841000	13.014813000
C	11.180848000	9.473755000	4.475754000
H	10.937029000	10.188493000	5.274258000
C	7.226429000	5.253965000	4.397809000
C	10.300014000	7.744103000	9.279339000
H	11.063007000	8.529390000	9.228400000
H	10.161922000	7.497334000	10.338003000
H	9.358461000	8.148920000	8.896979000
C	10.124444000	4.479774000	2.617767000
H	9.099151000	4.280683000	2.934920000
H	10.409061000	3.679270000	1.925286000
H	10.134351000	5.426062000	2.065669000
C	8.691660000	2.174555000	10.459527000
C	9.897202000	2.985499000	10.923046000
H	10.252299000	3.584071000	10.075479000
C	8.268540000	-0.271385000	2.824266000
H	8.008282000	-1.095189000	2.164521000
C	1.142281000	1.464344000	4.332166000
H	1.108436000	0.393405000	4.102609000
H	0.272292000	1.703560000	4.954038000
H	2.043071000	1.660290000	4.922918000
C	1.126697000	2.310098000	3.050943000
H	1.065329000	3.360544000	3.349324000
C	8.915830000	1.851320000	4.486168000
H	9.171084000	2.674026000	5.144195000
C	11.024712000	8.084677000	5.058871000
C	8.445002000	1.905266000	9.093918000
C	10.731968000	6.488054000	8.518767000
H	10.015626000	5.694451000	8.760958000
C	6.848688000	3.636509000	0.632762000
H	7.210475000	3.074044000	1.500265000
H	7.479874000	4.523887000	0.512426000
H	6.987633000	3.017163000	-0.260506000
C	1.953735000	3.779987000	10.832545000
H	2.328881000	3.460854000	11.809566000
H	0.970976000	3.317566000	10.702714000
H	1.831078000	4.868261000	10.842256000
C	4.744433000	9.113506000	0.797976000
H	3.715310000	9.270024000	1.133379000
H	4.724582000	8.861471000	-0.268780000
H	5.285228000	10.059915000	0.915672000
C	9.898051000	0.941136000	4.111161000
H	10.913682000	1.069826000	4.476325000
C	4.877722000	4.757389000	-0.466070000
H	5.535260000	5.586925000	-0.749863000
H	3.866833000	5.152818000	-0.325240000
H	4.852268000	4.040184000	-1.295236000
C	3.020051000	1.784439000	9.770711000
H	3.697901000	1.414409000	8.997632000
H	2.033296000	1.334426000	9.615363000
H	3.406489000	1.466681000	10.744941000
C	12.541596000	4.506315000	3.302509000
H	12.728968000	5.372972000	2.658545000
H	12.740597000	3.600955000	2.717635000
H	13.256011000	4.548753000	4.131226000
C	8.122045000	-0.558339000	6.932510000
H	9.176499000	-0.300610000	7.053101000
H	7.967636000	-0.861328000	5.890680000

H	7.897474000	-1.413670000	7.581319000
C	6.861360000	7.798977000	1.055910000
H	7.466840000	8.706190000	1.158759000
H	6.814584000	7.560761000	-0.012632000
H	7.382911000	6.986141000	1.565061000
C	6.624904000	-0.939824000	12.874215000
H	6.977426000	-1.704808000	12.174669000
H	5.968031000	-1.417722000	13.610045000
H	7.496852000	-0.540278000	13.405095000
C	4.282108000	-1.828814000	1.785499000
H	4.988256000	-1.501512000	2.555944000
H	4.599239000	-2.813699000	1.425073000
H	3.300591000	-1.947577000	2.257664000
C	10.212709000	9.718098000	3.312427000
H	10.485148000	9.118939000	2.436170000
H	10.230596000	10.771816000	3.011937000
H	9.189330000	9.451513000	3.594741000
C	3.726545000	7.234819000	7.580133000
H	4.546178000	6.513129000	7.509082000
H	2.907492000	6.770464000	8.141179000
H	4.088705000	8.089778000	8.162292000
C	3.223083000	-1.301878000	-0.445254000
H	3.503766000	-2.290436000	-0.825775000
H	3.188591000	-0.603229000	-1.287532000
H	2.213187000	-1.374855000	-0.025359000
C	2.130718000	8.728614000	6.322819000
H	2.520041000	9.632174000	6.806707000
H	1.299994000	8.346252000	6.927907000
H	1.739592000	9.012968000	5.339969000
C	-0.116992000	1.997650000	2.207291000
H	-0.152195000	2.620450000	1.307161000
H	-1.028186000	2.179565000	2.788363000
H	-0.123587000	0.948579000	1.889927000
C	12.632008000	9.726161000	4.042038000
H	13.323171000	9.589896000	4.880355000
H	12.750613000	10.745505000	3.656871000
H	12.921100000	9.026580000	3.248880000
C	11.039655000	2.046963000	11.349474000
H	10.718531000	1.425086000	12.193711000
H	11.912325000	2.629862000	11.666735000
H	11.349130000	1.382676000	10.539272000
B	6.740703000	4.109900000	5.205854000

Coordinates of compound **7** (CPCM(cyclohexane))

Ge	-4.821747000	-4.797854000	-17.080868000
Ge	-1.227586000	-5.363512000	-15.437158000
Cl	-4.071820000	-5.159993000	-13.838014000
O	-2.089057000	-4.864621000	-18.244445000
O	-4.046241000	-2.958170000	-16.755262000
C	-5.747789000	0.466355000	-16.342228000
C	-6.906756000	-9.845268000	-16.174719000
C	-0.078449000	-1.857918000	-11.856566000
H	-0.668617000	-1.082266000	-11.371879000
C	-0.615816000	-3.139523000	-11.986031000
C	-7.014661000	-8.182927000	-17.947663000
C	-2.001612000	-3.398857000	-11.424456000
H	-2.313806000	-4.398053000	-11.745688000
C	-0.290266000	-5.578076000	-12.639978000
C	-6.867789000	-9.503884000	-17.517860000
H	-6.712245000	-10.278531000	-18.263147000
C	-4.310272000	-4.937334000	-18.980751000
C	-6.825966000	-1.638441000	-15.760160000
C	-6.803421000	-4.612430000	-17.252057000
C	-8.687241000	-3.276499000	-18.012830000
H	-9.119185000	-2.294939000	-18.190528000
C	-6.312076000	-0.393920000	-15.403249000
H	-6.365278000	-0.084155000	-14.363686000
C	-5.223844000	1.830968000	-15.945559000
H	-4.552762000	2.162249000	-16.750208000
C	0.285790000	-11.065579000	-18.442575000
H	1.355780000	-11.316069000	-18.464251000
C	-1.992314000	-3.368982000	-9.888148000
H	-1.707950000	-2.375967000	-9.520459000
H	-2.990469000	-3.599852000	-9.498837000
H	-1.287041000	-4.094705000	-9.471885000
C	-5.218874000	-4.981011000	-20.038645000
H	-6.282173000	-4.888191000	-19.838662000
C	-1.775509000	-1.164726000	-15.944838000
C	-3.413781000	-5.276380000	-21.614885000
H	-3.092578000	-5.414480000	-22.642405000
C	-0.382925000	-8.605708000	-14.939225000
C	-0.226179000	-6.239724000	-11.408368000
H	0.002796000	-5.662573000	-10.516890000
C	-0.556834000	-6.312445000	-13.821474000
C	-0.418089000	-7.610643000	-11.319475000
H	-0.404723000	-8.106121000	-10.352630000
C	-1.027904000	-0.385561000	-15.052527000
H	-0.636397000	-0.845746000	-14.149532000
C	-1.455429000	-8.950533000	-15.778051000
C	-7.089404000	-8.820615000	-15.245441000
H	-7.117058000	-9.086291000	-14.192369000
C	1.183549000	-1.527700000	-12.338910000
C	1.437380000	-3.827058000	-13.107641000
C	-7.584895000	-5.774739000	-17.430753000
C	0.970063000	-6.364037000	-19.556393000
H	1.473109000	-6.584975000	-20.492352000
C	-7.393684000	-3.349041000	-17.488080000
C	-4.774670000	-5.149227000	-21.345813000
H	-5.490598000	-5.188003000	-22.161870000
C	-5.719820000	0.056665000	-17.671236000
H	-5.285243000	0.724665000	-18.413076000

C	0.904764000	-9.121962000	-15.204981000
C	-8.877220000	-5.659881000	-17.961368000
H	-9.468263000	-6.563642000	-18.084560000
C	-7.197878000	-7.158049000	-16.998096000
C	-2.465579000	-5.200712000	-20.593121000
C	-0.539798000	-8.350297000	-12.487231000
H	-0.584842000	-9.434966000	-12.445146000
C	0.978100000	-6.420028000	-17.141863000
H	1.464552000	-6.691166000	-16.211771000
C	1.593170000	-6.703062000	-18.357621000
H	2.563067000	-7.192710000	-18.373272000
C	-0.274567000	-5.731222000	-19.564362000
C	0.046615000	-10.232489000	-17.200252000
C	-1.223273000	-9.748883000	-16.896517000
H	-2.055749000	-10.001568000	-17.547058000
C	-0.861230000	-5.489591000	-18.323274000
C	-7.480253000	-6.434685000	-14.543261000
H	-6.906153000	-5.541802000	-14.819876000
C	1.088918000	-9.924239000	-16.333039000
H	2.080021000	-10.314994000	-16.552208000
C	-0.956591000	-5.185018000	-20.815890000
C	-9.415595000	-4.425505000	-18.287170000
H	-10.415641000	-4.356371000	-18.706127000
C	-2.297171000	-0.560474000	-17.095628000
H	-2.885091000	-1.143442000	-17.793650000
C	-6.795031000	-11.277833000	-15.692722000
H	-6.306001000	-11.244460000	-14.708193000
C	-2.954130000	-5.015706000	-19.300613000
C	2.363930000	-4.877910000	-13.700258000
H	1.753946000	-5.719556000	-14.040646000
C	-1.919188000	-2.617618000	-15.694972000
C	-6.960054000	-7.920988000	-19.442600000
H	-7.061371000	-6.843944000	-19.599463000
C	2.096220000	-8.872487000	-14.288416000
H	1.846947000	-8.037212000	-13.623876000
C	-4.722941000	-1.506370000	-20.098629000
H	-4.057333000	-2.153531000	-19.519652000
H	-4.707352000	-1.853327000	-21.138191000
H	-4.320556000	-0.487006000	-20.077626000
C	-6.216408000	-1.183688000	-18.075995000
C	-0.560198000	-7.726266000	-13.737560000
C	-6.153616000	-1.556650000	-19.546656000
H	-6.505981000	-2.588742000	-19.647318000
C	-0.278535000	-5.822782000	-17.102724000
C	-6.761333000	-2.045538000	-17.109395000
C	-3.129121000	-3.378538000	-15.963519000
C	-0.873868000	-3.410901000	-15.328607000
H	0.109657000	-2.962197000	-15.198544000
C	-3.032757000	-2.394570000	-11.958180000
H	-2.838128000	-1.382936000	-11.584397000
H	-3.030826000	-2.362725000	-13.051837000
H	-4.037251000	-2.682821000	-11.630755000
C	0.143514000	-4.141939000	-12.625576000
C	1.925172000	-2.529313000	-12.958958000
H	2.919566000	-2.300408000	-13.328952000
C	-7.233821000	-7.486787000	-15.617002000
C	-7.010005000	-6.857468000	-13.148525000
H	-7.673879000	-7.613193000	-12.712174000
H	-5.990616000	-7.253153000	-13.164085000
H	-7.021935000	-5.987757000	-12.483370000

C	-1.298052000	1.549123000	-16.467404000
H	-1.112887000	2.600015000	-16.672032000
C	-0.794507000	0.960173000	-15.309869000
H	-0.219717000	1.551406000	-14.601947000
C	-2.048155000	0.783152000	-17.354996000
H	-2.445047000	1.232645000	-18.261501000
C	-3.525029000	-9.618936000	-14.557970000
H	-4.540311000	-9.316183000	-14.280194000
H	-3.587066000	-10.566400000	-15.106962000
H	-2.948916000	-9.791461000	-13.642817000
C	-7.527553000	-2.480349000	-14.707392000
H	-7.560023000	-3.512931000	-15.068239000
C	-2.867871000	-8.536805000	-15.429044000
H	-2.819718000	-7.626527000	-14.819123000
C	-4.414013000	1.798031000	-14.645657000
H	-3.645735000	1.019735000	-14.680800000
H	-3.919276000	2.761878000	-14.482215000
H	-5.057802000	1.607379000	-13.779479000
C	-0.525277000	-3.705039000	-20.976345000
H	0.560782000	-3.643094000	-21.106704000
H	-1.016110000	-3.262847000	-21.850635000
H	-0.801010000	-3.121246000	-20.091866000
C	-0.037883000	-10.267567000	-19.713401000
H	0.529263000	-9.331234000	-19.743042000
H	0.202842000	-10.852314000	-20.608595000
H	-1.103349000	-10.012605000	-19.752973000
C	-0.556581000	-5.964250000	-22.071567000
H	-0.842231000	-7.018691000	-21.993608000
H	-1.028854000	-5.536626000	-22.959808000
H	0.522690000	-5.904078000	-22.234203000
C	2.357367000	-10.108519000	-13.411489000
H	1.471373000	-10.388497000	-12.835323000
H	2.635726000	-10.964585000	-14.037494000
H	3.178287000	-9.915462000	-12.711208000
C	-8.966012000	-6.042468000	-14.475771000
H	-9.125916000	-5.316579000	-13.669867000
H	-9.318045000	-5.596218000	-15.409316000
H	-9.579111000	-6.926884000	-14.265148000
C	-8.119525000	-8.606461000	-20.179607000
H	-9.088895000	-8.294649000	-19.777550000
H	-8.092448000	-8.355369000	-21.246090000
H	-8.054160000	-9.696714000	-20.090092000
C	-5.613388000	-8.357256000	-20.037501000
H	-5.476059000	-9.441269000	-19.953431000
H	-5.564286000	-8.091947000	-21.099302000
H	-4.778571000	-7.866303000	-19.528043000
C	1.724685000	-0.124927000	-12.148436000
H	0.854297000	0.540989000	-12.053114000
C	3.385837000	-8.506204000	-15.036444000
H	4.172049000	-8.260862000	-14.314221000
H	3.752952000	-9.339451000	-15.644707000
H	3.252495000	-7.642449000	-15.694317000
C	3.302846000	-5.403867000	-12.603266000
H	2.731674000	-5.827293000	-11.770064000
H	3.964349000	-6.182057000	-13.000522000
H	3.925045000	-4.590202000	-12.211709000
C	-7.086797000	-0.666219000	-20.379890000
H	-6.767699000	0.381538000	-20.336699000
H	-7.079223000	-0.979144000	-21.430389000
H	-8.116839000	-0.718146000	-20.011619000

C	-6.378273000	2.839430000	-15.843170000
H	-6.000563000	3.838659000	-15.597000000
H	-6.934574000	2.901216000	-16.784496000
H	-7.078923000	2.536192000	-15.056087000
C	-3.715709000	-8.235570000	-16.662152000
H	-4.665501000	-7.785552000	-16.362303000
H	-3.196501000	-7.546831000	-17.338723000
H	-3.961072000	-9.144457000	-17.220921000
C	2.523698000	-0.038489000	-10.838326000
H	1.912793000	-0.343525000	-9.982476000
H	3.397466000	-0.699459000	-10.882912000
H	2.877230000	0.984488000	-10.665560000
C	-8.197588000	-11.876673000	-15.498231000
H	-8.791928000	-11.274776000	-14.803165000
H	-8.729798000	-11.911263000	-16.456260000
H	-8.133053000	-12.897497000	-15.104552000
C	-5.952260000	-12.171969000	-16.604451000
H	-5.787400000	-13.144153000	-16.128209000
H	-6.454864000	-12.358281000	-17.560365000
H	-4.975270000	-11.723665000	-16.815040000
C	3.164110000	-4.380286000	-14.908877000
H	3.907895000	-3.626840000	-14.628334000
H	3.707317000	-5.217294000	-15.361249000
H	2.510123000	-3.948912000	-15.674655000
C	-0.505046000	-12.380021000	-18.404907000
H	-1.584125000	-12.187501000	-18.408531000
H	-0.271786000	-12.995502000	-19.281141000
H	-0.268796000	-12.956611000	-17.504460000
C	-6.808150000	-2.490370000	-13.355800000
H	-7.271294000	-3.231469000	-12.694205000
H	-5.752278000	-2.751705000	-13.470715000
H	-6.871162000	-1.519191000	-12.852059000
C	2.568348000	0.366241000	-13.328527000
H	3.520599000	-0.172021000	-13.390138000
H	2.041464000	0.233536000	-14.279249000
H	2.802097000	1.429539000	-13.207994000
B	-3.309337000	-4.910389000	-15.516660000
C	-8.980891000	-2.007137000	-14.544670000
H	-9.006556000	-0.967007000	-14.198559000
H	-9.522984000	-2.063910000	-15.494404000
H	-9.507448000	-2.627750000	-13.810301000

Coordinates of compound **6-Terph** (CPCM(cyclohexane))

Ge	4.433908000	4.186417000	4.769282000
Ge	7.573798000	4.583755000	6.936728000
Cl	7.676405000	6.809268000	6.874125000
O	4.750482000	3.512235000	7.630875000
O	7.299268000	5.786172000	3.184323000
C	11.840006000	4.215479000	7.455324000
H	12.726613000	4.776790000	7.172627000
C	3.444299000	3.917967000	7.468506000
C	3.960774000	7.182610000	1.752434000
H	4.128724000	8.252312000	1.663896000
C	0.873842000	4.766900000	7.054917000
H	-0.146006000	5.104049000	6.894546000
C	5.117604000	2.419952000	4.328247000
H	4.647767000	1.508782000	3.961556000
C	3.074798000	4.276356000	6.180268000
C	4.201674000	8.358781000	6.349885000
H	3.643535000	8.356509000	7.282051000
C	11.948971000	3.106958000	8.280343000
H	12.920518000	2.795414000	8.653501000
C	2.596867000	3.989635000	8.574721000
C	3.318133000	5.090876000	0.771603000
H	2.984457000	4.509501000	-0.083912000
C	3.569951000	6.448894000	0.642663000
H	3.444114000	6.939378000	-0.318484000
C	11.195205000	8.156660000	5.750738000
H	11.569453000	9.092923000	6.155449000
C	1.757122000	4.697104000	5.981500000
H	1.427866000	5.010024000	4.992672000
C	5.251974000	9.250511000	6.163996000
C	5.951118000	9.246255000	4.959573000
H	6.783905000	9.927849000	4.810514000
C	5.601948000	8.358481000	3.950316000
C	7.520820000	1.741690000	4.001306000
C	3.461154000	4.456877000	2.010334000
C	2.588432000	0.261630000	2.188468000
C	10.598396000	4.626685000	6.952754000
C	6.660076000	4.415047000	8.672918000
C	4.546216000	7.452144000	4.125153000
C	1.293943000	4.426448000	8.341536000
H	0.592062000	4.507982000	9.165320000
C	3.883013000	5.187107000	3.143502000
C	11.130517000	7.031967000	6.562880000
C	4.124121000	6.573657000	3.004268000
C	5.350871000	3.977279000	8.785740000
C	3.849640000	7.470529000	5.338343000
C	6.463560000	0.597604000	7.883551000
H	5.798410000	0.224387000	7.109514000
C	3.538095000	0.744529000	1.290556000
H	4.072403000	0.057223000	0.640315000
C	9.426486000	3.919629000	7.302130000
C	10.625671000	5.823230000	6.070397000
C	4.609749000	4.028163000	9.968782000
C	5.261568000	4.509571000	11.101764000
H	4.733764000	4.575002000	12.047701000
C	7.234206000	0.573611000	3.273763000
H	6.204207000	0.330608000	3.028234000
C	7.530245000	1.418400000	7.531065000

C	10.810911000	2.385029000	8.603475000
H	10.884851000	1.492167000	9.218401000
C	10.227844000	5.758148000	4.734320000
C	3.153056000	3.006182000	2.073576000
C	1.909776000	1.151872000	3.017384000
H	1.158106000	0.786792000	3.711594000
C	6.594364000	4.917917000	11.036911000
H	7.087027000	5.286932000	11.931809000
C	6.257952000	0.258968000	9.215956000
C	6.446538000	2.645548000	4.449404000
C	7.125411000	0.747203000	10.192916000
H	6.964138000	0.495576000	11.237588000
C	2.186379000	2.513717000	2.955947000
C	10.300703000	6.882215000	3.916479000
H	9.986260000	6.812524000	2.879267000
C	3.160871000	3.547398000	9.921710000
C	3.816009000	2.106144000	1.231018000
C	9.554913000	2.770786000	8.121095000
C	7.285129000	4.881850000	9.831395000
H	8.312334000	5.237120000	9.785735000
C	9.586008000	0.037620000	3.132678000
H	10.380598000	-0.622339000	2.796660000
C	7.059670000	5.084196000	4.059337000
C	8.192392000	1.562213000	9.839102000
C	8.253879000	-0.266022000	2.848727000
H	8.010868000	-1.163012000	2.285610000
C	8.864359000	2.034868000	4.268709000
H	9.110175000	2.919809000	4.847352000
C	10.774771000	8.087055000	4.423931000
C	8.403363000	1.916393000	8.500366000
C	2.337431000	4.077135000	11.095363000
H	2.753068000	3.723868000	12.043241000
H	1.311094000	3.702899000	11.041471000
H	2.312917000	5.171872000	11.109599000
C	9.887267000	1.193738000	3.845141000
H	10.918901000	1.443950000	4.076495000
C	3.151303000	1.999378000	9.958280000
H	3.722613000	1.585487000	9.123253000
H	2.121060000	1.631601000	9.897497000
H	3.603502000	1.646171000	10.891727000
B	6.635893000	4.127233000	5.106487000
H	6.162953000	8.350765000	3.019930000
H	4.575324000	2.477878000	0.547642000
H	2.374720000	-0.802260000	2.238055000
H	1.642947000	3.203535000	3.594734000
H	5.427242000	-0.381971000	9.496863000
H	7.709048000	1.641565000	6.485611000
H	8.850554000	1.960364000	10.606797000
H	11.441610000	7.091490000	7.602689000
H	10.825122000	8.965903000	3.787399000
H	5.531846000	9.939599000	6.955566000
H	2.997142000	6.816423000	5.477723000
H	9.882592000	4.816262000	4.318047000

Coordinates of compound **7-Terph** (CPCM(cyclohexane))

Ge	4.600389000	4.806241000	17.189343000
Ge	1.235133000	5.053159000	15.303120000
Cl	4.140945000	4.732660000	13.869799000
O	1.927233000	5.064143000	18.232144000
O	3.703900000	2.968051000	17.226747000
C	5.336753000	-0.322791000	15.961726000
C	5.999500000	9.590170000	16.338515000
C	1.118130000	2.362953000	11.663133000
H	2.059428000	1.857819000	11.463590000
C	1.126002000	3.697060000	12.058595000
C	6.946819000	8.130066000	18.012642000
C	-0.074698000	5.801073000	12.709762000
C	6.544359000	9.396950000	17.607266000
H	6.656505000	10.239382000	18.284023000
C	4.099279000	5.465858000	18.969983000
C	6.041878000	1.956132000	15.615281000
C	6.559784000	4.528479000	17.277020000
C	8.483854000	3.183266000	17.882682000
H	8.949029000	2.204892000	17.970562000
C	5.452962000	0.792043000	15.136045000
H	5.080433000	0.757370000	14.115789000
C	4.972347000	5.907372000	19.963261000
H	6.046507000	5.838717000	19.813221000
C	1.850240000	0.913430000	15.909787000
C	3.093147000	6.527951000	21.354696000
H	2.731557000	6.942675000	22.290429000
C	1.024645000	8.175987000	15.467141000
C	-0.738822000	6.700708000	11.866501000
H	-1.203155000	6.325524000	10.958062000
C	0.535924000	6.259707000	13.892196000
C	-0.791450000	8.053112000	12.172977000
H	-1.296481000	8.744712000	11.504365000
C	1.462439000	0.079403000	14.854122000
H	1.236193000	0.520312000	13.886460000
C	2.351358000	7.944615000	15.843973000
C	5.842875000	8.504905000	15.483034000
H	5.421509000	8.645094000	14.491742000
C	-0.087332000	1.679327000	11.525582000
C	-1.280016000	3.678604000	12.162987000
C	7.326686000	5.689321000	17.506297000
C	-1.353704000	6.413055000	19.077405000
H	-1.933134000	6.779087000	19.919071000
C	7.173320000	3.267143000	17.396303000
C	4.469279000	6.445763000	21.144844000
H	5.150622000	6.797637000	21.913863000
C	5.819392000	-0.268378000	17.266747000
H	5.723165000	-1.133288000	17.917340000
C	0.191408000	8.885018000	16.341688000
C	8.637498000	5.579686000	17.981743000
H	9.222988000	6.481069000	18.142649000
C	6.801094000	7.030350000	17.156754000
C	2.183592000	6.064522000	20.401998000
C	-0.189593000	8.518863000	13.334337000
H	-0.220275000	9.577030000	13.581133000
C	-1.236288000	5.894520000	16.719220000
H	-1.703623000	5.887720000	15.736536000
C	-1.958642000	6.336164000	17.824986000

H	-2.995131000	6.640352000	17.709849000
C	-0.028488000	6.014541000	19.262981000
C	1.964446000	9.019593000	17.969911000
C	2.812745000	8.353215000	17.092240000
H	3.839956000	8.152213000	17.378943000
C	0.640325000	5.542370000	18.135738000
C	0.655824000	9.300988000	17.583123000
H	-0.013477000	9.825236000	18.259834000
C	0.673588000	5.989357000	20.619365000
C	9.199761000	4.329102000	18.203242000
H	10.217845000	4.248282000	18.573494000
C	2.155669000	0.342823000	17.150917000
H	2.461203000	0.978180000	17.974934000
C	2.729892000	5.549322000	19.228679000
C	1.915843000	2.374676000	15.693064000
C	6.410375000	0.895563000	17.747839000
C	0.470781000	7.639135000	14.197909000
C	0.095257000	5.505657000	16.857384000
C	6.515302000	2.024453000	16.929922000
C	3.026097000	3.204122000	16.160871000
C	0.941934000	3.103592000	15.079445000
H	0.045330000	2.608419000	14.707505000
C	-0.072691000	4.368616000	12.315090000
C	-1.287017000	2.341110000	11.778150000
H	-2.231761000	1.814500000	11.675486000
C	6.234950000	7.232559000	15.889084000
C	1.680371000	-1.858056000	16.273949000
H	1.615542000	-2.933152000	16.416505000
C	1.382264000	-1.296595000	15.033967000
H	1.088134000	-1.932402000	14.203364000
C	2.061292000	-1.033198000	17.328947000
H	2.292970000	-1.463844000	18.299308000
C	0.362324000	4.630585000	21.294949000
H	-0.717650000	4.526382000	21.447546000
H	0.867495000	4.568338000	22.265332000
H	0.705380000	3.798951000	20.671117000
C	0.181812000	7.126049000	21.522998000
H	0.390543000	8.103139000	21.074620000
H	0.661868000	7.078642000	22.503951000
H	-0.893652000	7.043727000	21.698632000
B	3.301775000	4.641911000	15.538657000
H	5.690922000	10.582633000	16.023182000
H	6.156186000	6.397010000	15.197569000
H	7.371913000	7.984948000	19.002384000
H	6.772912000	0.941347000	18.771859000
H	6.136725000	2.824540000	14.968283000
H	4.858239000	-1.226187000	15.594268000
H	2.066505000	4.228554000	12.163690000
H	-0.093315000	0.636381000	11.220777000
H	-2.216484000	4.193172000	12.364209000
H	3.025939000	7.442886000	15.155690000
H	2.324710000	9.320042000	18.950163000
H	-0.843340000	9.063278000	16.061375000

Coordinates of compound **6-C_6H_5** (CPCM(cyclohexane))

Ge	-4.130056000	-4.202437000	-4.702955000
Ge	-7.320401000	-4.545256000	-6.851007000
Cl	-7.614876000	-6.753002000	-6.960581000
O	-4.552616000	-3.393507000	-7.513702000
O	-6.972521000	-6.071721000	-3.357702000
C	-11.454125000	-3.862541000	-6.168001000
H	-12.276406000	-4.379226000	-5.680202000
C	-3.250954000	-3.839446000	-7.427101000
C	-2.639570000	-7.390962000	-2.347503000
H	-2.286884000	-8.403729000	-2.522594000
C	-0.696182000	-4.777811000	-7.164789000
H	0.319490000	-5.149536000	-7.066536000
C	-4.840560000	-2.458035000	-4.216578000
H	-4.428752000	-1.534390000	-3.809993000
C	-2.848631000	-4.296242000	-6.178434000
C	-11.658406000	-2.608148000	-6.738844000
H	-12.639352000	-2.142852000	-6.693289000
C	-2.440956000	-3.831880000	-8.560609000
C	-3.157316000	-5.590623000	-0.829410000
H	-3.206403000	-5.195140000	0.181506000
C	-2.695916000	-6.885679000	-1.050422000
H	-2.384680000	-7.503021000	-0.212263000
C	-1.536865000	-4.761088000	-6.054227000
H	-1.174910000	-5.122672000	-5.095117000
C	-7.250560000	-1.722683000	-4.341504000
C	-3.559097000	-4.801049000	-1.904213000
C	-10.196849000	-4.457899000	-6.223528000
C	-6.516993000	-4.117773000	-8.587103000
C	-1.145095000	-4.323979000	-8.405267000
H	-0.468435000	-4.353016000	-9.253441000
C	-3.496125000	-5.293354000	-3.212239000
C	-3.038779000	-6.600142000	-3.421418000
C	-5.194391000	-3.711489000	-8.692905000
C	-9.133648000	-3.807726000	-6.855846000
C	-4.490865000	-3.648827000	-9.896539000
C	-5.201363000	-3.955806000	-11.055468000
H	-4.705950000	-3.926053000	-12.020643000
C	-7.047392000	-0.351818000	-4.558261000
H	-6.066082000	-0.001656000	-4.867360000
C	-10.605098000	-1.953155000	-7.370921000
H	-10.760511000	-0.975061000	-7.818035000
C	-6.551973000	-4.302205000	-10.996992000
H	-7.088628000	-4.525740000	-11.914163000
C	-6.146874000	-2.683346000	-4.492146000
C	-3.022814000	-3.233854000	-9.839708000
C	-9.349009000	-2.551021000	-7.430161000
C	-7.204811000	-4.394452000	-9.772382000
H	-8.243852000	-4.713668000	-9.734372000
C	-9.359955000	0.100246000	-4.035264000
H	-10.178159000	0.806071000	-3.923591000
C	-6.728759000	-5.222143000	-4.090957000
C	-8.094108000	0.549570000	-4.408416000
H	-7.924975000	1.607176000	-4.591360000
C	-8.531276000	-2.162003000	-3.983299000
H	-8.709869000	-3.223282000	-3.831223000
C	-2.250188000	-3.670135000	-11.084319000
H	-2.671430000	-3.203935000	-11.979384000

H	-1.208427000	-3.343752000	-11.019210000
H	-2.271186000	-4.757604000	-11.211007000
C	-9.573716000	-1.258722000	-3.819071000
H	-10.559224000	-1.619010000	-3.538489000
C	-2.954667000	-1.690132000	-9.720229000
H	-3.502220000	-1.338159000	-8.841058000
H	-1.910856000	-1.370345000	-9.630874000
H	-3.393531000	-1.228093000	-10.611151000
B	-6.302974000	-4.193628000	-5.059430000
H	-3.925341000	-3.792596000	-1.721772000
H	-2.994017000	-7.008724000	-4.429250000
H	-10.047550000	-5.438987000	-5.777962000
H	-8.532801000	-2.030106000	-7.927129000

Coordinates of compound **7-C_6H_5** (CPCM(cyclohexane))

Ge	4.645713000	4.778932000	17.511379000
Ge	1.352781000	5.282906000	15.620654000
Cl	4.249160000	5.096576000	14.171889000
O	1.902160000	4.807444000	18.553717000
O	3.867913000	2.910096000	17.194686000
C	0.643790000	5.743800000	12.832006000
C	4.091606000	5.131902000	19.347525000
C	6.574493000	4.519970000	17.460586000
C	8.588519000	3.486331000	18.324032000
H	9.074002000	2.826724000	19.038053000
C	4.953883000	5.496505000	20.385807000
H	6.028616000	5.500545000	20.222670000
C	2.028475000	1.071306000	15.554325000
C	3.058688000	5.905786000	21.832798000
H	2.681921000	6.216891000	22.801855000
C	0.279699000	6.491036000	11.714465000
H	0.179915000	6.006083000	10.747118000
C	0.775095000	6.348611000	14.086244000
C	0.049633000	7.858859000	11.836488000
H	-0.232594000	8.443900000	10.965443000
C	1.480532000	0.460081000	14.418343000
H	1.111392000	1.080432000	13.605787000
C	7.339790000	5.163270000	16.481129000
C	-1.138636000	6.604742000	19.477177000
H	-1.690079000	6.937381000	20.350620000
C	7.211564000	3.678585000	18.381808000
C	4.436998000	5.880545000	21.619672000
H	5.108802000	6.171313000	22.421726000
C	8.719362000	4.978987000	16.432258000
H	9.306009000	5.484264000	15.670176000
C	2.166640000	5.537346000	20.825446000
C	0.188976000	8.476288000	13.077389000
H	0.017043000	9.544816000	13.176110000
C	-0.952051000	6.480014000	17.068250000
H	-1.349397000	6.718981000	16.085016000
C	-1.641697000	6.885402000	18.208217000
H	-2.577069000	7.428505000	18.109535000
C	0.052916000	5.896093000	19.631113000
C	0.710565000	5.508649000	18.463928000
C	0.650092000	5.464008000	20.967679000
C	9.343034000	4.140282000	17.351908000

H	10.418551000	3.991932000	17.309378000
C	2.537868000	0.262739000	16.579029000
H	2.961274000	0.718587000	17.466415000
C	2.722418000	5.160564000	19.604543000
C	2.044886000	2.546627000	15.638001000
C	0.552141000	7.726191000	14.192872000
C	0.259872000	5.792963000	17.178897000
C	3.157421000	3.316018000	16.207573000
C	1.026074000	3.358786000	15.249815000
H	0.095613000	2.920213000	14.888095000
C	1.929858000	-1.721534000	15.340810000
H	1.893314000	-2.804042000	15.258504000
C	1.431389000	-0.923944000	14.312995000
H	1.010919000	-1.381624000	13.422048000
C	2.480387000	-1.123055000	16.470486000
H	2.869144000	-1.738579000	17.276852000
C	0.262200000	3.983224000	21.210992000
H	-0.827241000	3.891351000	21.277300000
H	0.706964000	3.629692000	22.147657000
H	0.614759000	3.343773000	20.396338000
C	0.136630000	6.308851000	22.133565000
H	0.385382000	7.367564000	22.005364000
H	0.565347000	5.958703000	23.076742000
H	-0.948518000	6.211759000	22.226262000
B	3.402194000	4.848448000	15.816570000
H	6.858452000	5.804479000	15.746862000
H	6.631717000	3.163624000	19.144983000
H	0.833601000	4.677619000	12.721421000
H	0.659175000	8.223175000	15.155162000

Coordinates of compound **6-CH$_3$** (CPCM(cyclohexane))

Ge	4.429742000	4.004594000	4.716064000
Ge	7.394427000	3.806671000	7.059851000
Cl	9.360341000	4.856489000	7.151299000
O	4.632017000	3.344997000	7.713571000
O	7.208063000	6.520871000	4.323751000
C	3.327856000	3.701294000	7.419760000
C	0.752105000	4.391207000	6.785772000
H	-0.272044000	4.652995000	6.536557000
C	5.320842000	2.447840000	3.956289000
H	5.008999000	1.592174000	3.358240000
C	3.021348000	3.916279000	6.081271000
C	2.423867000	3.888089000	8.467302000
C	1.698442000	4.254398000	5.774811000
H	1.407935000	4.440088000	4.744040000
C	7.827771000	2.127071000	3.793476000
C	6.485999000	4.408467000	8.690054000
C	1.118379000	4.233288000	8.121638000
H	0.374604000	4.388992000	8.896404000
C	5.161279000	4.014292000	8.807699000
C	4.356824000	4.266252000	9.915428000
C	4.943660000	4.977640000	10.961927000
H	4.366565000	5.214737000	11.850029000
C	7.802028000	0.796946000	3.343118000
H	6.860870000	0.254849000	3.323660000

C	6.274799000	5.389194000	10.885488000
H	6.711480000	5.940655000	11.712987000
C	6.599080000	2.813392000	4.221959000
C	2.937947000	3.704091000	9.893122000
C	7.048060000	5.102025000	9.762146000
H	8.082479000	5.430810000	9.713284000
C	10.189611000	0.836601000	2.987198000
H	11.102305000	0.334292000	2.679686000
C	6.969409000	5.447841000	4.658717000
C	8.969212000	0.161284000	2.944400000
H	8.931738000	-0.870457000	2.605754000
C	9.062021000	2.788278000	3.841837000
H	9.109596000	3.810969000	4.207680000
C	2.033859000	4.375929000	10.926029000
H	2.429111000	4.219858000	11.933741000
H	1.033948000	3.933265000	10.905444000
H	1.945704000	5.452552000	10.746319000
C	10.231175000	2.152642000	3.437199000
H	11.176649000	2.685444000	3.482737000
C	3.010703000	2.187451000	10.201096000
H	3.653558000	1.667541000	9.485179000
H	2.008162000	1.748938000	10.149981000
H	3.414800000	2.031751000	11.207191000
B	6.554186000	4.132534000	5.166844000
C	7.816249000	1.906329000	7.277845000
H	6.890740000	1.331937000	7.168796000
H	8.531232000	1.581367000	6.519091000
H	8.231355000	1.743348000	8.275990000
C	3.795013000	5.245330000	3.328222000
H	4.590073000	5.411813000	2.596107000
H	2.929858000	4.821502000	2.808520000
H	3.506011000	6.203271000	3.770293000

Coordinates of compound **7-CH_3** (CPCM(cyclohexane))

Ge	4.634682000	4.907376000	17.447949000
Ge	1.299017000	5.360067000	15.586738000
Cl	4.229245000	5.210885000	14.157844000
O	1.880664000	4.829875000	18.513767000
O	3.969006000	3.006058000	17.080474000
C	4.073194000	5.170086000	19.298210000
C	4.937460000	5.494592000	20.348082000
H	6.012417000	5.506282000	20.185066000
C	2.048185000	1.145474000	15.611298000
C	3.048267000	5.839948000	21.817749000
H	2.673995000	6.114673000	22.798732000
C	1.524316000	0.495504000	14.486101000
H	1.162040000	1.088733000	13.650374000
C	-1.147026000	6.616791000	19.500728000
H	-1.689565000	6.931438000	20.386302000
C	4.425878000	5.827761000	21.598843000
H	5.099799000	6.088084000	22.409587000
C	2.154243000	5.500144000	20.802345000
C	-0.972260000	6.556693000	17.088984000
H	-1.372075000	6.833290000	16.116542000
C	-1.649837000	6.943663000	18.242989000
H	-2.574936000	7.507445000	18.164704000
C	0.036787000	5.889729000	19.627626000

C	0.684640000	5.528443000	18.446592000
C	0.638648000	5.416146000	20.948048000
C	2.544272000	0.373574000	16.670103000
H	2.946542000	0.861456000	17.550454000
C	2.705636000	5.168046000	19.566056000
C	2.048636000	2.623394000	15.654077000
C	0.226692000	5.843655000	17.171152000
C	3.167530000	3.416827000	16.167393000
C	1.003354000	3.411188000	15.285490000
H	0.071089000	2.941592000	14.968506000
C	1.975850000	-1.653000000	15.482572000
H	1.949595000	-2.737840000	15.433215000
C	1.488887000	-0.891906000	14.422270000
H	1.087055000	-1.380545000	13.539156000
C	2.499973000	-1.015350000	16.603610000
H	2.877727000	-1.602627000	17.435926000
C	0.255798000	3.927265000	21.144999000
H	-0.833272000	3.829731000	21.209175000
H	0.702448000	3.545526000	22.069623000
H	0.609532000	3.315143000	20.310159000
C	0.126285000	6.221108000	22.142269000
H	0.371601000	7.284192000	22.047948000
H	0.558369000	5.841889000	23.072606000
H	-0.958416000	6.117863000	22.234705000
B	3.340146000	4.968250000	15.795030000
C	6.581015000	4.779147000	17.357924000
H	6.947576000	4.049613000	18.086017000
H	6.882807000	4.479813000	16.351678000
H	7.024340000	5.755064000	17.581589000
C	0.623315000	6.394987000	14.062303000
H	1.234555000	6.181037000	13.181788000
H	-0.415845000	6.129442000	13.844461000
H	0.676876000	7.466638000	14.274963000

Coordinates of compound **6-H** (CPCM(cyclohexane))

Ge	-4.155683000	-3.840669000	-4.897050000
Ge	-7.223947000	-3.624661000	-7.097859000
Cl	-9.146712000	-4.736897000	-7.112031000
O	-4.456200000	-3.158803000	-7.857310000
O	-7.085949000	-6.163559000	-4.192187000
C	-3.159252000	-3.585811000	-7.630990000
C	-0.606446000	-4.447151000	-7.121780000
H	0.407472000	-4.781892000	-6.923736000
C	-4.943708000	-2.224893000	-4.155542000
H	-4.562477000	-1.360037000	-3.615077000
C	-2.810261000	-3.858106000	-6.314240000
C	-2.306821000	-3.781638000	-8.718153000
C	-1.502136000	-4.287621000	-6.068856000
H	-1.189100000	-4.524541000	-5.054816000
C	-7.426635000	-1.754808000	-3.961555000
C	-6.388702000	-4.113775000	-8.798558000
C	-1.012195000	-4.215297000	-8.435397000
H	-0.308184000	-4.383722000	-9.243848000
C	-5.056029000	-3.760580000	-8.952875000
C	-4.307597000	-3.999321000	-10.102885000

C	-4.964590000	-4.638166000	-11.153847000
H	-4.432597000	-4.859825000	-12.073500000
C	-7.313415000	-0.419661000	-3.540045000
H	-6.340157000	0.062665000	-3.536775000
C	-6.307650000	-4.998654000	-11.041771000
H	-6.799837000	-5.493354000	-11.873789000
C	-6.246552000	-2.529480000	-4.372912000
C	-2.862024000	-3.509846000	-10.113723000
C	-7.021645000	-4.736728000	-9.874799000
H	-8.063876000	-5.032712000	-9.795681000
C	-9.694480000	-0.302775000	-3.160783000
H	-10.570406000	0.261234000	-2.853412000
C	-6.774763000	-5.148169000	-4.624176000
C	-8.433910000	0.295326000	-3.143324000
H	-8.327986000	1.328634000	-2.824698000
C	-8.700543000	-2.337531000	-3.985799000
H	-8.818705000	-3.364355000	-4.323681000
C	-2.032487000	-4.181617000	-11.207524000
H	-2.451044000	-3.957702000	-12.192804000
H	-1.009446000	-3.795115000	-11.202794000
H	-1.998668000	-5.268611000	-11.079337000
C	-9.823336000	-1.621632000	-3.584242000
H	-10.800525000	-2.095064000	-3.609784000
C	-2.865917000	-1.979446000	-10.356166000
H	-3.448799000	-1.457252000	-9.592311000
H	-1.839748000	-1.597240000	-10.332046000
H	-3.303062000	-1.760611000	-11.336249000
B	-6.290991000	-3.900377000	-5.243689000
H	-3.617036000	-4.795448000	-3.813209000
H	-7.663382000	-2.153039000	-7.164845000

Coordinates of compound **7-H** (CPCM(cyclohexane))

Ge	4.615374000	4.900058000	17.450781000
Ge	1.298353000	5.346573000	15.602008000
Cl	4.222690000	5.214369000	14.146114000
O	1.875514000	4.827761000	18.516662000
O	3.976870000	3.008619000	17.066068000
C	4.069085000	5.160133000	19.298197000
C	4.939519000	5.482128000	20.344038000
H	6.013743000	5.484947000	20.176527000
C	2.060473000	1.138285000	15.586582000
C	3.053336000	5.843893000	21.814759000
H	2.682979000	6.124036000	22.795663000
C	1.521309000	0.495170000	14.464733000
H	1.143281000	1.092635000	13.639150000
C	-1.144819000	6.630854000	19.496829000
H	-1.686412000	6.952187000	20.380556000
C	4.430703000	5.822364000	21.593786000
H	5.107209000	6.080483000	22.402952000
C	2.154254000	5.506055000	20.802849000
C	-0.970963000	6.560540000	17.084642000
H	-1.366568000	6.833309000	16.109210000
C	-1.646848000	6.953558000	18.237420000
H	-2.569584000	7.520693000	18.156917000
C	0.036507000	5.900445000	19.628569000

C	0.681925000	5.530688000	18.449332000
C	0.638066000	5.432577000	20.951433000
C	2.578198000	0.361443000	16.631188000
H	2.992377000	0.843654000	17.509139000
C	2.701781000	5.165854000	19.567808000
C	2.056417000	2.615389000	15.639722000
C	0.224233000	5.842805000	17.173596000
C	3.172494000	3.410799000	16.150774000
C	1.007040000	3.403396000	15.281586000
H	0.072622000	2.937182000	14.968902000
C	2.000674000	-1.658314000	15.436919000
H	1.979762000	-2.742821000	15.379131000
C	1.492228000	-0.891773000	14.390736000
H	1.078898000	-1.375626000	13.510376000
C	2.540033000	-1.027047000	16.554283000
H	2.934999000	-1.618810000	17.375268000
C	0.246677000	3.947499000	21.159684000
H	-0.842789000	3.857277000	21.227140000
H	0.693052000	3.569963000	22.086120000
H	0.594661000	3.326926000	20.328656000
C	0.133095000	6.249876000	22.140408000
H	0.385433000	7.310512000	22.037804000
H	0.564219000	5.874479000	23.072678000
H	-0.952073000	6.154472000	22.235085000
B	3.342293000	4.962234000	15.774600000
H	6.151367000	4.790684000	17.425884000
H	0.739009000	6.161365000	14.425172000

Optimization of compound **6**.

On the basis of the molecular structure of **6** determined in the solid state the structure was optimized using the program Orca 6.0.1[36-42] along with BP86,[43, 44] Grimme´s dispersion correction and Becke-Johnson damping (D3BJ) with suitable RI approximations (RI/ RIJCOSX).[29] The basis sets employed were def2-TZVP for Ge, B as implemented in ORCA 5.0.3, and def2-SVP on all other elements.[32, 34, 45, 46] For all calculations, tight or very tight convergence criteria were applied for optimization and SCF convergence, respectively. Analyses of the electronic structures were performed using NBO7, plots were generated using ChemCraft.[47, 48]

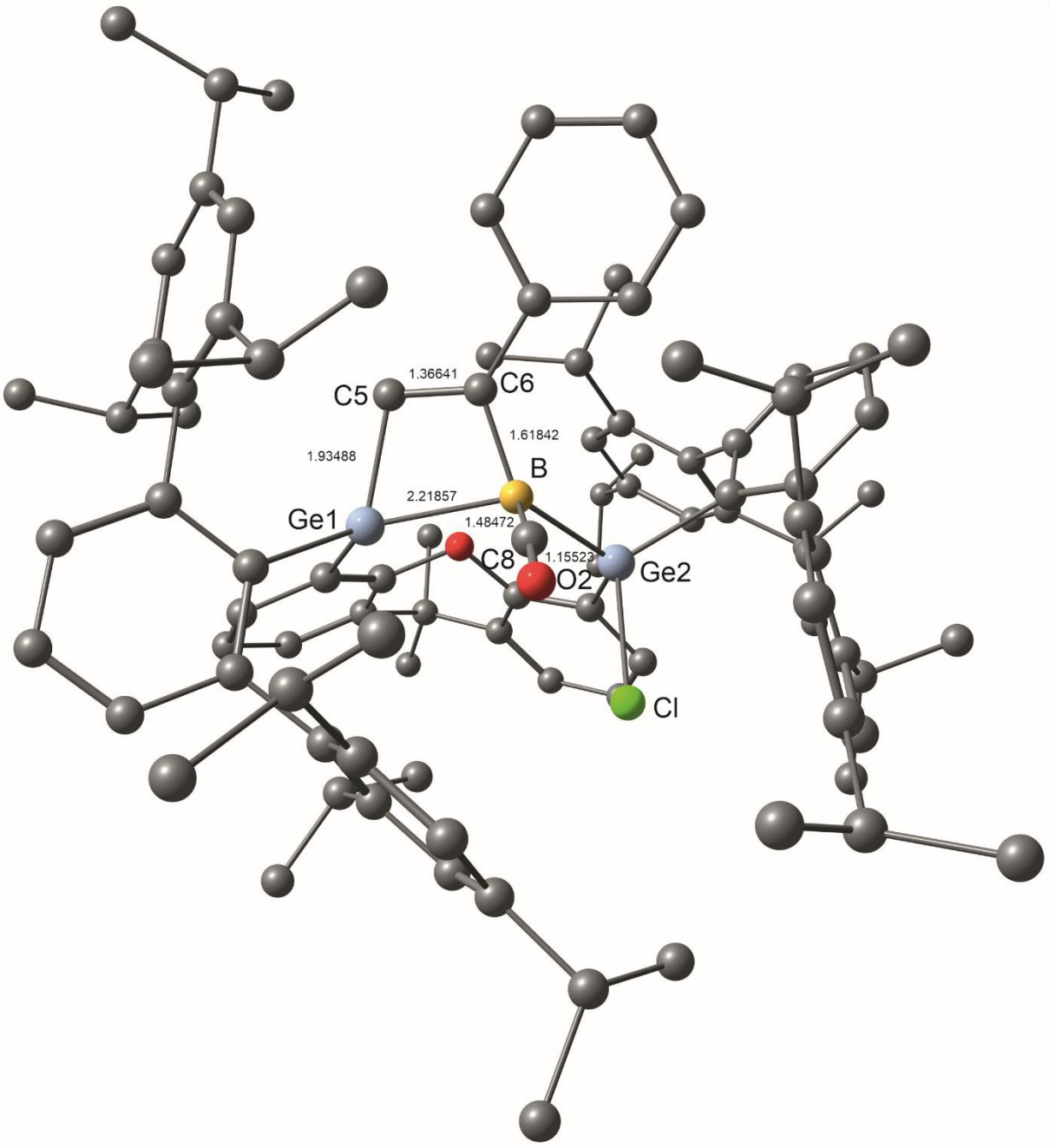

Figure S59. Optimized structure **6**, distances in Å.

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Coordinates from ORCA-job bp86optfreq_hnumac E -8516.143914952969

Ge	4.59027897589753	4.27856063951734	4.68932463387493
Ge	7.52835349483331	4.48403013012415	7.08443373488437
Cl	7.55344193608939	6.71089010583732	7.04908219145154
O	4.68653230687753	3.32507062372266	7.54662102327992
O	7.57216563147691	6.20432720096791	3.76772086253215
C	11.64043909484761	3.30894791022948	6.55041275546109
H	12.53372389460269	3.70791273486342	6.04804812554113
C	3.38419564491771	3.73334841336404	7.28874678094977
C	2.42344735035721	7.34179453727054	2.71964350327397
H	2.25067893572923	8.42121336522914	2.84522375058444
C	0.83189825106437	4.62774597853926	6.71960135822431
H	-0.18446122756334	4.98180309166704	6.49152222002975
C	5.24111603845617	2.53664100934332	4.15463914315108
H	4.76017601374577	1.65317032204352	3.70998852496402
C	3.12477557164494	4.20519242610602	6.00088399775872
C	5.37704416661246	9.03157186126998	5.84714027328729
H	5.31850045656856	9.32935048563762	6.90453718758865
C	11.65399788856693	2.02216708323414	7.09551290181639
H	12.54241077780376	1.38075632944176	6.99374420262955
C	2.43744455454891	3.73689772872583	8.32981410926947
C	1.87749210753836	5.23475294187197	1.66066200008188
H	1.28642155085737	4.64740174657011	0.94159204834146
C	1.58066514502657	6.58327021551628	1.89567168129123
H	0.72317385432141	7.05786845635373	1.39487174659573
C	10.76379850418795	7.90143234055399	6.40186028141734
H	10.80351628188881	8.76810210530028	7.07741303469356
C	1.81786895443076	4.65064699155484	5.72260494601807
H	1.57712085387743	5.05533401796602	4.72936543832887
C	6.35296160967273	9.60799630515974	5.02136877971372
C	6.39485963476727	9.20730883671589	3.67668574308267
H	7.14872946082582	9.66310376045173	3.01705341923553
C	5.50710173690193	8.25637626111136	3.14644467270791
C	7.61620462718678	1.72996463122573	4.00542319740961
C	2.93911154990988	4.60607223177426	2.34433949989660
C	3.97391628683533	0.53566018618023	1.24864626823820
C	7.29963098211240	10.67977492378031	5.54152532382948
H	8.09019913171983	10.80939150058265	4.77055151599550
C	10.49312866379828	4.12654562183412	6.63243841427976
C	6.47633474822759	4.32845974430214	8.73539045117682
C	4.52691876641740	7.68200138182622	4.00767480400781
C	1.14504584915611	4.19012703265741	8.01857475917799
H	0.37150830012586	4.21423315543838	8.79902183444569
C	3.71752948339962	5.35111484430993	3.27233600249102
C	10.64214790127354	6.61586954243244	6.94418225411461
C	10.98889431767500	4.55275650166448	3.67663828197033
H	10.87945170303704	3.60290564311797	4.22975483617853
C	3.52446551705866	6.75472070228327	3.37916378551565
C	5.17846319263855	3.81763327941462	8.74915817687630
C	5.66370861132348	0.29675965415265	6.77003967158776
H	5.31155033334482	-0.62382700278551	7.28037552466911
H	5.59857196370869	0.10936052079418	5.68027984246823
H	4.97421257257103	1.12612573359620	7.01172687037679
C	4.45789221635255	8.08537460916116	5.36413805589645
C	6.44604787552294	0.58797107040741	9.60240554678430
H	5.61142254214372	-0.07344834786221	9.32823805026721
C	4.79146187068764	1.62251909041638	0.89441773224749
H	5.71493325737227	1.42151032449987	0.33217196023539
C	9.33275877361426	3.65377626358853	7.31312193313438
C	10.59680910346187	5.50085678723881	6.05519929482360
C	6.56480856274576	12.02689206320464	5.68521605701115
H	6.10366711483900	12.33810391193965	4.72616366122357
H	7.25942025782385	12.82855271971733	6.01309243788004
H	5.75248841076180	11.95217241983670	6.43837424568926
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B	6.75301474730504	4.11610466899003	5.15649936332235

References

1. R. H. Kern, M. Schneider, K. Eichele, H. Schubert, H. F. Bettinger and L. Wesemann, *Angew. Chem., Int. Ed.*, 2023, **62**, e202301593.
2. R. K. Harris, E. D. Becker, S. M. C. d. Menezes, R. Goodfellow and P. Granger, *Pure Appl. Chem.*, 2001, **73**, 1795-1818.
3. L. J. Farrugia, *J. Appl. Crystallogr.*, 1997, **30**, 565.
4. L. J. Farrugia, *J. Appl. Crystallogr.*, 1999, **32**, 837-838.
5. L. J. Farrugia, *J. Appl. Crystallogr.*, 2012, **45**, 849-854.
6. C. B. Hübschle, G. M. Sheldrick and B. Dittrich, *J. Appl. Crystallogr.*, 2011, **44**, 1281-1284.
7. G. M. Sheldrick, *Program for crystal-structure refinement. University of Gottingen, Germany.*, 1997.
8. G. M. Sheldrick, *Acta Cryst., Sect. A*, 2008, **64**, 112-122.
9. G. M. Sheldrick, *Journal*, 1996.
10. S. Grimme, A. Hansen, S. Ehlert and J.-M. Mewes, *J. Chem. Phys.*, 2021, **154**, 064103.
11. J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew and J. Sun, *The Journal of Physical Chemistry Letters*, 2020, **11**, 8208-8215.
12. J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew and J. Sun, *The Journal of Physical Chemistry Letters*, 2020, **11**, 9248-9248.
13. E. Caldeweyher, C. Bannwarth and S. Grimme, *J. Chem. Phys.*, 2017, **147**, 034112.
14. E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth and S. Grimme, *J. Chem. Phys.*, 2019, **150**, 154122.
15. H. Kruse and S. Grimme, *J. Chem. Phys.*, 2012, **136**, 154101.
16. S. Grimme, *Chem.-Eur. J.*, 2012, **18**, 9955-9964.
17. V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995-2001.
18. C. Riplinger and F. Neese, *J. Chem. Phys.*, 2013, **138**, 034106.
19. C. Riplinger, B. Sandhoefer, A. Hansen and F. Neese, *J. Chem. Phys.*, 2013, **139**, 134101.
20. C. Riplinger, P. Pinski, U. Becker, E. F. Valeev and F. Neese, *J. Chem. Phys.*, 2016, **144**, 024109.
21. G. Santra, N. Sylvetsky and J. M. L. Martin, *J. Phys. Chem. A*, 2019, **123**, 5129-5143.
22. S. Grimme, *J. Chem. Phys.*, 2006, **124**.
23. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
24. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
25. P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627.
26. Y. Zhao and D. G. J. T. C. A. Truhlar, *Theor. Chem. Account*, 2008, **120**, 215-241.
27. J.-D. Chai and M. Head-Gordon, *J. Chem. Phys.*, 2008, **128**.
28. N. Mardirossian and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2014, **16**, 9904-9924.
29. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
30. W. Hujo and S. Grimme, *J. Chem. Theo. Comp.*, 2011, **7**, 3866-3871.
31. O. A. Vydrov and T. Van Voorhis, *J. Chem. Phys.*, 2010, **133**, 244103.
32. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
33. F. Weigend, M. Häser, H. Patzelt and R. Ahlrichs, *Chem. Phys. Lett.*, 1998, **294**, 143-152.
34. F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065.
35. F. Weigend, *J. Comput. Chem.*, 2008, **29**, 167-175.
36. F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2018, **8**, e1327.
37. F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2012, **2**, 73-78.
38. F. Neese, *WIREs Comput Mol Sci.*, 2022, **12**, e1606.
39. F. Neese, *J. Comput. Chem.*, 2003, **24**, 1740-1747.
40. D. Bykov, T. Petrenko, R. Izsák, S. Kossmann, U. Becker, E. Valeev and F. Neese, *Mol. Phys.*, 2015, **113**, 1961-1977.
41. F. Neese, *J. Comput. Chem.*, 2023, **44**, 381-396.

42. F. Neese, F. Wennmohs, U. Becker and C. Riplinger, *J. Chem. Phys.*, 2020, **152**, 224108.
43. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.
44. J. P. Perdew and W. Yue, *Phys. Rev. B*, 1986, **33**, 8800-8802.
45. B. Metz, H. Stoll and M. Dolg, *J. Chem. Phys.*, 2000, **113**, 2563-2569.
46. D. Andrae, U. Häussermann, M. Dolg, H. Stoll and H. Preuß, *Theoret. Chim. Acta*, 1990, **77**, 123-141.
47. G. A. Zhurko, *CHEMCRAFT (http://www.chemcraftprog.com)*.
48. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis and F. Weinhold, NBO 7.0, 2018.