

Supporting Information

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Tetrylidyne Coordination Modes: Vinyl-Type Germa-Ruthena Anion [Ru=Ge:]⁻ and its Reaction with Monofluorobenzene

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Experimental

General information. All manipulations were performed under argon (99.999 %) atmosphere using standard Schlenk techniques or an MBraun glovebox. Additionally, the argon for Schlenk techniques is dried through SICAPENT®. All solvents were degassed via three “freeze-pump-thaw” cycles and dried with various methods. *n*-Hexane and *n*-pentane were obtained from an MBRAUN solvent purification system (SPS). Diethyl ether, tetrahydrofuran and toluene were obtained from a MBraun solvent purification system (SPS) and analogous to benzene-*d*₆ and toluene-*d*₈ distilled from a Na/K alloy. Benzene, benzene-*d*₆ and *o*-difluorobenzene were dried over activated aluminium oxide. [Ar*GeCl]₂ and [(Ph₃P)ClRuGeCl₂(C₆H₃-2- η^6 -Trip)-6-Trip)] were synthesized according to literature procedures.^{1, 2} Commercially purchased chemicals (*sigma aldrich*, *abcr* and *apollo scientific*) were used as received. All air and moisture sensitive chemicals were stored under argon atmosphere.

NMR spectroscopy. NMR spectra were recorded using one of the following spectrometers with the respective equipment:

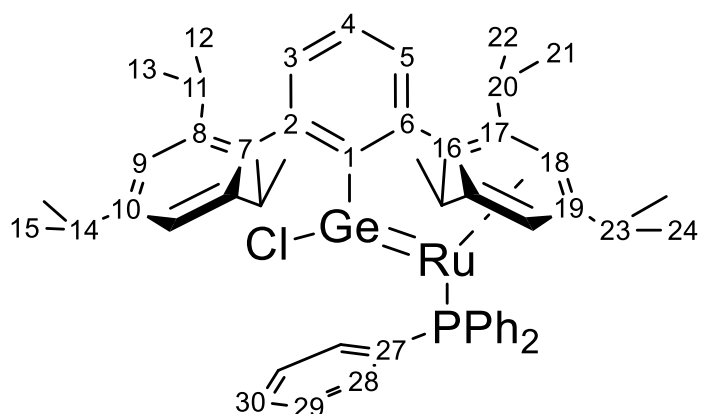
- Bruker Avance III HD 300 NanoBay Spectrometer, 5 mm BBFO ATM probe head, operating at 300.13 (¹H), 75.47 (¹³C), 282.40 (¹⁹F) and 121.49 (³¹P) MHz.
- Bruker AVII+400, 5 mm H-1,X+F-19 BBFO ATM head (Quad Systems), operating at 400.11 (¹H), 100.61 (¹³C), 376.48 (¹⁹F) and 161.97 (³¹P) MHz.
- Bruker AVII+500, 5 mm TBO probe head operating at 500.13 (¹H) MHz.
- Bruker Avance III HDX 600, 5 mm Prodigy BBO Cryo probe head, operating at 600.13 (¹H), 150.92 (¹³C), 564.63 (¹⁹F) MHz.
- Bruker Avance III HDX 700, 5 mm TXI probe head operating at 700.29 (¹H), 176.09 (¹³C) MHz.

Chemical shifts are reported as δ in ppm relative to the following external standards: Me₄Si (¹H, ¹³C), BF₃·Et₂O (¹¹B), CCl₃F (¹⁹F), 85% H₃PO₄ (³¹P).³ The chemical shifts were referenced using the chemical shift of the solvents ²H resonance frequency as followed: $\Xi = 25.145020$ % for ¹³C, $\Xi = 94.094011$ % for ¹⁹F, $\Xi = 40.480742$ for ³¹P.³ The multiplicity of the signals is abbreviated as s = singlet, d = doublet, t = triplet, sept = septet and m = multiplet or br = broad/unresolved. The proton and carbon signals were assigned via detailed analysis of ¹H, ¹³C{¹H} UDEFT, ¹³C{¹H} DEPT135, ¹³C{¹⁹F}, ¹H-¹H COSY, ¹H-¹³C HSQC and ¹H-¹³C HMBC NMR spectra.

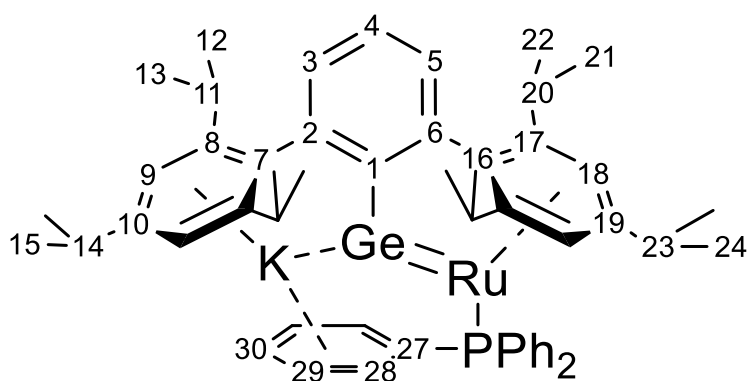
Crystal structure determination. X-ray data were collected with a Bruker Smart APEX II diffractometer with graphite monochromated Mo-K α radiation. Programs used were Bruker APEX2 v2011.8-0 including SADABS for absorption correction, SAINT for data reduction, SHELXS for structure solution and SHELXL or WinGX suite of programs v1.70.01 including SHELXL for structure refinement.⁴⁻¹⁰

UV/Vis spectroscopy. The absorption spectrum was recorded on a PerkinElmer *Lambda 35* spectrophotometer in 1 cm quartz cuvettes sealed by Teflon stoppers or Teflon lined screw caps.

Elemental analysis. The elemental analysis was performed at the Department for Inorganic Chemistry at the University of Tübingen using a vario MICRO CUBE or UNICUBE by *elementar*.

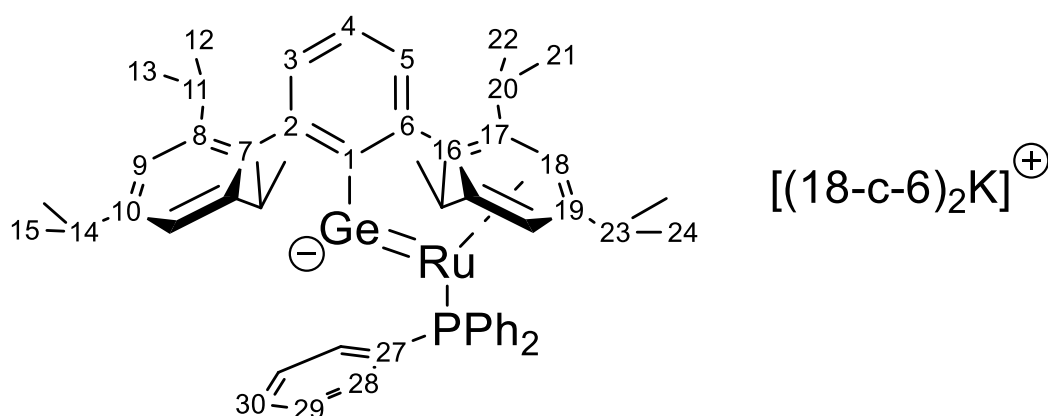
Compound 2: Ar*GeClRuPPh₃

To a mixture of Ar*GeCl₂RuClPPh₃·0.5 C₇H₈ (0.500 g, 0.468 mmol, 1.0 eq.) and KC₈ (168 mg, 1.24 mmol, 2.7 eq.) benzene (4 ml) was added at room temperature. After stirring the reaction mixture for 90 minutes the volatiles were removed under reduced pressure from the blue suspension. The product was extracted with benzene (2 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with frozen benzene (2 ml). The product was crystallized from a highly saturated benzene solution at room temperature to yield Ar*GeClRuPPh₃ · 2 C₆H₆ (0.431 g, 0.388 mmol, 83 %) as blue crystals suitable for X-ray diffraction. **Characterization:** **¹H-NMR** (400.11 MHz, C₆D₆, 300.00 K): δ = 0.74 (d, 6H, ³J_{H-H} = 6.8 Hz, H-24), 1.19 (d, 6H, ³J_{H-H} = 6.8 Hz, H-12), 1.23 (d, 6H, ³J_{H-H} = 6.9 Hz, H-15), 1.25 (d, 6H, ³J_{H-H} = 6.8 Hz, H-21), 1.34 (d, 6H, ³J_{H-H} = 6.8 Hz, H-22), 1.36 (d, 6H, ³J_{H-H} = 6.8 Hz, H-13), 1.62 (sept, 1H, ³J_{H-H} = 6.8 Hz, H-23), 2.46 (sept, 2H, ³J_{H-H} = 6.7 Hz, H-20), 2.83 (sept, 1H, ³J_{H-H} = 6.4 Hz, H-14), 2.93 (sept, 2H, ³J_{H-H} = 6.9 Hz, H-11), 5.31 (s, 2H, H-18), 6.96 (m, 3H, H-30), 7.04 (m, 6H, H-29), 7.14 (m, 1H, H-3), 7.15 (s, 2H, H-9), 7.18 (m, 1H, H-4), 7.74 (m, 1H, H-5), 7.82 (m, 6H, H-28) ppm. **¹³C{¹H}-NMR** (100.61 MHz, C₆D₆, 300.00 K): δ = 22.8 (s, C-24), 23.5 (s, C-13), 24.1 (s, C-15), 24.4 (s, C-22), 24.5 (s, C-12), 26.5 (s, C-21), 30.2 (s, C-20), 30.5 (s, C-23), 30.9 (s, C-11), 34.5 (s, C-14), 73.8 (s, C-18), 98.0 (d, J_{P-C} = 9.9 Hz, C-16), 110.3 (s, C-19), 115.7 (d, J_{P-C} = 3.8 Hz, C-17), 120.4 (s, C-9), 126.7 (s, C-4), 126.8 (s, C-5), 127.0 (d, ³J_{P-C} = 9.4 Hz, C-29), 128.3 (d, ⁴J_{P-C} = 5.3 Hz, C-30), 130.5 (s, C-3), 134.2 (d, ²J_{P-C} = 12.9 Hz, C-28), 136.8 (s, C-7), 139.2 (s, C-6), 141.0 (d, ¹J_{P-C} = 38.3 Hz, C-27), 141.8 (s, C-2), 145.7 (s, C-8), 147.9 (s, C-10), 172.2 (d, ³J_{P-C} = 16.5 Hz, C-1) ppm. **³¹P{¹H}-NMR** (161.97 MHz, C₆D₆, 300.00 K): δ = 56.0 (s) ppm. **UV-Vis** (n-pentane, c = 10.8 μmol · l⁻¹): λ (nm) [ε (l · mol⁻¹ · cm⁻¹)]: 309 [88237], 622 [21800]. **Elemental analysis** calculated for C₅₄H₆₄ClGePRu (%): C 68.04, H 6.77 Found: C 68.55, H 6.42

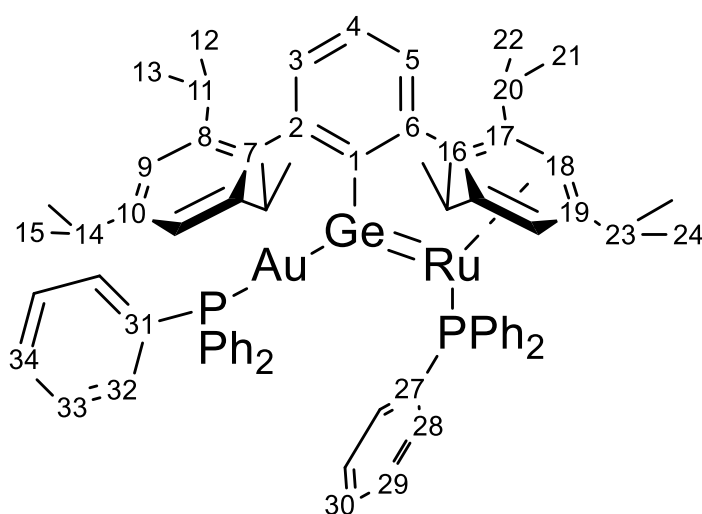
Compound **3a**: Ar*GeKRuPPh₃

To a mixture of Ar*GeCl₂RuClPPh₃ (0.456 g, 0.445 mmol, 1.0 eq.) and KC₈ (302 mg, 2.23 mmol, 5.0 eq.) thf (9 ml) was added at room temperature. After stirring the reaction mixture for one hour the volatiles were removed under reduced pressure from the dark green suspension. The product was extracted with pentane (10 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with pentane (5 times 2 ml) and frozen benzene (3 times 2 ml). The product was crystallized from a concentrated toluene solution at -40 °C to yield Ar*GeKRuPPh₃ · 0.5 C₇H₈ (0.387 g, 0.193 mmol, 87 %) as dark green crystals suitable for X-ray diffraction. **Characterization:** **¹H-NMR** (400.11 MHz, C₆D₆, 300.00 K): δ = 0.85 (d, 6H, ³J_{H-H} = 6.7 Hz, H-12), 0.88 (d, 6H, ³J_{H-H} = 6.9 Hz, H-15), 0.99 (d, 6H, ³J_{H-H} = 6.9 Hz, H-24), 1.07 (d, 6H, ³J_{H-H} = 6.9 Hz, H-13), 1.31 (d, 6H, ³J_{H-H} = 7.0 Hz, H-22), 1.60 (d, 6H, ³J_{H-H} = 6.8 Hz, H-21), 2.36 (sept, 1H, ³J_{H-H} = 6.8 Hz, H-23), 2.43 (sept, 1H, ³J_{H-H} = 6.9 Hz, H-14), 2.85 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-20), 3.23 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-14), 5.17 (s, 2H, H-18), 6.65 (s, 2H, H-9), 6.86 (m, 3H, H-30), 7.05 (m, 6H, H-29), 7.14 (m, 1H, H-3), 7.27 (m, 1H, H-4), 8.14 (m, 6H, H-28), 8.15 (m, 1H, H-5) ppm. **¹³C{¹H}-NMR** (100.61 MHz, C₆D₆, 300.00 K): δ = 23.0 (s, C-12), 23.9 (s, C-13), 23.9 (s, C-24), 24.1 (s, C-15), 25.4 (s, C-22), 26.9 (s, C-21), 30.1 (s, C-11), 30.3 (s, C-20), 32.8 (s, C-23), 33.7 (s, C-14), 73.9 (s, C-18), 103.1 (d, J_{P-C} = 12.6 Hz, C-16), 106.9 (s, C-19), 112.3 (d, J_{P-C} = 3.7 Hz, C-17), 118.4 (s, C-9), 123.5 (s, C-4), 125.6 (d, ³J_{P-C} = 8.4 Hz, C-29), 126.2 (s, C-30), 126.3 (s, C-3), 128.3 (s, C-5), 135.2 (d, ²J_{P-C} = 12.9 Hz, C-28), 140.5 (s, C-2), 144.9 (s, C-6), 145.6 (s, C-10), 145.9 (s, C-7), 146.7 (d, ¹J_{P-C} = 26.8 Hz, C-27), 148.6 (s, C-8), 181.9 (d, ³J_{P-C} = 16.5 Hz, C-1) ppm. **³¹P{¹H}-NMR** (161.97 MHz, C₆D₆, 300.00 K): δ = 54.6 (s) ppm. **UV-Vis** (n-pentane, c = 12.5 μmol · l⁻¹): λ (nm) [ε (l · mol⁻¹ · cm⁻¹)]: 366 [37819], 598 [13962]. **Elemental analysis** calculated for C₅₄H₆₄GeKRu + 0.5 C₇H₈(%): C 68.86, H 6.83 Found: C 69.00, H 6.44.

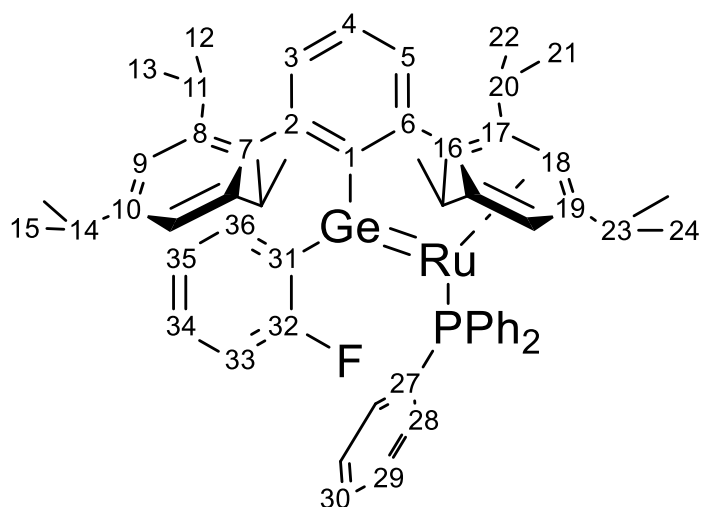
Compound **3b**: [Ar*GeRuPPh₃][K(18-c-6)₂]



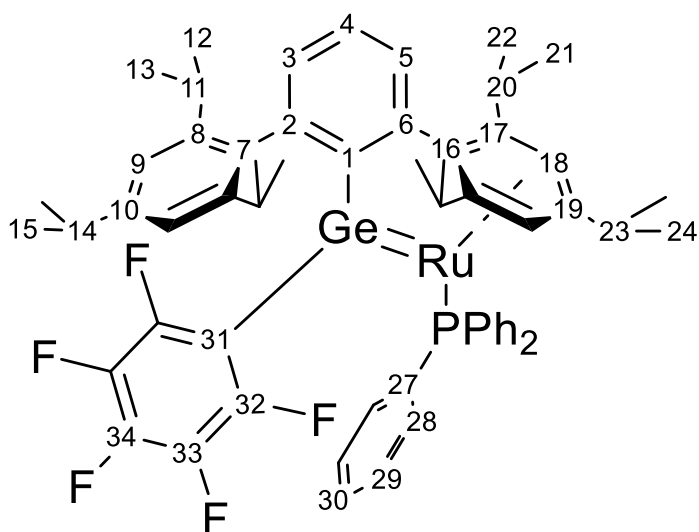
To a mixture of Ar*GeRuPPh₃ (36.2.0 mg, 37.8 μ mol, 1.0 eq.) and 18-c-6 (20.0 mg, 75.7 μ mol, 2.0 eq.) benzene (4 ml) was added at room temperature. After stirring the reaction mixture for 90 minutes the volatiles were removed under reduced pressure from the dark green suspension. The product was extracted with benzene (2 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with frozen benzene (2 ml). The product was crystallized from a saturated toluene solution at -40 $^{\circ}$ C to yield [Ar*GeRuPPh₃][K(18-c-6)₂] (51.0 mg, 34.3 μ mol, 91 %) as dark green crystals suitable for X-ray diffraction. **¹H-NMR** (400.11 MHz, C₆D₆, 300.00 K): δ = 0.94 (d, 6H, ³J_{H-H} = 6.8 Hz, H-24), 1.30 (d, 6H, ³J_{H-H} = 7.5 Hz, H-12), 1.31 (d, 6H, ³J_{H-H} = 7.0 Hz, H-15), 1.37 (d, 6H, ³J_{H-H} = 6.9 Hz, H-13), 1.41 (d, 6H, ³J_{H-H} = 7.0 Hz, H-21), 1.68 (d, 6H, ³J_{H-H} = 6.8 Hz, H-22), 1.73 (sept, 1H, ³J_{H-H} = 6.7 Hz, H-23), 2.89 (sept, 1H, ³J_{H-H} = 7.0 Hz, H-14), 3.13 (s, 48H, H-18-c-6), 3.17 (sept, 2H, ³J_{H-H} = 6.9 Hz, H-20), 3.66 (sept, 2H, ³J_{H-H} = 6.9 Hz, H-11), 5.21 (s, 2H, H-18), 7.02 (m, 3H, H-30), 7.10 (s, 2H, H-9), 7.17 (m, 6H, H-29), 7.36 (m, 1H, H-3), 7.48 (m, 1H, H-4), 8.31 (m, 1H, H-5), 8.48 (m, 6H, H-28) ppm. **¹³C{¹H}-NMR** (100.61 MHz, C₆D₆, 300.00 K): δ = 23.6 (s, C-24), 23.7 (s, C-12), 24.3 (s, C-15), 24.6 (s, C-13), 25.2 (s, C-21), 27.5 (s, C-22), 30.4 (s, C-11), 30.5 (s, C-20), 31.3 (s, C-23), 34.5 (s, C-14), 70.2 (s, C-18-c-6), 73.6 (s, C-18), 104.5 (d, ¹J_{P-C} = 12.8 Hz, C-16), 106.3 (s, C-19), 109.9 (s, C-17), 119.2 (s, C-9), 122.2 (s, C-4), 125.6 (s, C-30), 125.8 (d, ³J_{P-C} = 7.2 Hz, C-29), 127.5 (s, C-3), 127.9 (s, C-5), 135.3 (d, ²J_{P-C} = 12.9 Hz, C-28), 143.5 (s, C-6), 143.9 (s, C-2), 144.2 (s, C-7), 144.3 (s, C-10), 146.6 (s, C-8), 148.2 (d, ¹J_{P-C} = 21.8 Hz, C-27), 183.5 (d, ³J_{P-C} = 17.0 Hz, C-1) ppm. **³¹P{¹H}-NMR** (161.97 MHz, C₆D₆, 300.00 K): δ = 48.8 (s) ppm. **Elemental analysis** calculated for C₇₈H₁₁₂GeKO₁₂PRu (%): C 63.07, H 7.60 Found: C 63.45, H 7.15.

Compound 4: Ar*Ge(AuPPh₃)RuPPh₃

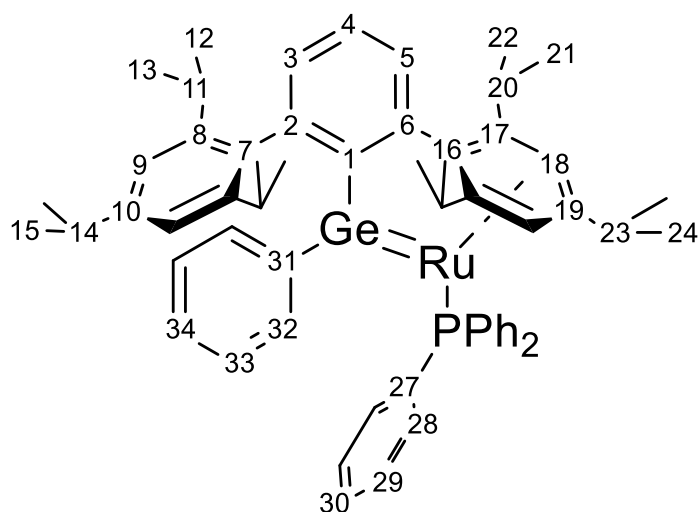
A mixture of Ar*GeKRuPPh₃ (50.2 mg, 52.5 μmol, 1.0 eq.) and AuCl(PPh₃) (27.0 mg, 54.6 μmol, 1.0 eq.) in benzene (1.0 ml) was stirred at room temperature for 40 minutes. The volatiles were removed under reduced pressure from the green suspension. The product was extracted with benzene (0.5 ml), the volatiles were removed under reduced pressure and the solid is coevaporated with frozen benzene (1 ml). The product was crystallized from a concentrated toluene solution at -40 °C to yield Ar*Ge(AuPPh₃)RuPPh₃ (13.8 mg, 10.0 μmol, 19 %) as green crystals suitable for X-ray diffraction. **¹H-NMR** (400.11 MHz, C₆D₆, 300.00 K): δ = 0.80 (d, 6H, ³J_{H-H} = 6.7 Hz, H-24), 0.81 (d, 6H, ³J_{H-H} = 6.5 Hz, H-15), 1.26 (d, 6H, ³J_{H-H} = 6.9 Hz, H-12), 1.40 (d, 6H, ³J_{H-H} = 6.9 Hz, H-21), 1.43 (d, 6H, ³J_{H-H} = 6.9 Hz, H-13), 1.48 (d, 6H, ³J_{H-H} = 6.7 Hz, H-22), 1.57 (sept, 1H, ³J_{H-H} = 6.8 Hz, H-23), 2.03 (sept, 1H, ³J_{H-H} = 6.7 Hz, H-14), 2.83 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-20), 3.36 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-11), 5.19 (br. s, 2H, H-18), 6.85 (m, 3H, H-30), 6.89 (m, 6H, H-29), 6.92 (m, 6H, H-32), 6.96 (m, 6H, H-33), 6.96 (s, 2H, H-9), 7.02 (m, 3H, H-34), 7.15 (m, 1H, H-3), 7.35 (m, 1H, H-4), 8.04 (m, 6H, H-28), 8.05 (m, 1H, H-5) ppm. **¹³C{¹H}-NMR** (100.61 MHz, C₆D₆, 300.00 K): δ = 23.2 (s, C-24), 23.5 (s, C-15), 23.8 (s, C-13), 24.4 (s, C-12), 24.7 (s, C-21), 27.1 (s, C-22), 30.2 (s, C-23), 30.5 (s, C-20), 30.5 (s, C-11), 33.0 (s, C-14), 73.4 (br. s, C-18), 103.0 (s, C-16), 109.7 (s, C-19), 112.9 (br. s, C-17), 120.5 (s, C-9), 124.9 (s, C-4), 126.3 (d, ³J_{P-C} = 9.0 Hz, C-29), 127.3 (s, C-5), 127.4 (m (overlapping with solvent signal), C-30), 128.2 (d, ³J_{P-C} = 10.3 Hz, C-33), 129.9 (s, C-3), 130.1 (d, ⁴J_{P-C} = 1.6 Hz, C-34), 131.7 (d, ¹J_{P-C} = 40.5 Hz, C-31), 134.5 (d, ²J_{P-C} = 14.5 Hz, C-32), 135.0 (d, ²J_{P-C} = 12.8 Hz, C-28), 141.3 (s, C-6), 141.7 (s, C-7), 143.4 (s, C-2), 144.4 (d, ¹J_{P-C} = 32.1 Hz, C-27), 145.3 (s, C-10), 145.7 (s, C-8), 181.8 (s, C-1) ppm. **³¹P{¹H}-NMR** (161.97 MHz, C₆D₆, 300.00 K): δ = 46.9 (d, ⁴J_{P-P} = 6.3 Hz, P-31), 55.7 (d, ⁴J_{P-P} = 7.7 Hz, P-27) ppm. **UV-Vis** (*n*-pentane, c = 8.71 μmol · l⁻¹): λ (nm) [ε (l · mol⁻¹ · cm⁻¹)]: 351 [111435], 620 [14321]. EA calculated for C₇₂H₇₉AuGeP₂Ru (%): C 62.80, H 5.78 Found: C 62.89, H 5.43.

Compound 5: Ar*Ge(C₆H₄F)RuPPh₃

To a mixture of Ar*GeKRuPPh₃ (50.0 mg, 52.3 μmol, 1.0 eq.) and 18-c-6 (13.8 mg, 52.3 μmol, 1.0 eq.) in benzene (0.5 ml) *o*-difluorobenzene (0.50 ml, 579 mg, 5.07 mmol, 97.1 eq.) was added at room temperature. After stirring the reaction mixture for 60 minutes the volatiles were removed under reduced pressure from the green suspension. The product was extracted with benzene (0.5 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with frozen benzene (1 ml). The product was crystallized from a concentrated diethylether solution at -40 °C to yield Ar*Ge(C₆H₄F)RuPPh₃ (44.1 mg, 43.5 μmol, 83 %) as green crystals suitable for X-ray diffraction. **¹H-NMR** (400.11 MHz, C₆D₆, 300.00 K): δ = 0.77 (d, 6H, ³J_{H-H} = 6.8 Hz, H-24), 1.05 (d, 6H, ³J_{H-H} = 6.8 Hz, H-12), 1.15 (d, 6H, ³J_{H-H} = 6.9 Hz, H-15), 1.28 (d, 6H, ³J_{H-H} = 6.8 Hz, H-13), 1.36 (d, 6H, ³J_{H-H} = 6.8 Hz, H-21), 1.44 (d, 6H, ³J_{H-H} = 6.9 Hz, H-22), 1.66 (sept, 1H, ³J_{H-H} = 6.8 Hz, H-23), 2.65 (sept, 1H, ³J_{H-H} = 6.8 Hz, H-14), 2.67 (br. m, 2H, H-20), 2.98 (sept, 2H, ³J_{H-H} = 6.7 Hz, H-11), 5.33 (br. s, 2H, H-18), 6.14 (m, 1H, H-36), 6.20 (m, 1H, H-35), 6.20 (m, 1H, H-33), 6.51 (m, 1H, H-34), 6.76 (s, 2H, H-9), 6.93 (m, 3H, H-30), 6.96 (m, 6H, H-29), 7.20 (m, 1H, H-3), 7.26 (m, 1H, H-4), 7.69 (m, 6H, H-28), 7.90 (m, 1H, H-5) ppm. **¹³C{¹H}-NMR** (100.61 MHz, C₆D₆, 300.00 K): δ = 22.4 (s, C-13), 22.8 (s, C-24), 23.9 (s, C-15), 24.2 (s, C-22), 25.9 (s, C-12), 26.7 (s, C-21), 30.3 (s, C-20), 30.3 (s, C-11), 30.5 (s, C-23), 34.2 (s, C-14), 73.9 (br. s, C-18), 100.7 (d, *J*_{P-C} = 10.6 Hz, C-16), 109.9 (s, C-19), 113.8 (d, ²*J*_{F-C} = 26.1 Hz, C-33), 114.9 (d, *J*_{P-C} = 4.0 Hz, C-17), 119.9 (s, C-9), 122.5 (d, ⁴*J*_{F-C} = 1.8 Hz, C-35), 125.4 (s, C-4), 126.6 (d, ³*J*_{P-C} = 10.1 Hz, C-29), 127.1 (s, C-5), 127.7 (m (overlapping with solvent signal), C-34), 127.8 (m (overlapping with solvent signal), C-30), 130.9 (s, C-3), 132.9 (d, ³*J*_{F-C} = 9.6 Hz, C-36), 134.1 (d, ²*J*_{P-C} = 12.9 Hz, C-28), 137.0 (d, ²*J*_{F-C} = 36.5 Hz, C-31), 138.1 (s, C-7), 140.8 (s, C-6), 141.9 (s, C-2), 142.2 (d, ¹*J*_{P-C} = 36.2 Hz, C-27), 145.4 (s, C-8), 146.7 (s, C-10), 160.5 (d, ¹*J*_{F-C} = 234.7 Hz, C-32), 172.2 (s, C-1) ppm. **¹⁹F{¹H}-NMR** (376.48 MHz, C₆D₆, 300.00 K): δ = -97.0 (d, ⁵*J*_{P-F} = 2.5 Hz) ppm. **³¹P{¹H}-NMR** (161.97 MHz, C₆D₆, 300.00 K): δ = 54.9 (d, ⁵*J*_{P-F} = 2.5 Hz) ppm. **UV-Vis** (n-pentane, c = 11.8 μmol · l⁻¹): λ (nm) [ε (l · mol⁻¹ · cm⁻¹)]: 378 [54559], 620 [17742]. **Elemental analysis** calculated for C₆₀H₆₈FGePRu (%): C 71.15, H 6.77 Found: C 70.07, H 6.67.

Compound **6**: Ar*Ge(C₆F₅)RuPPh₃

To a mixture of Ar*GeKRuPPh₃ (102 mg, 106 μmol, 1.0 eq.) and hexafluorobenzene (20.0 mg, 106 μmol, 1.0 eq.) benzene (1.0 ml) was added at room temperature. After stirring the reaction mixture for 5 minutes the volatiles were removed under reduced pressure from the green suspension. The product was extracted with benzene (0.5 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with frozen benzene (1 ml). The product Ar*Ge(C₆F₅)RuPPh₃ (110 mg, 101 μmol, 95 %) was obtained as green solid and crystals suitable for X-ray diffraction were obtained from a mixture of toluene and hexane. **¹H-NMR** (300.13 MHz, C₆D₆, 300.00 K): δ = 0.71 (d, 6H, ³J_{H-H} = 6.7 Hz, H-24), 1.01 (d, 6H, ³J_{H-H} = 6.8 Hz, H-12), 1.22 (d, 6H, ³J_{H-H} = 6.9 Hz, H-15), 1.31 (d, 6H, ³J_{H-H} = 6.7 Hz, H-21), 1.32 (d, 6H, ³J_{H-H} = 6.5 Hz, H-13), 1.43 (d, 6H, ³J_{H-H} = 6.7 Hz, H-22), 1.61 (sept, 1H, ³J_{H-H} = 6.6 Hz, H-23), 2.62 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-20), 2.90 (sept, 2H, H-11), 2.75 (sept, 1H, ³J_{H-H} = 6.9 Hz, H-14), 5.22 (br. s, 2H, H-18), 6.90 (s, 2H, H-9), 6.90 (m, 3H, H-30), 6.93 (m, 6H, H-29), 7.22 (m, 1H, H-3), 7.23 (m, 1H, H-4), 7.66 (m, 6H, H-28), 7.83 (m, 1H, H-5) ppm. **¹³C{¹H}-NMR** (75.47 MHz, C₆D₆, 300.00 K): δ = 21.8 (d, J = 4.9 Hz, C-13), 22.8 (s, C-24), 23.6 (s, C-15), 24.3 (s, C-22), 26.2 (s, C-12), 26.5 (s, C-21), 30.2 (s, C-20), 30.4 (s, C-23), 30.5 (s, C-11), 34.0 (s, C-14), 74.2 (br. s, C-18), 99.9 (d, J_{P-C} = 10.2 Hz, C-16), 110.0 (s, C-19), 116.0 (d, J_{P-C} = 3.8 Hz, C-17), 119.7 (s, C-9), 120.1 (s, C-31), 125.7 (s, C-4), 126.7 (d, ³J_{P-C} = 9.3 Hz, C-29), 127.1 (s, C-5), 128.2 (m (overlapping with solvent signal), C-30), 131.6 (s, C-3), 134.0 (d, ²J_{P-C} = 12.7 Hz, C-28), 136.3 (d, ¹J_{F-C} = 247.1 Hz, C-33), 137.9 (s, C-7), 140.2 (d, ¹J_{F-C} = 247.2 Hz, C-34), 140.7 (s, C-2), 141.1 (d, ¹J_{P-C} = 37.2 Hz, C-27), 141.4 (s, C-6), 142.7 (d, ¹J_{F-C} = 234.1 Hz, C-32), 145.8 (d, C-8), 147.6 (s, C-10), 171.7 (s, C-1) ppm. **¹⁹F{¹H}-NMR** (282.40 MHz, C₆D₆, 300.00 K): δ = -162.5 (m, F-33), -156.8 (t, ³J_{F-F} = 20.6 Hz, F-34), -123.3 (m, F-32) ppm. **³¹P{¹H}-NMR** (121.49 MHz, C₆D₆, 300.00 K): δ = 51.7 (t, ⁵J_{F-P} = 3.7 Hz) ppm. **UV-Vis** (*n*-pentane, c = 11.1 μmol · l⁻¹): λ (nm) [ε (l · mol⁻¹ · cm⁻¹)]: 364 [69030], 618 [20855]. **Elemental analysis** calculated for C₆₀H₆₄F₅GePRu (%): C 66.43, H 5.95 Found: C 66.48, H 5.66.

Compound 7: Ar*Ge(C₆H₅)RuPPh₃

To a mixture of Ar*GeKRuPPh₃ (21.1 mg, 22.1 μmol, 1.0 eq.), 18-c-6 (10.5 mg, 39.7 μmol, 1.8 eq.), and fluorobenzene (0.05 ml, 529 μmol, 24.0 eq.) and benzene (0.5 ml) was added at room temperature. After stirring the reaction mixture for 3 days the volatiles were removed under reduced pressure from the green suspension. The product was extracted with benzene (0.5 ml), the volatiles were removed under reduced pressure and the solid was coevaporated with frozen benzene (1 ml). The product Ar*Ge(C₆H₅)RuPPh₃ (20.2 mg, 22.1 μmol, 92 %) was obtained as green solid. **Characterization:** ¹H-NMR (600.13 MHz, C₆D₆, 300.00 K): δ = 0.83 (d, 6H, ³J_{H-H} = 6.8 Hz, H-24), 1.09 (d, 6H, ³J_{H-H} = 6.2 Hz, H-12), 1.10 (d, 6H, ³J_{H-H} = 6.4 Hz, H-13), 1.26 (d, 6H, ³J_{H-H} = 6.9 Hz, H-15), 1.39 (d, 6H, ³J_{H-H} = 6.7 Hz, H-21), 1.46 (m, 1H, H-23), 1.47 (d, 1H, ³J_{H-H} = 6.9 Hz, H-22), 2.66 (sept, 2H, ³J_{H-H} = 6.7 Hz, H-20), 2.78 (sept, 1H, ³J_{H-H} = 6.9 Hz, H-14), 2.95 (sept, 2H, ³J_{H-H} = 6.8 Hz, H-11), 5.31 (br. s, 2H, H-18), 6.44 (m, 2H, H-32), 6.57 (m, 2H, H-33), 6.68 (m, 1H, H-34), 6.89 (s, 2H, H-9), 6.95 (m, 3H, H-30), 6.98 (m, 6H, H-29), 7.12 (m, 1H, H-3), 7.25 (m, 1H, H-4), 7.73 (m, 6H, H-28), 7.90 (m, 1H, H-5) ppm. ¹³C{¹H}-NMR (150.90 MHz, C₆D₆, 300.00 K): δ = 22.8 (s, C-13), 23.1 (s, C-24), 24.1 (s, C-15), 24.7 (s, C-22), 25.2 (s, C-12), 26.7 (s, C-21), 30.3 (s, C-23), 30.4 (s, C-20), 30.4 (s, C-11), 34.3 (s, C-14), 74.3 (br. s, C-18), 100.3 (d, J_{P-C} = 10.3 Hz, C-16), 109.9 (s, C-19), 114.6 (d, J_{P-C} = 3.6 Hz, C-20), 120.3 (s, C-9), 125.4 (s, C-34), 125.5 (s, C-4), 126.3 (s, C-33), 126.6 (d, ³J_{P-C} = 9.0 Hz, C-29), 127.0 (s, C-5), 127.9 (m (overlapping with solvent signal), C-30), 130.5 (s, C-3), 130.9 (s, C-32), 134.3 (d, ³J_{P-C} = 12.7 Hz, C-28), 139.1 (s, C-7), 140.8 (s, C-2), 142.0 (d, ²J_{P-C} = 35.7 Hz, C-27), 142.2 (s, C-6), 145.6 (s, C-8), 147.3 (s, C-10), 152.6 (s, C-31), 172.7 (s, C-1) ppm. ³¹P{¹H}-NMR (161.97 MHz, C₆D₆, 300.00 K): δ = 54.9 (s) ppm.

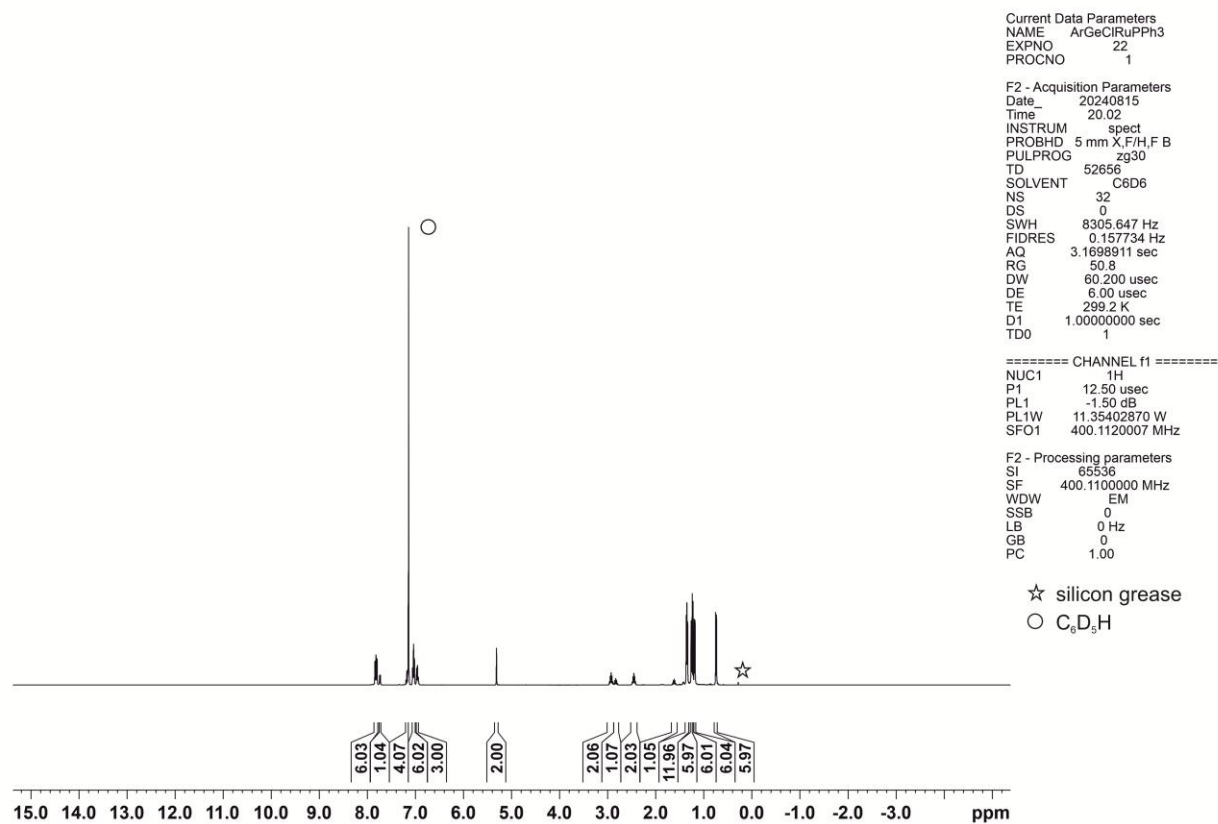
Data of crystal structure determinations

Table S11. Crystal structure refinement tables of **2**, **3a**, **3b**, **4**, **5** and **6**.

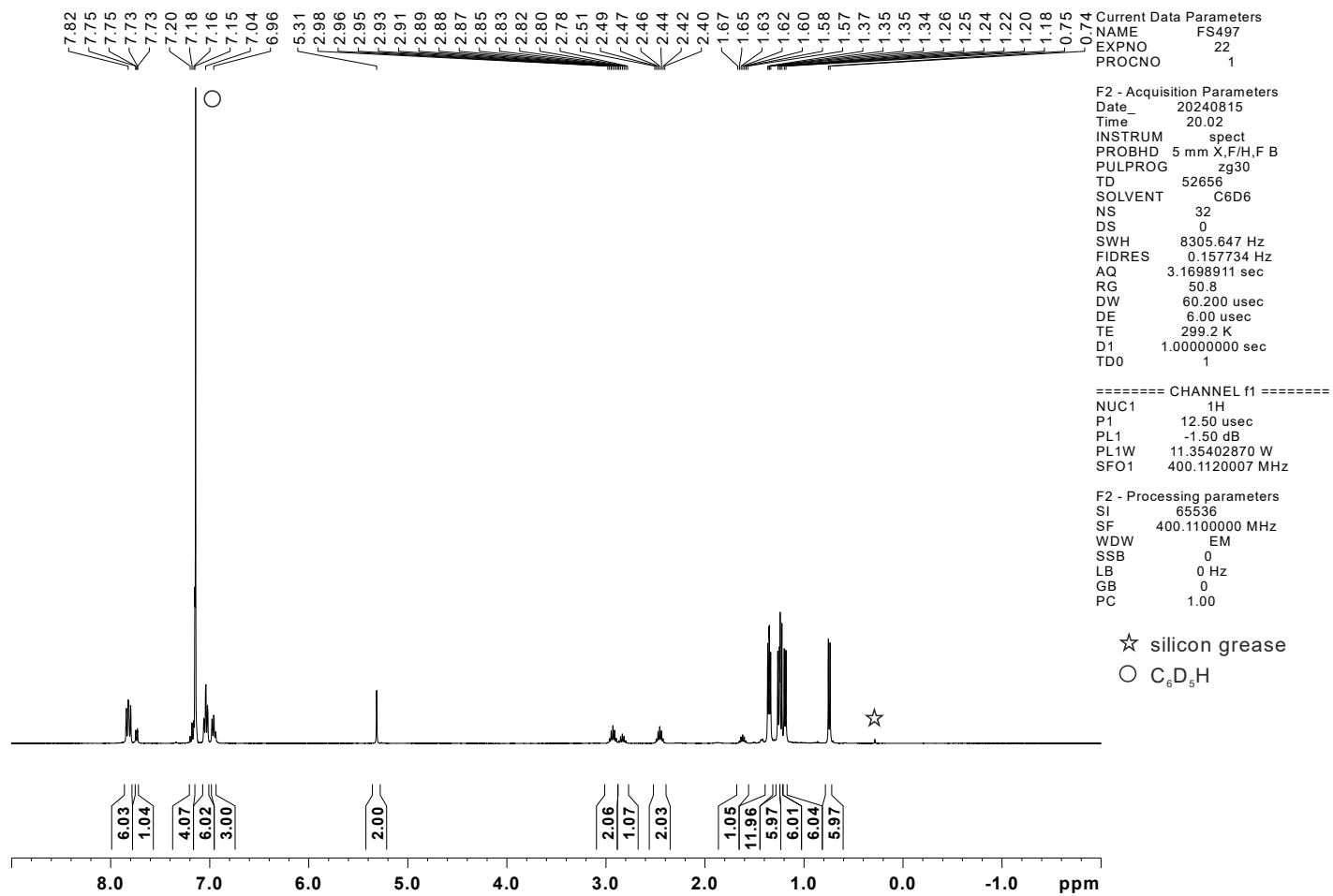
	2	3a	3b	4	5	6
Empirical formula	C ₅₄ H ₆₄ ClGePRu · 2 (C ₆ H ₆)	2 (C ₅₄ H ₆₄ GeKPRu) · C ₇ H ₈	C ₇₈ H ₁₁₂ GeKO ₁₂ PRu	2 (C ₇₂ H ₇₉ AuGeP ₂ Ru) · C ₇ H ₈	C ₆₀ H ₆₈ FGePRu	C ₆₀ H ₆₄ F ₅ GePRu
M _r / g mol ⁻¹	1109.34	2005.69	1485.40	2845.96	1012.77	1084.74
l / Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
T / K	100(2)	120(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triklin	monoclinic	triclinic	monoclinic	triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	Cc	<i>P</i> $\bar{1}$	<i>Pn</i>	<i>P</i> $\bar{1}$
Z	2	1	4	1	2	2
a / Å	12.4809(4)	13.1931(8)	18.1537(5)	12.5095(3)	13.0284(3)	12.9143(3)
b / Å	14.0176(5)	13.6074(8)	18.4660(4)	13.2731(4)	12.3512(3)	14.1030(4)
c / Å	17.7133(7)	15.3277(10)	23.0398(6)	21.4516(8)	17.2539(4)	16.5775(4)
a / °	91.403(2)	87.493(2)	90	89.463(2)	90	67.9240(10)
b / °	90.159(2)	77.894(2)	95.8450(10)	82.266(2)	111.9910(10)	75.6280(10)
g / °	113.144(2)	85.863(2)	90	65.4790(10)	90	68.5030(10)
V / Å ³	2848.46(18)	2682.3(3)	7683.4(3)	3206.83(17)	2574.43(11)	2581.82(12)
D _c / g cm ⁻³	1.293	1.242	1.284	1.474	1.306	1.395
m / mm ⁻¹	0.907	0.983	0.720	3.072	0.949	0.962
F(000)	1160	1046	3144	1442	1056	1120
Crystal size / mm	0.30 x 0.28 x 0.25	0.29 x 0.25 x 0.24	0.299 x 0.223 x 0.184	0.385 x 0.236 x 0.180	0.31 x 0.29 x 0.28	0.28 x 0.26 x 0.22
q range / °	1.580 - 28.560	1.501 - 27.142	1.753 - 25.348	1.689 - 26.449	1.649 - 30.519	1.337 - 30.550
Limiting indices	-16 ≤ h ≤ 16 -18 ≤ k ≤ 18 -23 ≤ l ≤ 23	-16 ≤ h ≤ 16 -17 ≤ k ≤ 17 -18 ≤ l ≤ 19	-21 ≤ h ≤ 21 -22 ≤ k ≤ 22 -27 ≤ l ≤ 27	-15 ≤ h ≤ 15 -15 ≤ k ≤ 16 -26 ≤ l ≤ 26	-18 ≤ h ≤ 18 -17 ≤ k ≤ 17 -24 ≤ l ≤ 24	-18 ≤ h ≤ 18 -20 ≤ k ≤ 20 -23 ≤ l ≤ 23
Reflects. collect.	159303	52111	113396	39031	95127	127602
Indepdnt Reflects	14309	11540	13931	13145	15122	15724
R _{int}	0.0225	0.0694	0.0403	0.0377	0.0248	0.0420
Completeness	0.985	0.971	1.000	0.993	0.994	0.993
Absorp. Corr.	multi-scan	multi-scan	multi-scan	numerical	multi-scan	multi-scan
Trans.(min., max.)	0.6942, 0.7457	0.5981, 0.7455	0.7710, 0.8403	0.6680, 0.9215	0.7075, 0.7461	0.6958, 0.7461
Parameters/restraints	643/0	617/193	836/1206	770/122	571/2	625/0
R ₁ , wR ₂ [I > 2s(I)]	0.0248, 0.0610	0.0853, 0.1844	0.0536, 0.1332	0.0377, 0.0713	0.0241, 0.0597	0.0261, 0.0608
R ₁ , wR ₂ (all data)	0.0268, 0.0626	0.1250, 0.1981	0.0563, 0.1353	0.0563, 0.0767	0.0252, 0.0605	0.0344, 0.0640
Goof on F ²	1.025	1.131	1.035	1.057	1.026	1.025
Dr _{max,min} / e · Å ⁻³	1.879, -0.619	1.183, -1.662	1.204, -1.445	2.303, -1.352	0.904, -0.812	0.973, -0.382
Flack parameter	-	-	0.016(16)	-	0.0049(15)	-
CCDC	2512268	2512263	2512267	2512264	2512265	2512266

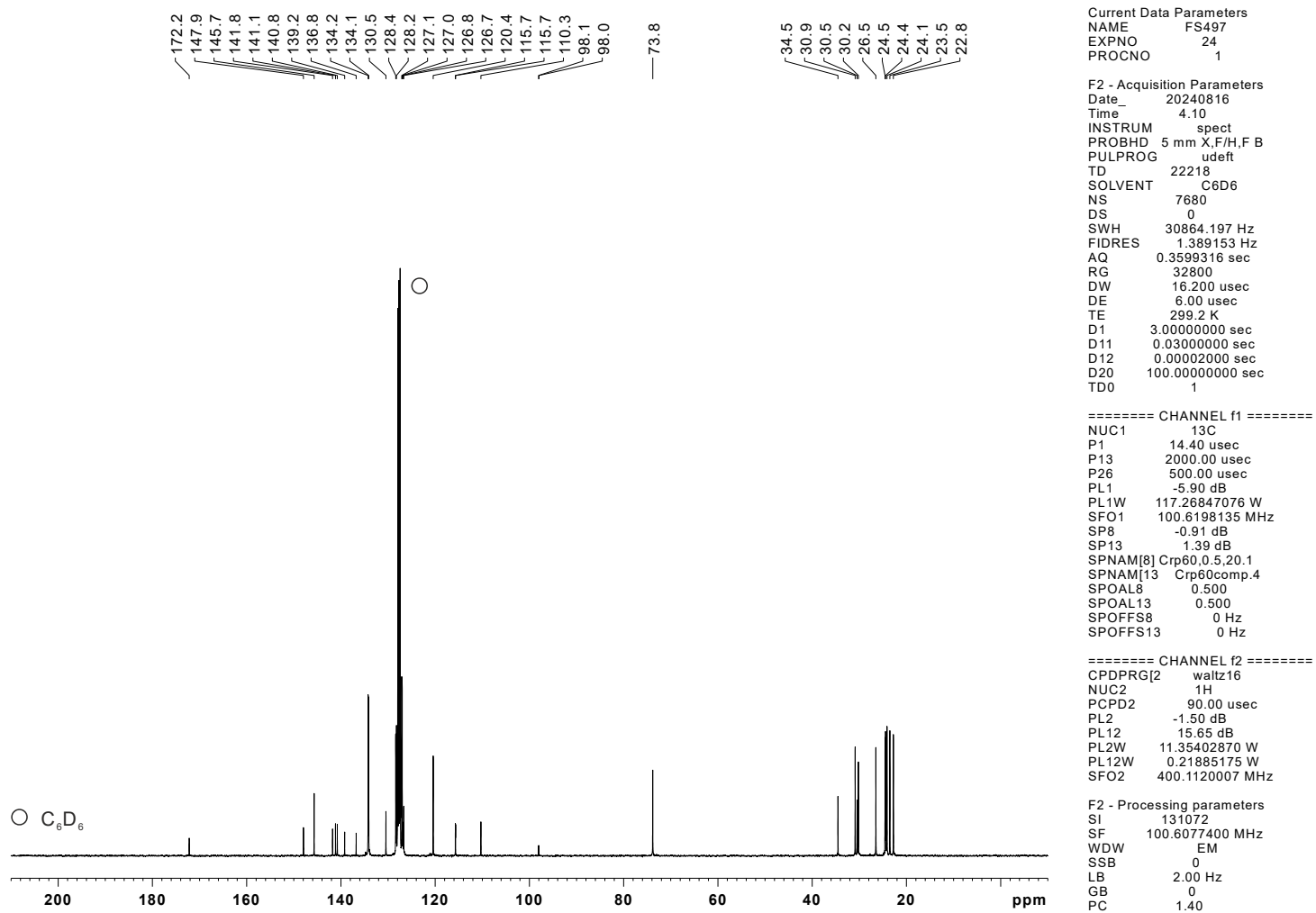
NMR spectroscopy

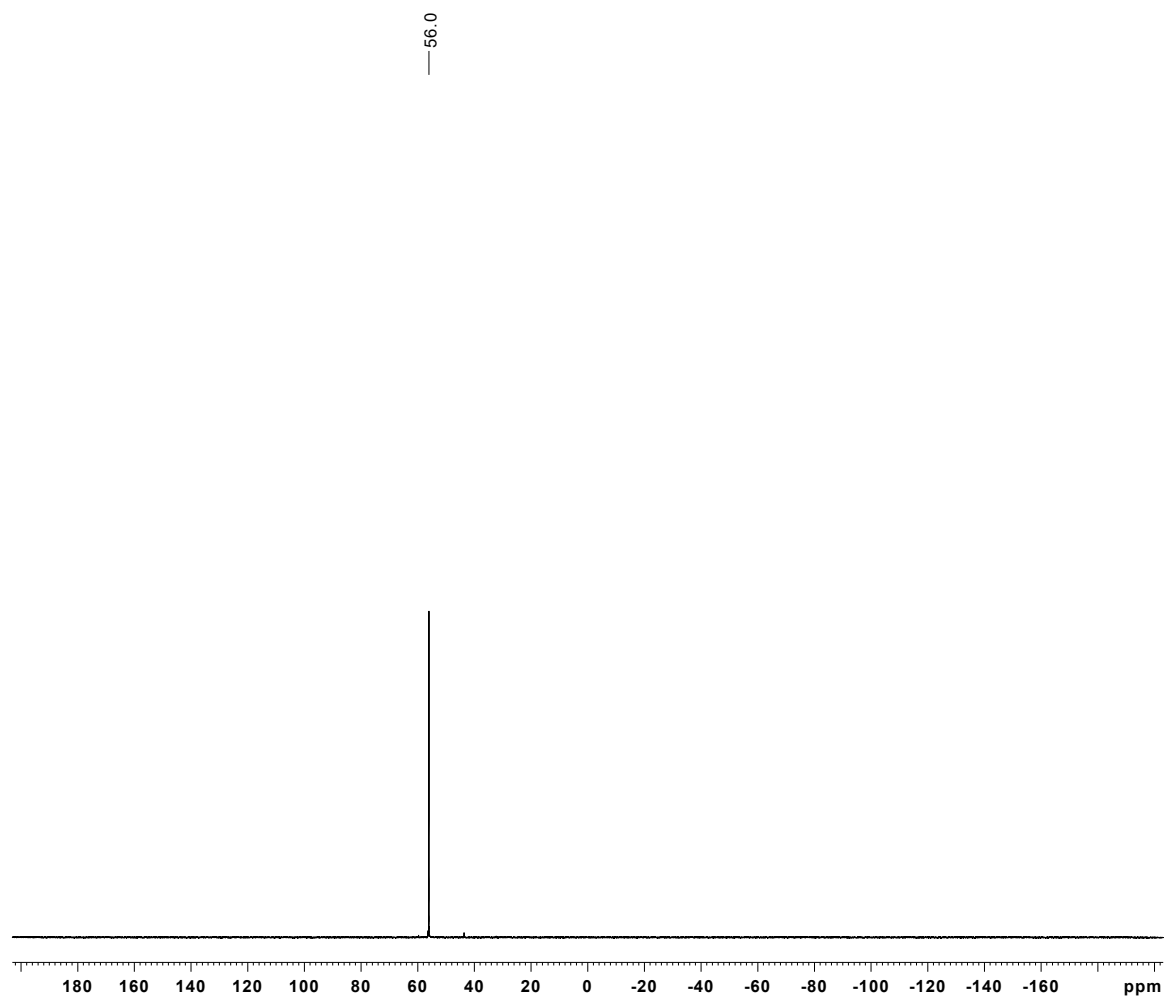
NMR spectra of compound **2**.



NMR Figure S11. ¹H NMR spectrum (-5 – 15 ppm) of compound **2**.

Figure S12. ¹H NMR spectrum of compound 2.

Figure S13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2**.



Current Data Parameters
NAME FS497
EXPNO 23
PROCNO 1

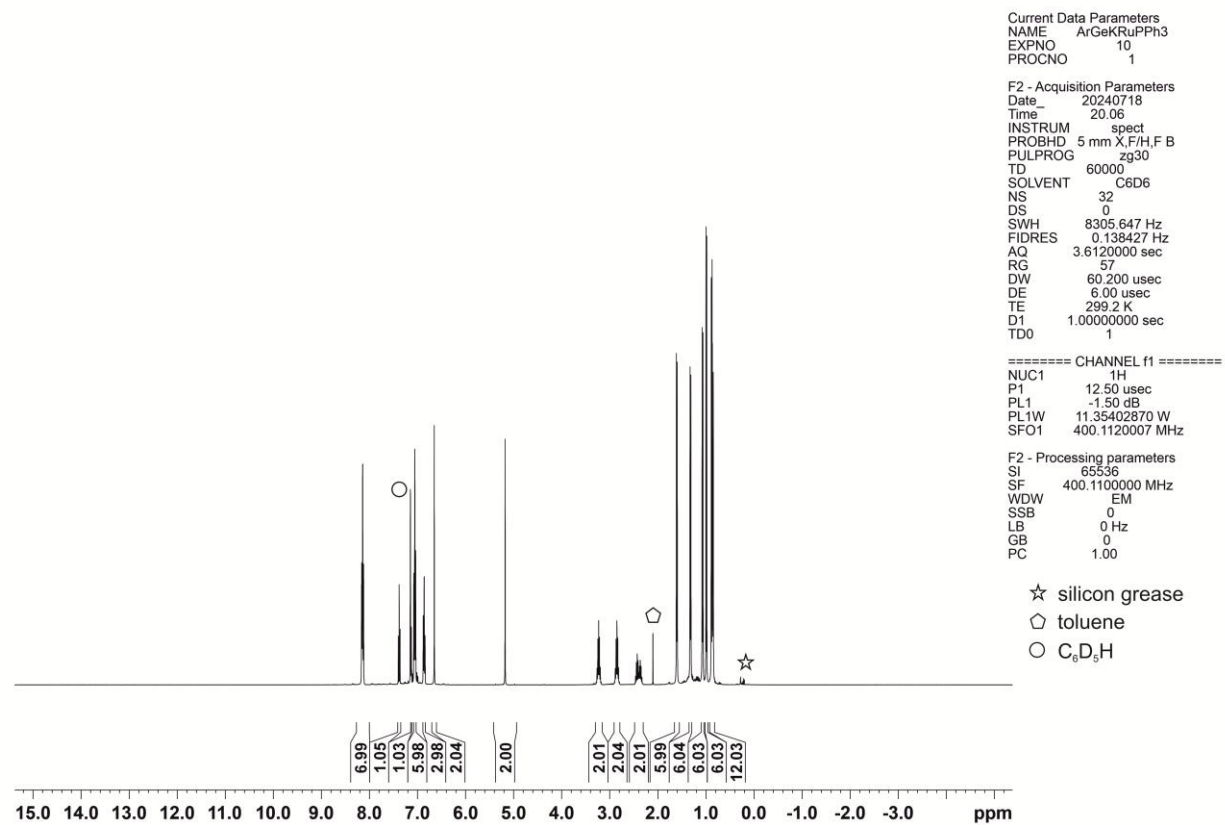
F2 - Acquisition Parameters
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Time 20.10
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PULPROG zgig30b
TD 88150
SOLVENT C6D6
NS 256
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

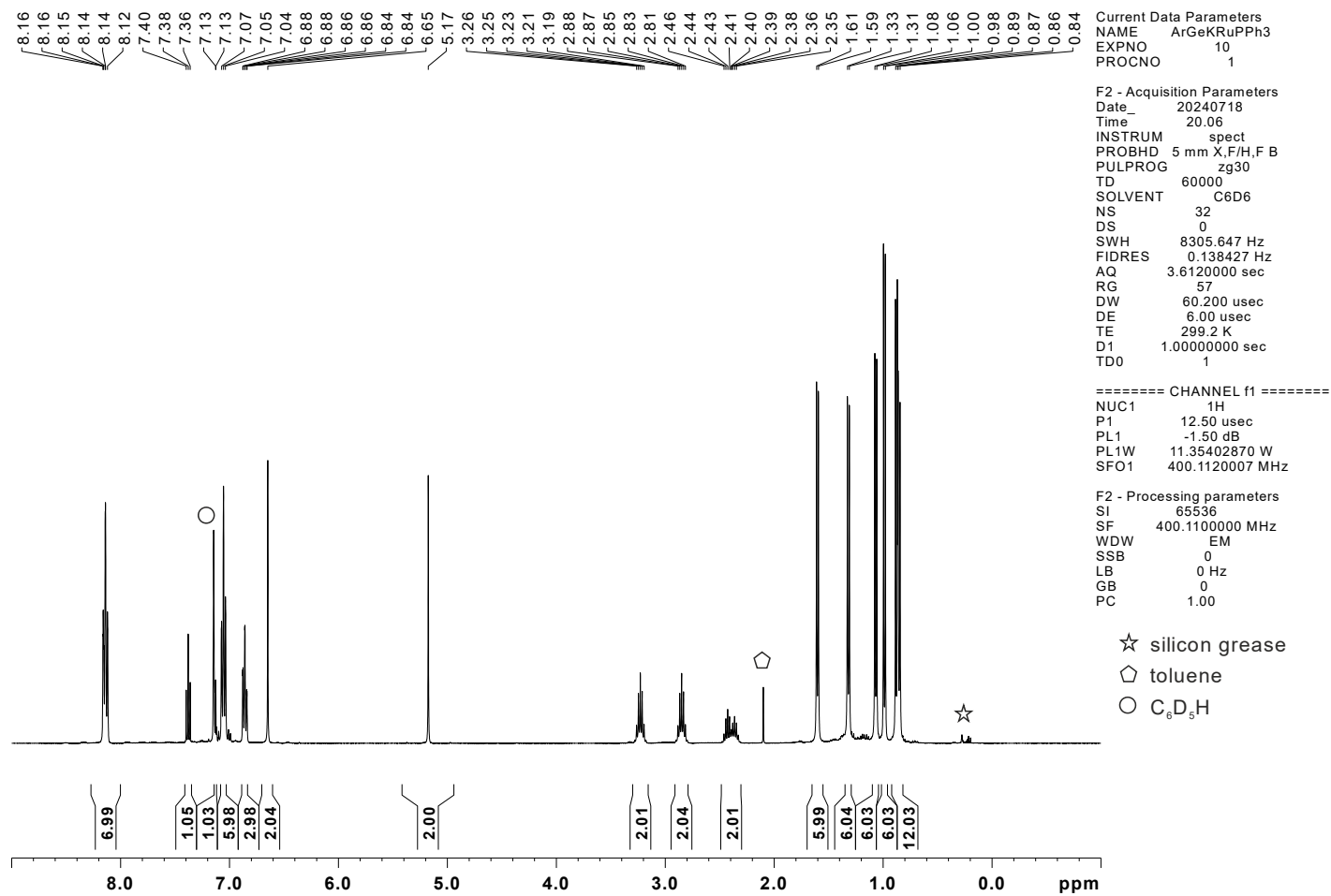
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PL1 -4.00 dB
PL1W 56.78615952 W
SFO1 161.9674970 MHz

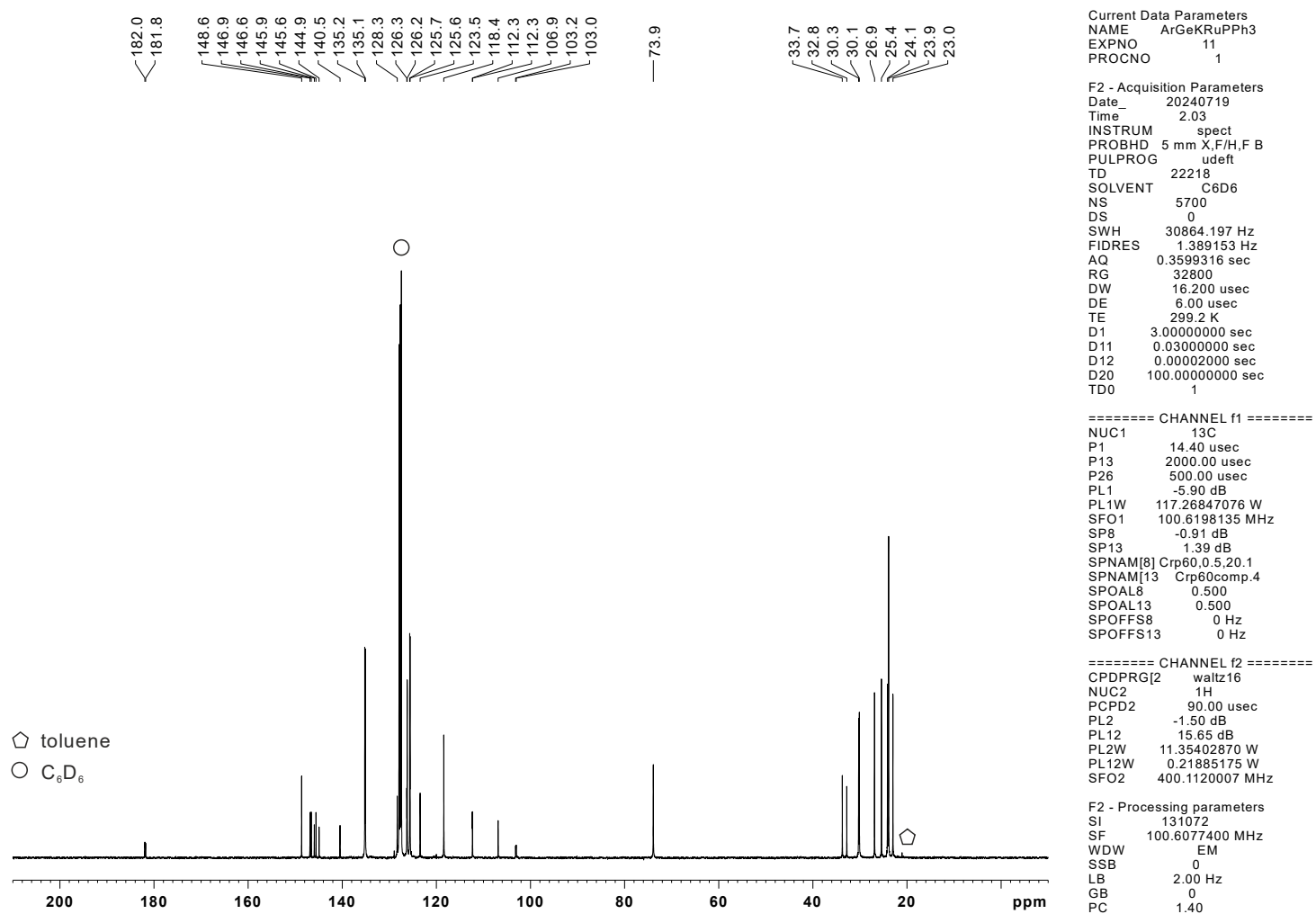
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 15.65 dB
PL2W 11.35402870 W
PL12W 0.21885175 W
SFO2 400.1120007 MHz

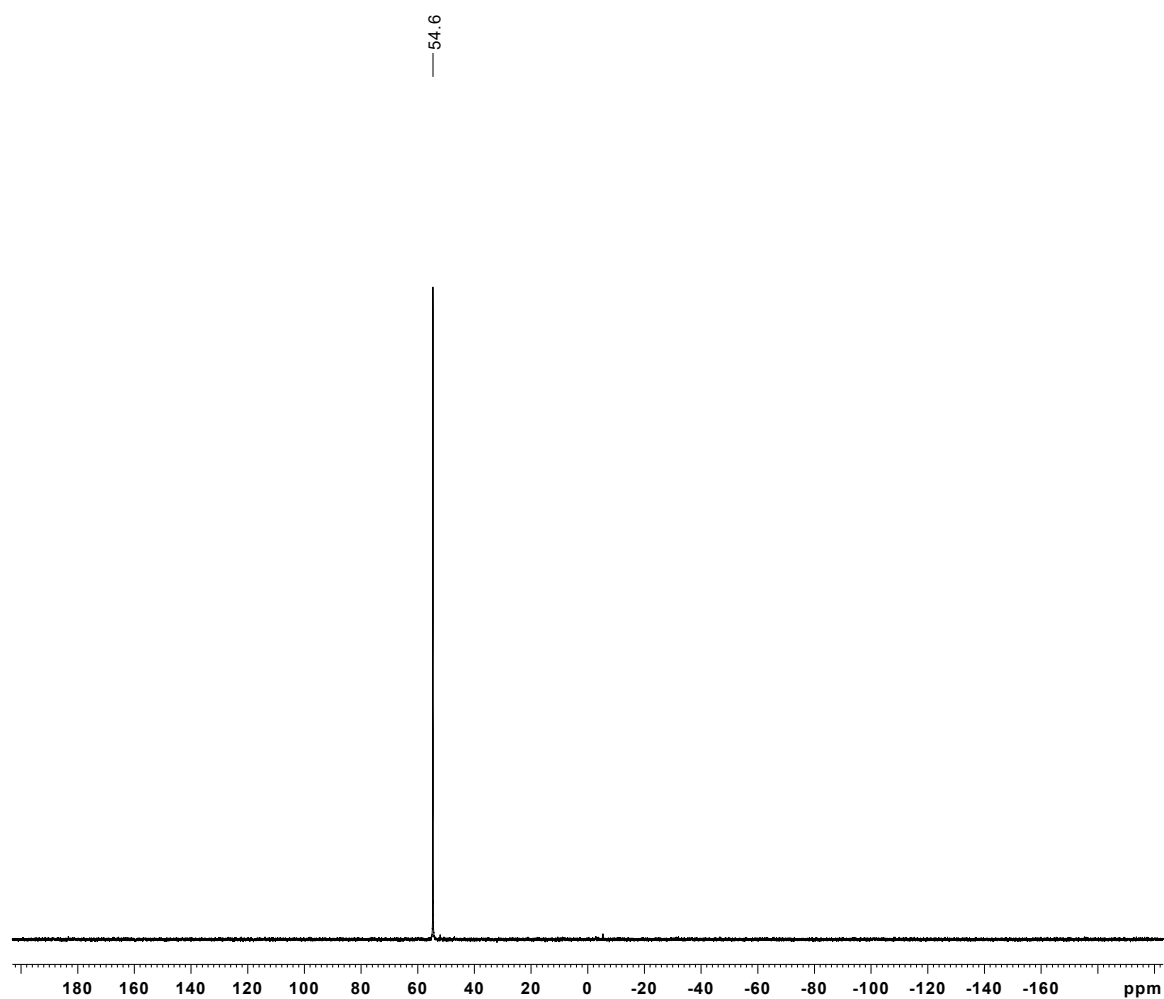
F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 2.

NMR spectra of compound **3a**.Figure S15. ¹H NMR spectrum (-5 – 15 ppm) of compound **3a**.

Figure S16. ¹H NMR spectrum of compound **3a**.

Figure S17. ¹³C{¹H} NMR spectrum of compound **3a**.



Current Data Parameters
NAME ArGeKRuPPh3
EXPNO 16
PROCNO 1

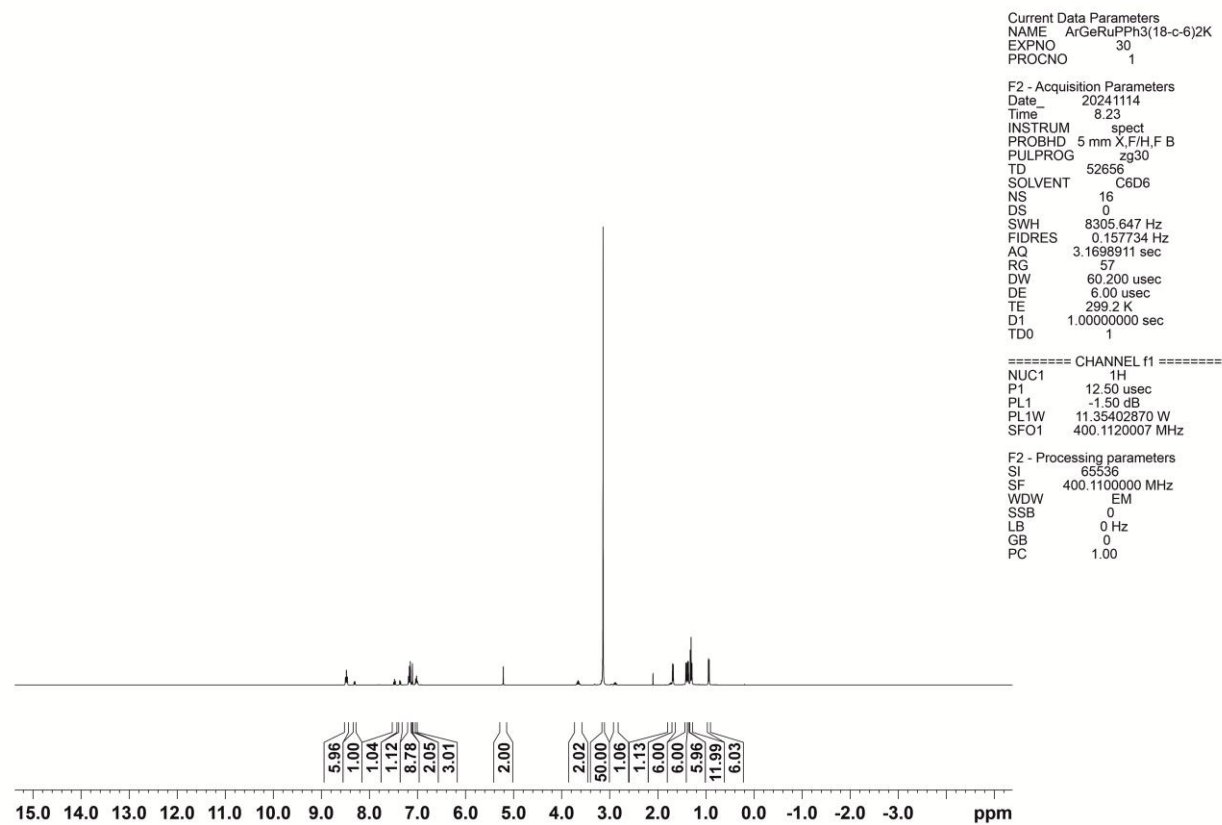
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TD 130000
SOLVENT C6D6
NS 256
DS 0
SWH 65789.477 Hz
FIDRES 0.506073 Hz
AQ 0.9880000 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

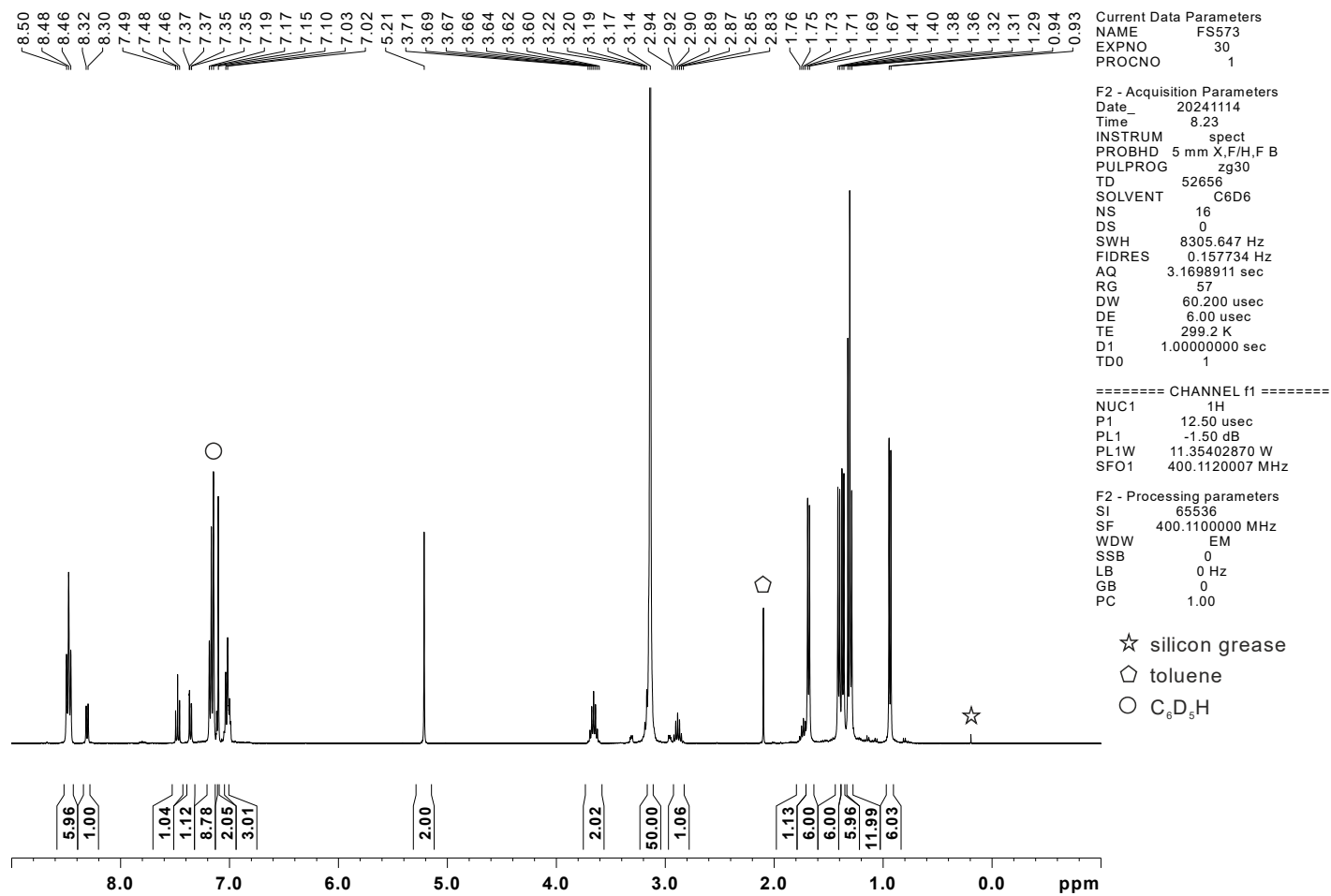
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P1 14.50 usec
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SFO1 161.9674970 MHz

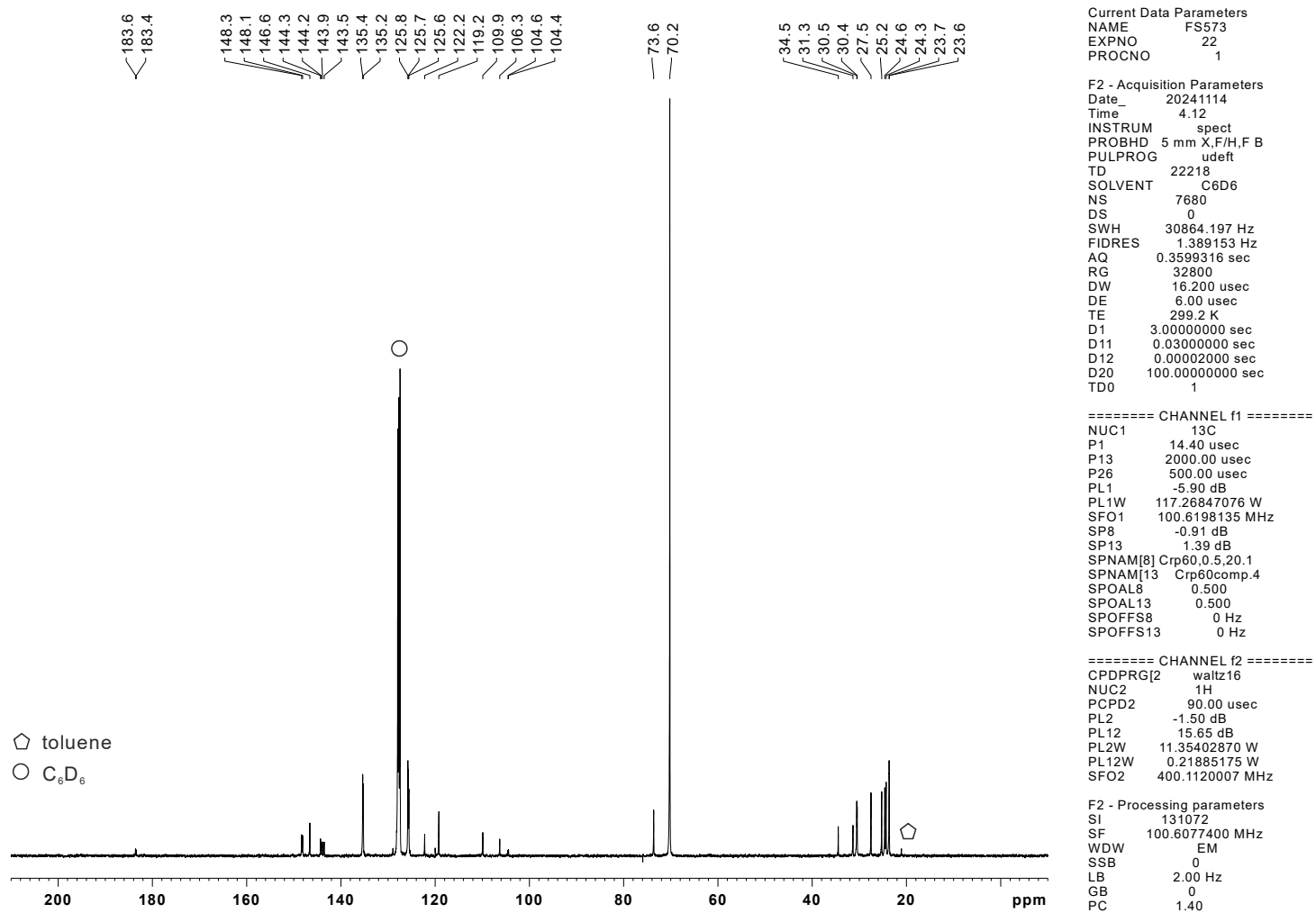
==== CHANNEL f2 =====
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NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 15.65 dB
PL2W 11.35402870 W
PL12W 0.21885175 W
SFO2 400.1120007 MHz

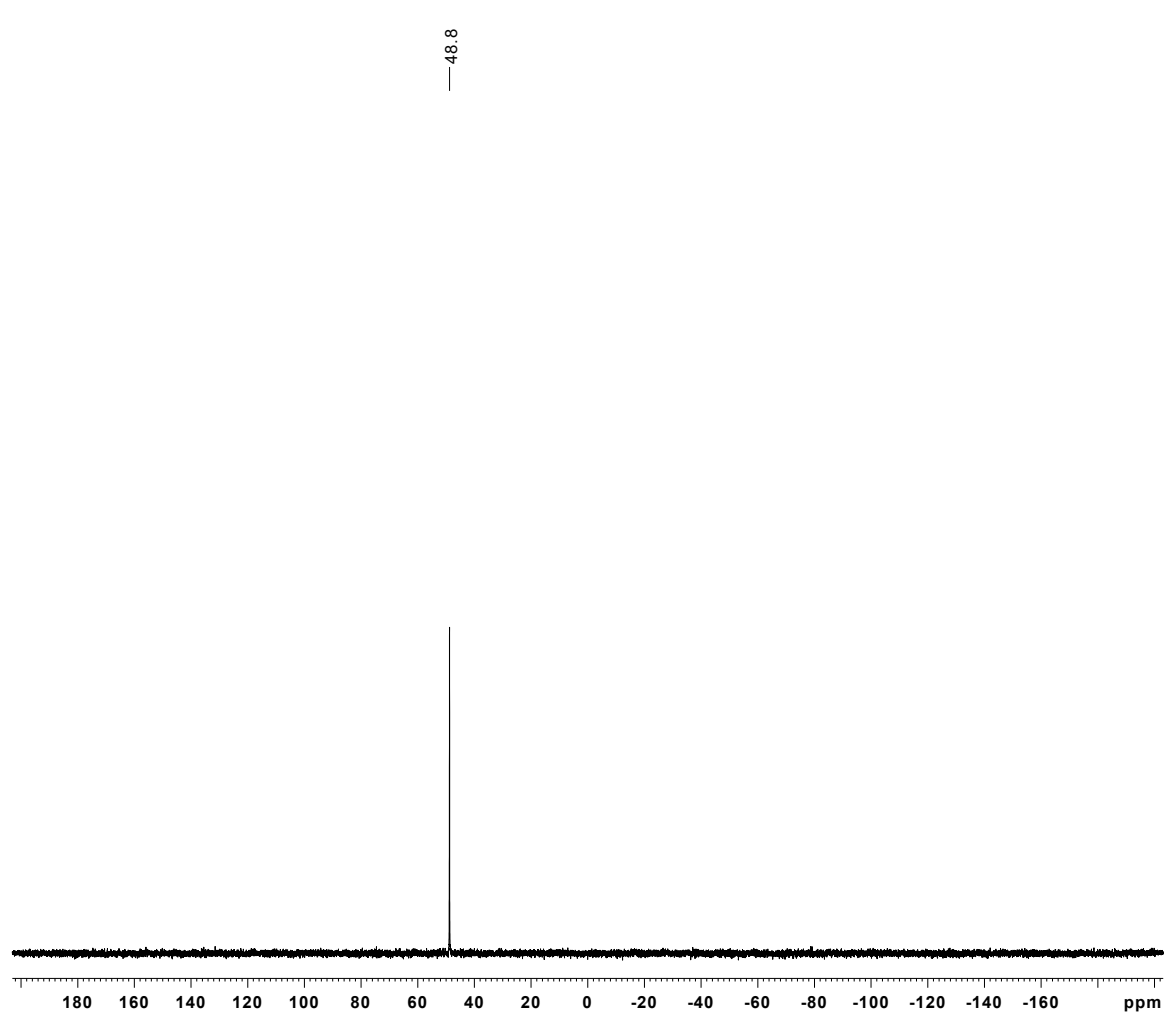
F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S18. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **3a**.

NMR spectra of compound **3b**.Figure S19. ¹H NMR spectrum (–5 – 15 ppm) of compound **3b**.

Figure S110. ¹H NMR spectrum of compound **3b**.

Figure S111. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3b**.



Current Data Parameters
NAME FS573
EXPNO 21
PROCNO 1

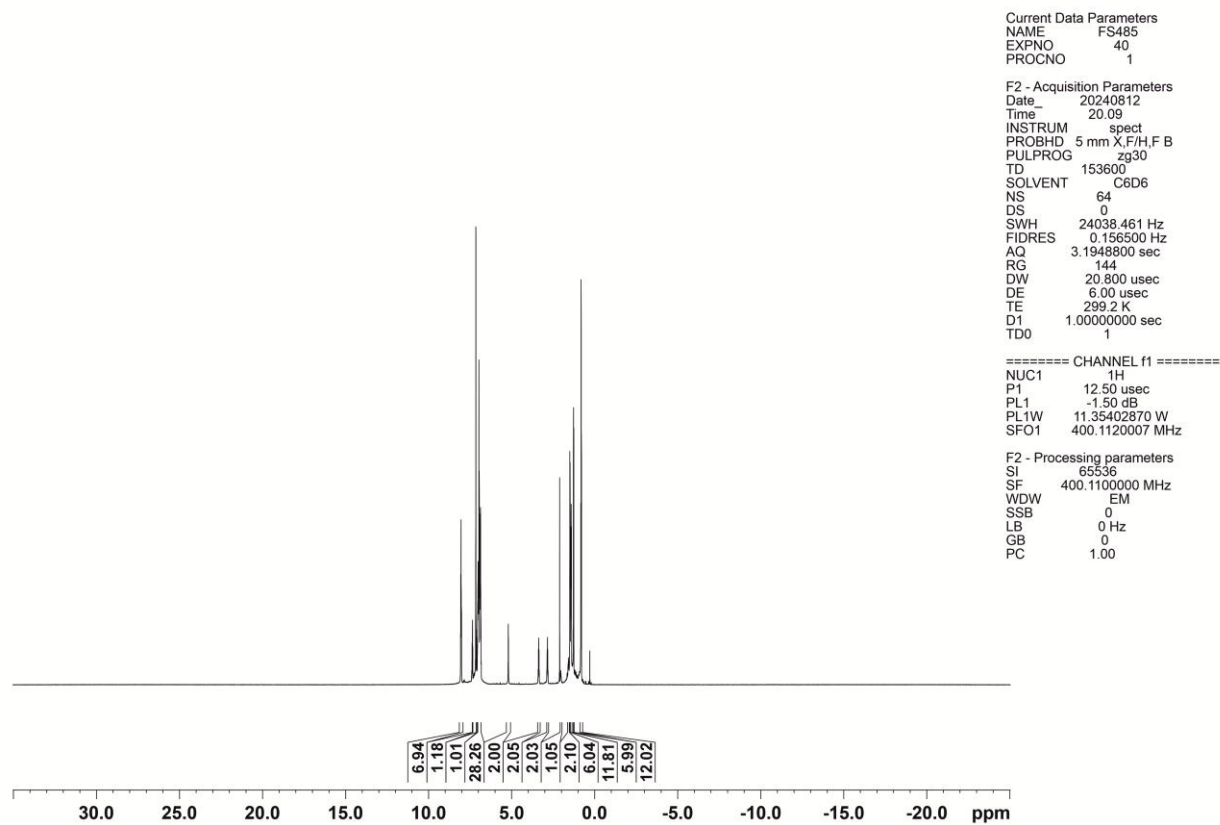
F2 - Acquisition Parameters
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Time 20.12
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TD 88150
SOLVENT C6D6
NS 128
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

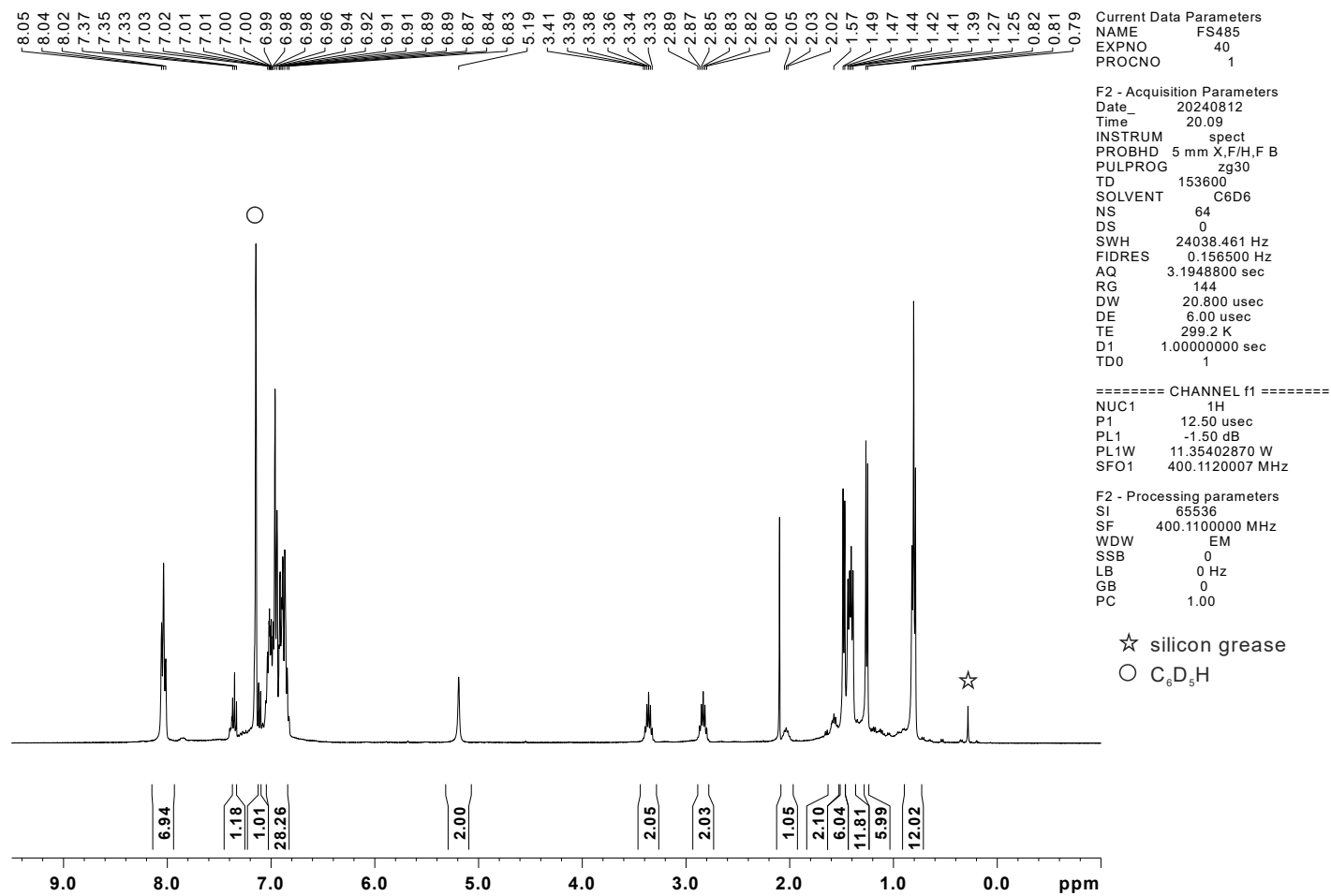
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PL1 -4.00 dB
PL1W 56.78615952 W
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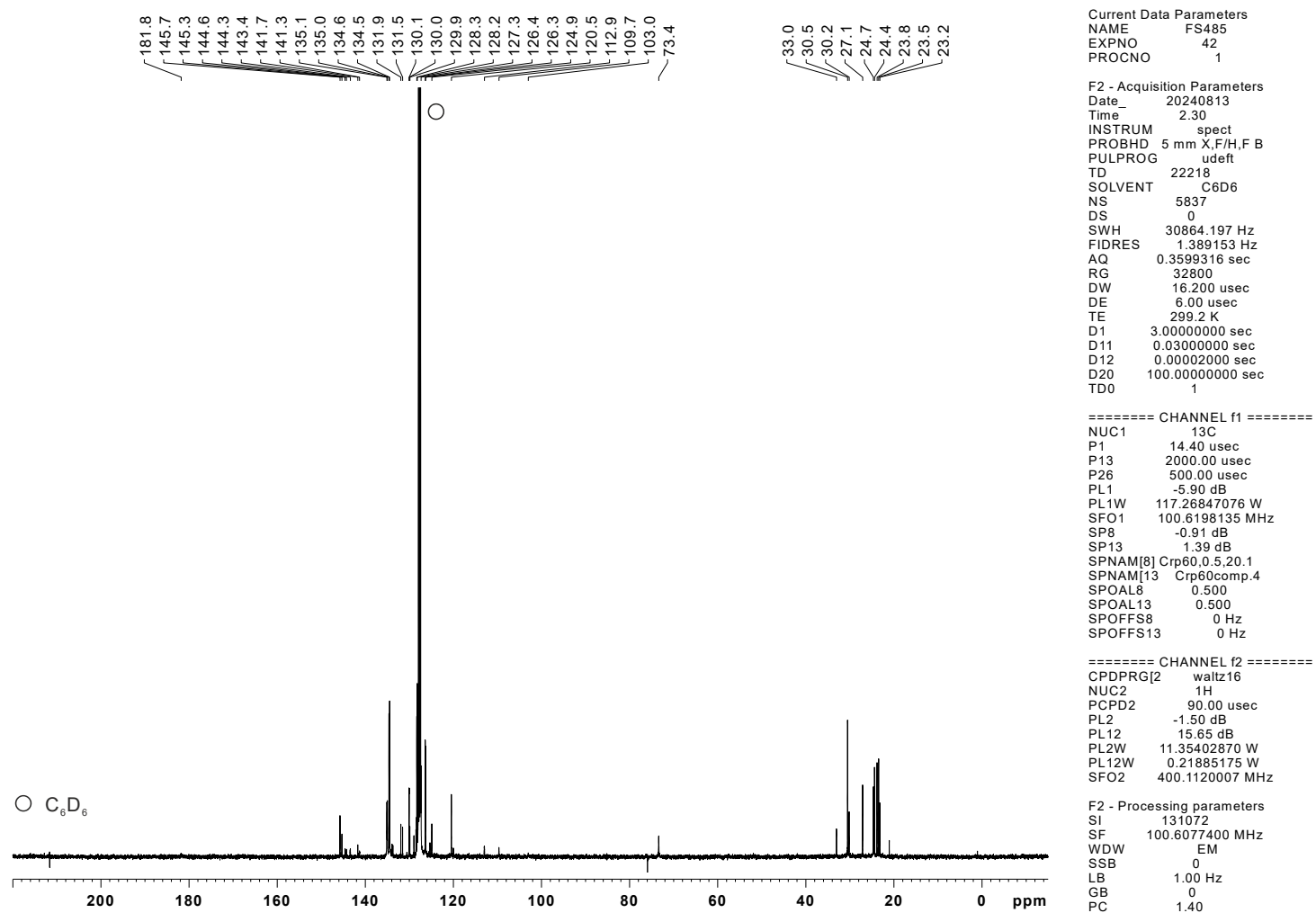
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CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 15.65 dB
PL2W 11.35402870 W
PL12W 0.21885175 W
SFO2 400.1120007 MHz

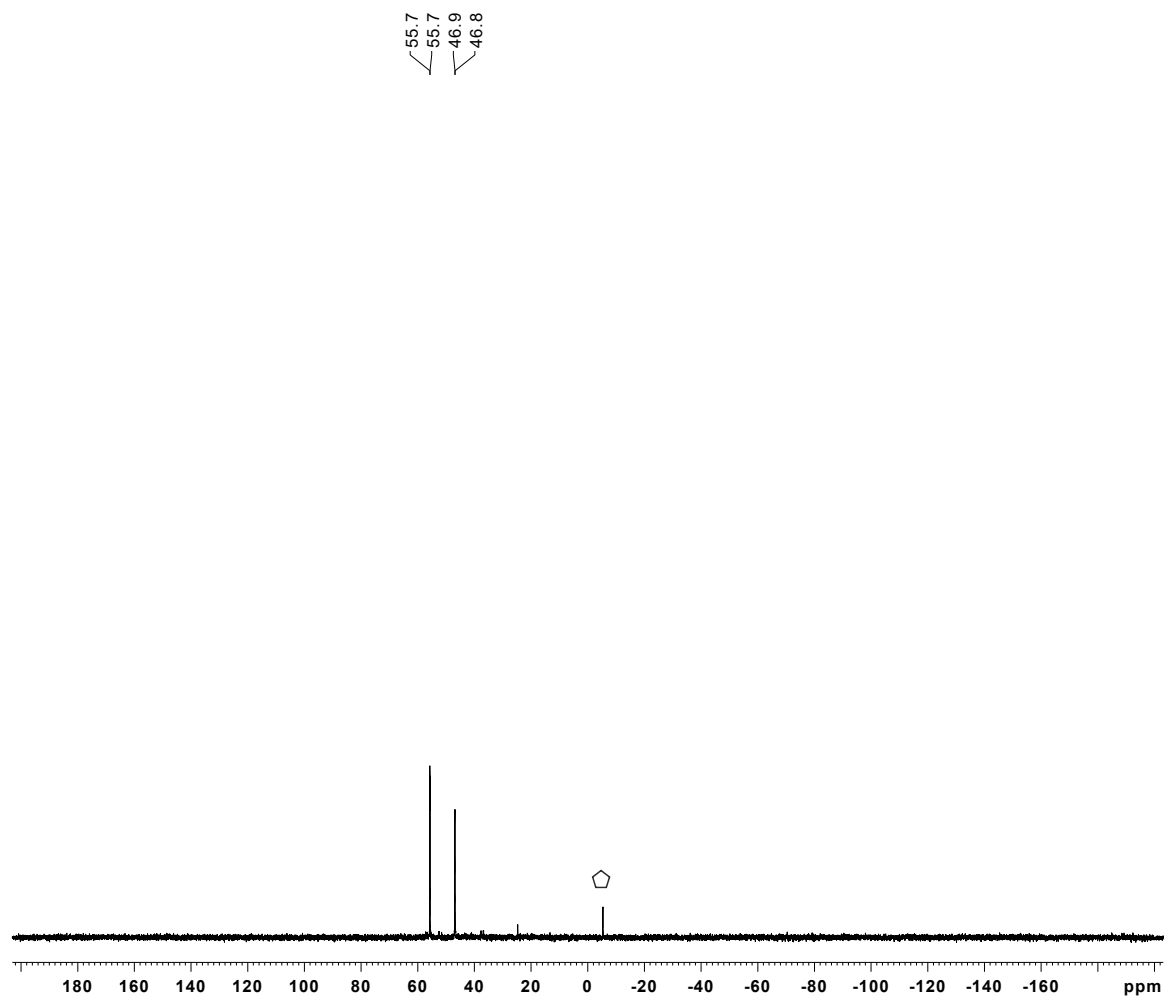
F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S112. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **3b**.

NMR spectra of compound **4**.Figure S113. ¹H NMR spectrum (-25 – 35 ppm) of compound **4**.

Figure S114. ¹H NMR spectrum of compound 4.

Figure S115. ¹³C{¹H} NMR spectrum of compound 4.



Current Data Parameters
 NAME FS485
 EXPNO 61
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240911
 Time 12.06
 INSTRUM spect
 PROBHD 5 mm X,F/H,F B
 PULPROG zgig30b
 TD 88150
 SOLVENT C6D6
 NS 128
 DS 0
 SWH 65789.477 Hz
 FIDRES 0.746336 Hz
 AQ 0.6699400 sec
 RG 23100
 DW 7.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

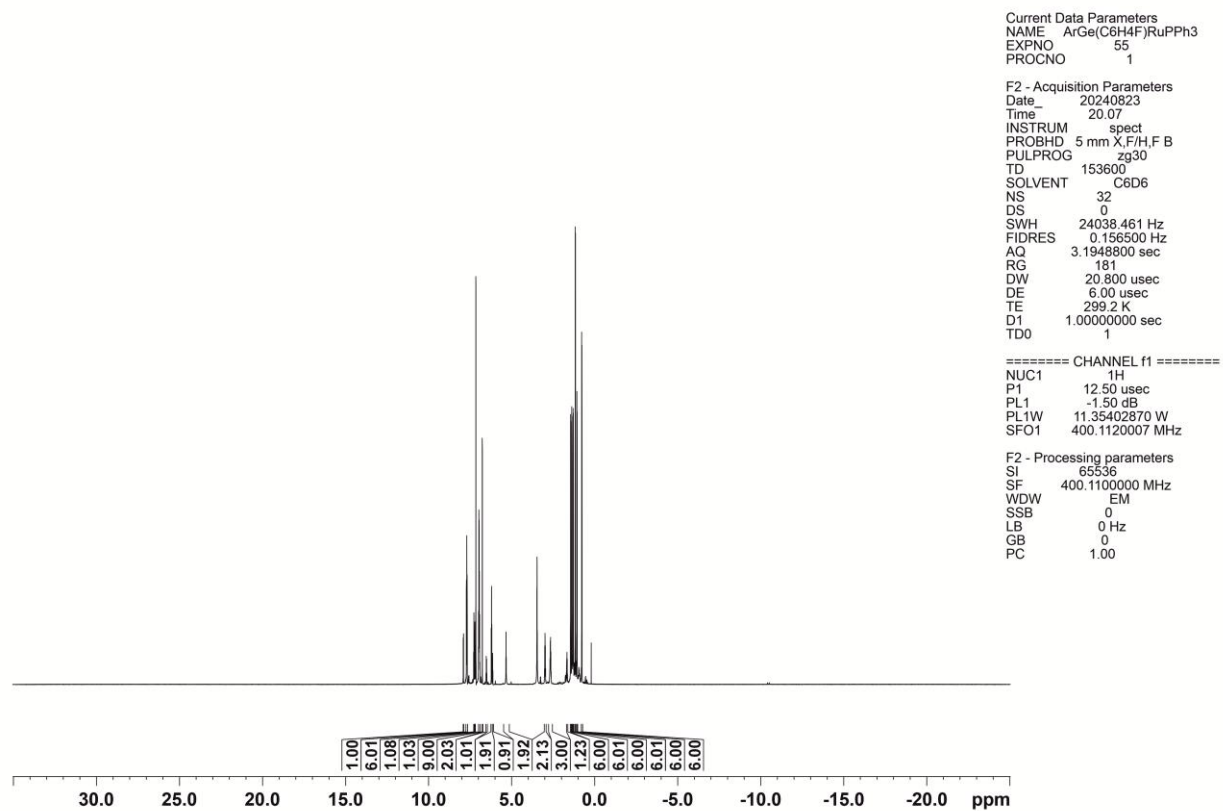
==== CHANNEL f1 =====
 NUC1 31P
 P1 14.50 usec
 PL1 -4.00 dB
 PL1W 56.78615952 W
 SFO1 161.9674970 MHz

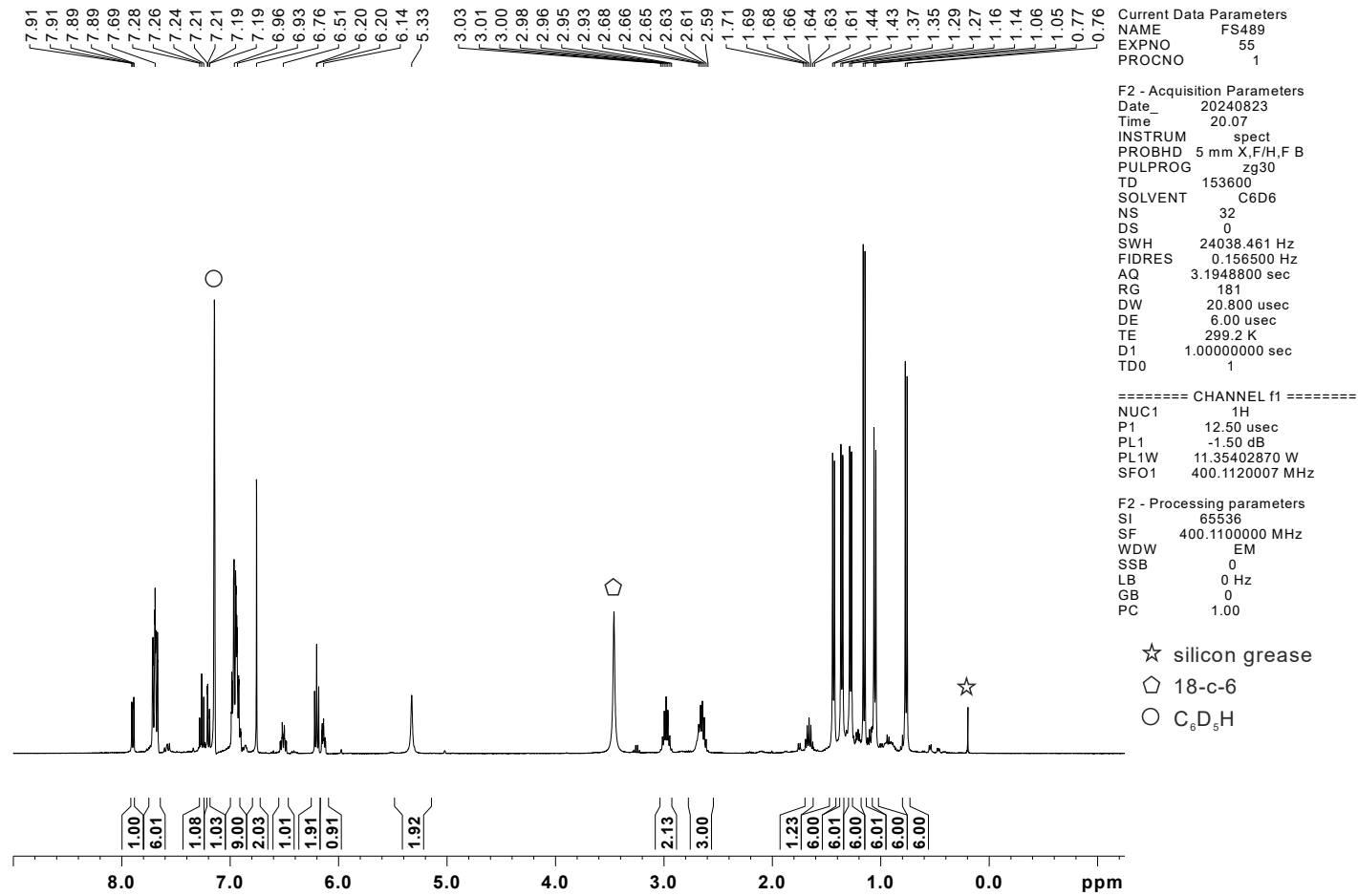
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.50 dB
 PL12 15.65 dB
 PL2W 11.35402870 W
 PL12W 0.21885175 W
 SFO2 400.1120007 MHz

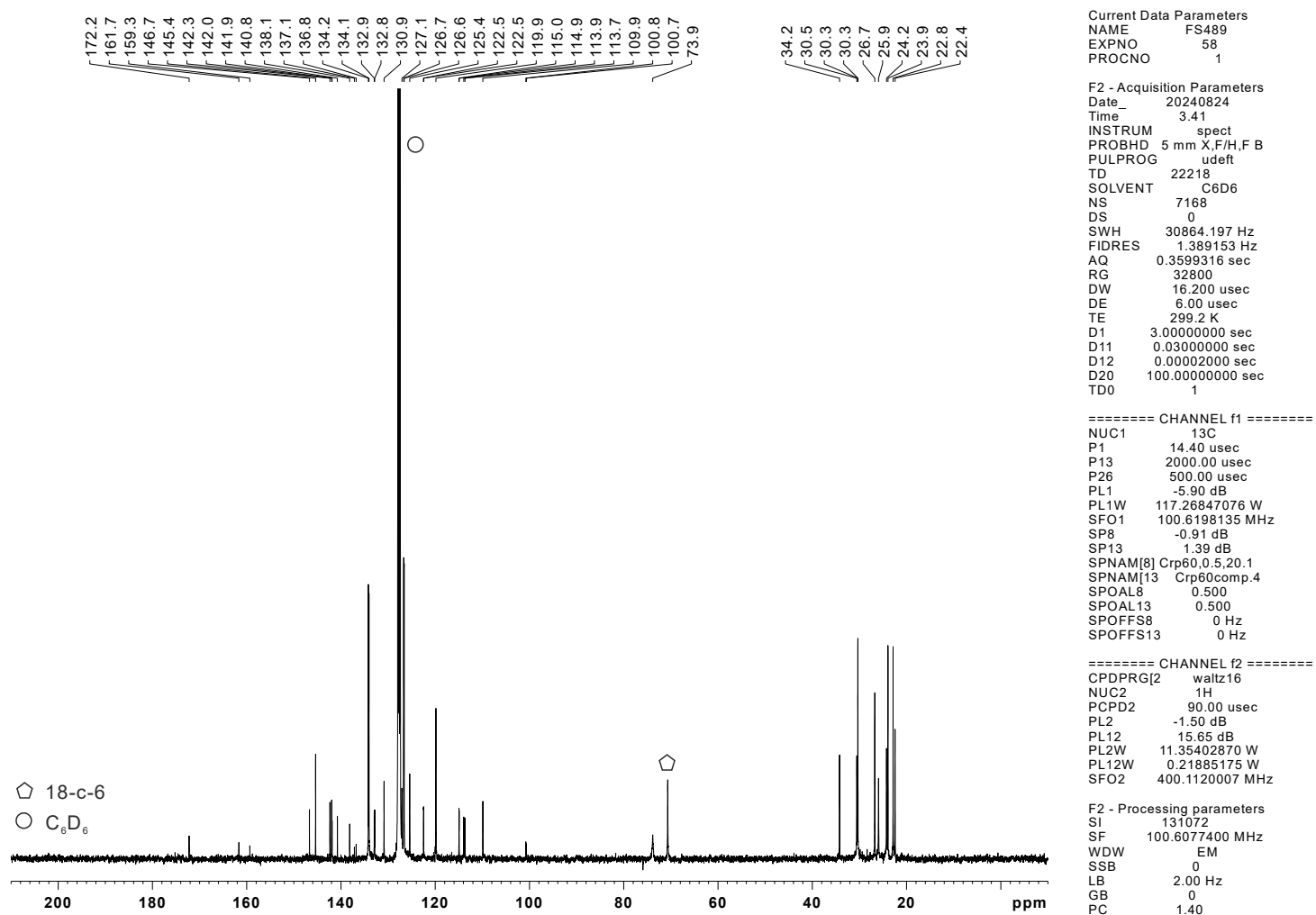
F2 - Processing parameters
 SI 131072
 SF 161.9674970 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

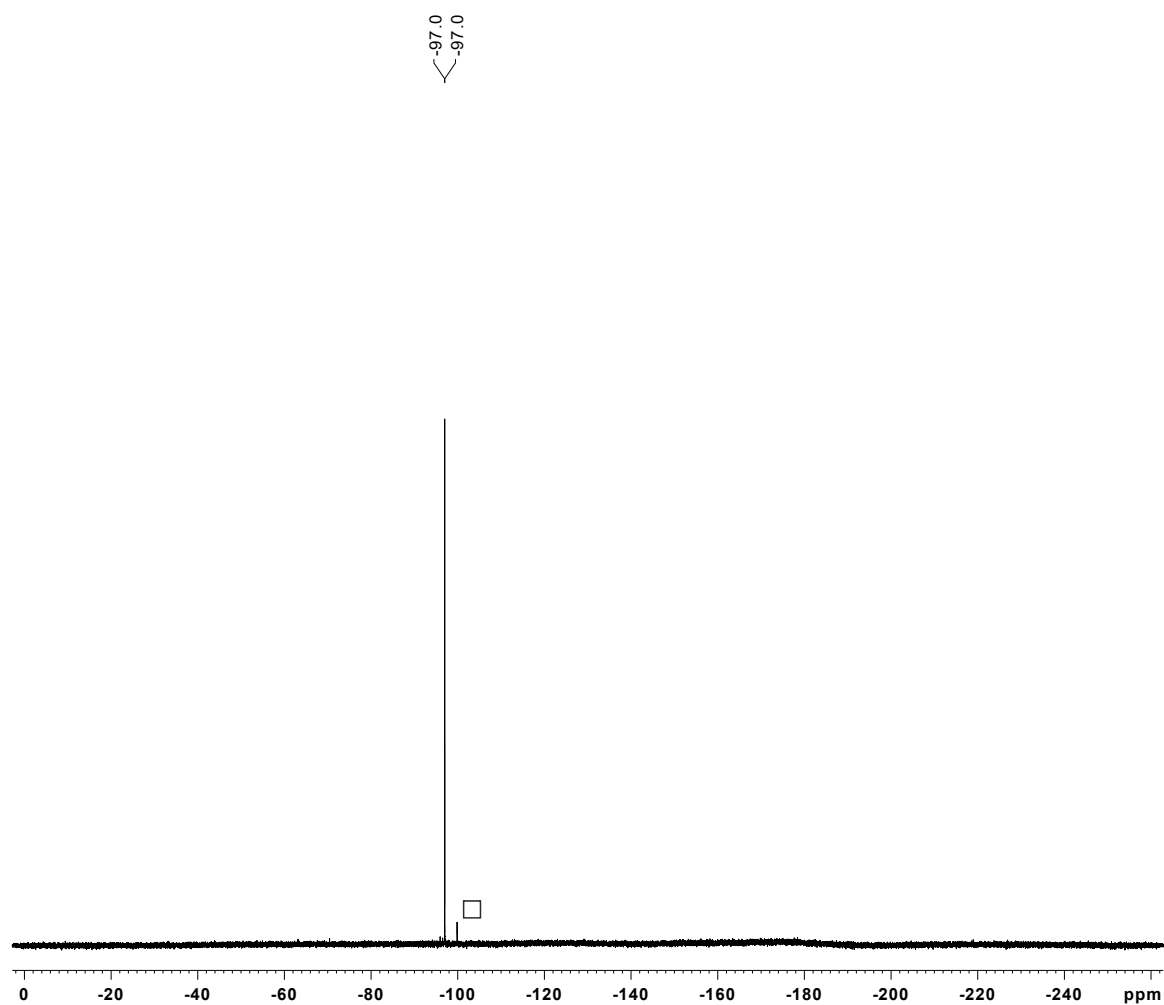
⬡ PPh₃ impurity

Figure S116. ³¹P{¹H} NMR spectrum of compound 4.

NMR spectra of compound **5**.Figure S117. ^1H NMR spectrum (-25 – 35 ppm) of compound **5**.

Figure S118. ¹H NMR spectrum of compound **5**.

Figure S119. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 5.



Current Data Parameters
 NAME FS489
 EXPNO 53
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240823
 Time 11.50
 INSTRUM spect
 PROBHD 5 mm X,F/H,F B
 PULPROG zgfhigqn
 TD 131072
 SOLVENT C6D6
 NS 64
 DS 0
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6553600 sec
 RG 4100
 DW 5.000 usec
 DE 6.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

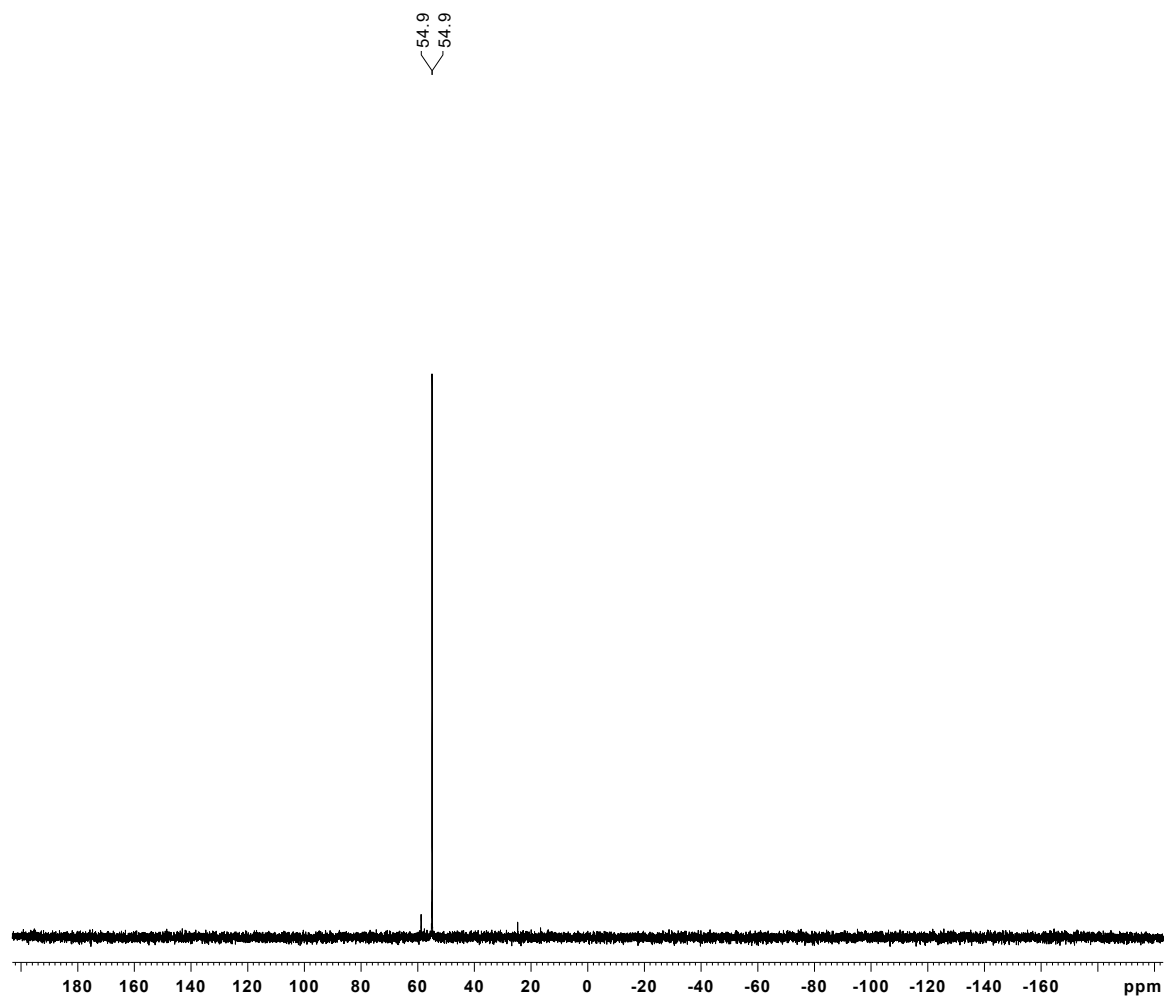
==== CHANNEL f1 =====
 NUC1 19F
 P1 19.70 usec
 PL1 -6.00 dB
 PL1W 62.00000000 W
 SFO1 376.4306030 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.50 dB
 PL12 15.65 dB
 PL2W 11.35402870 W
 PL12W 0.21885175 W
 SFO2 400.1120007 MHz

F2 - Processing parameters
 SI 262144
 SF 376.4795470 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

impurity

Figure S120. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of compound 5.



Current Data Parameters
NAME FS489
EXPNO 57
PROCNO 1

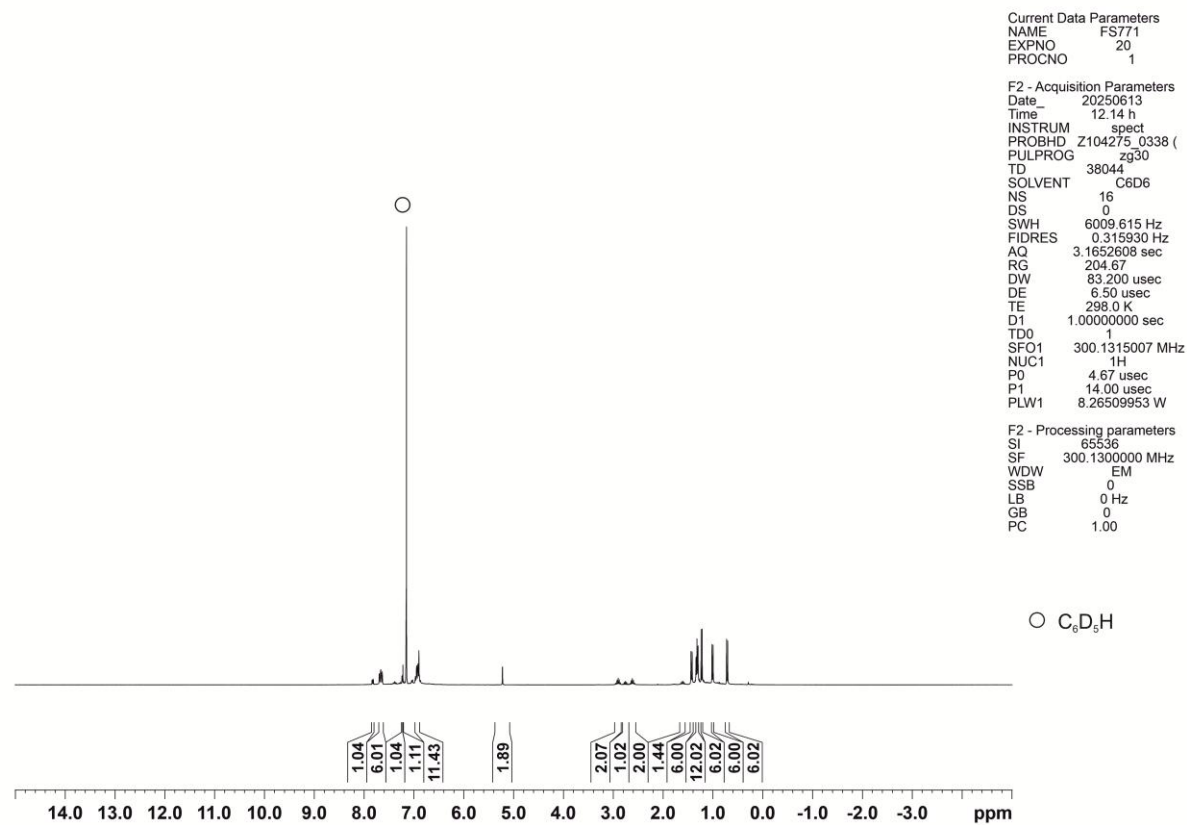
F2 - Acquisition Parameters
Date_ 20240823
Time 20.12
INSTRUM spect
PROBHD 5 mm X,F/H,F B
PULPROG zgig30b
TD 88150
SOLVENT C6D6
NS 128
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

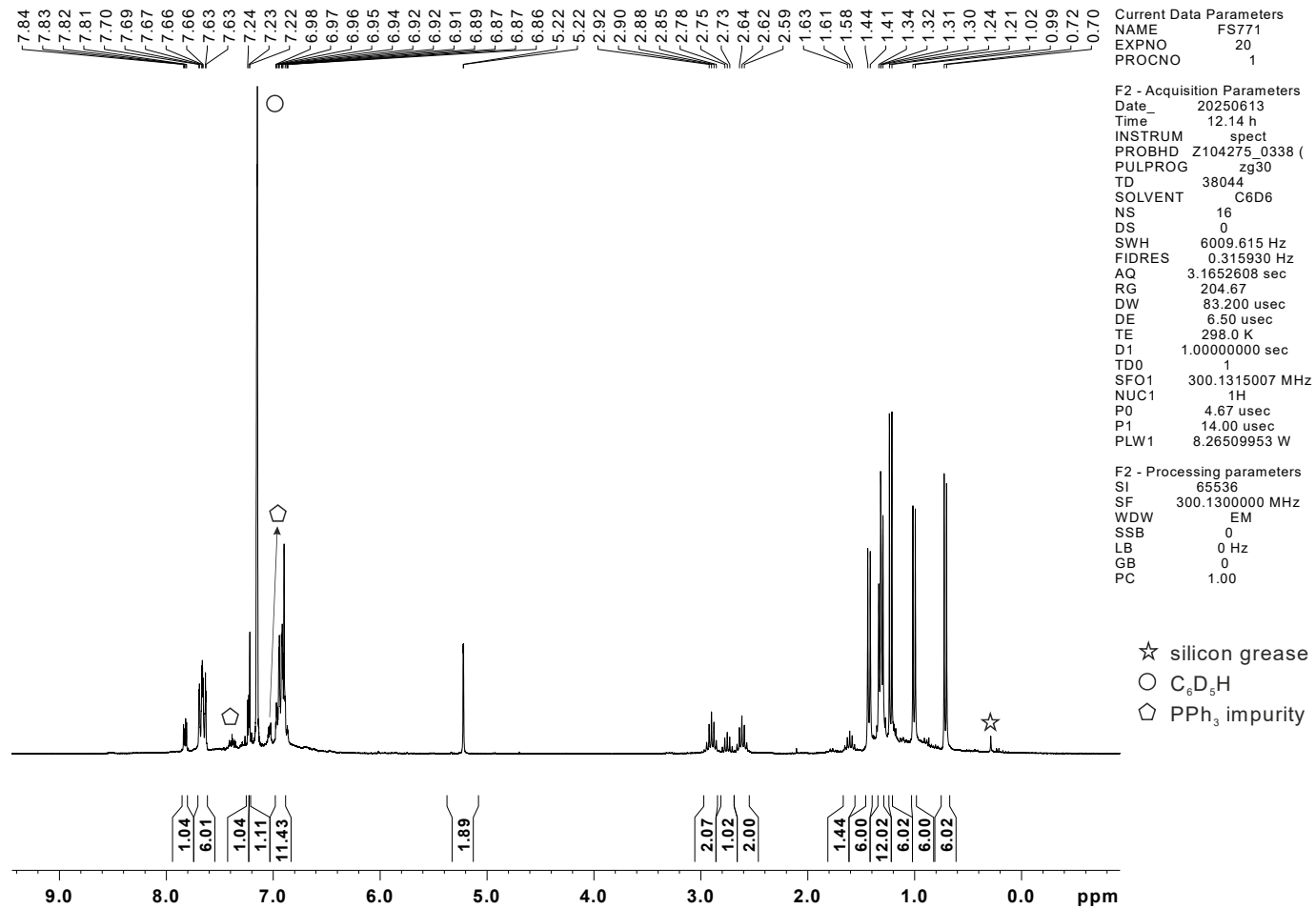
==== CHANNEL f1 =====
NUC1 31P
P1 14.50 usec
PL1 -4.00 dB
PL1W 56.78615952 W
SFO1 161.9674970 MHz

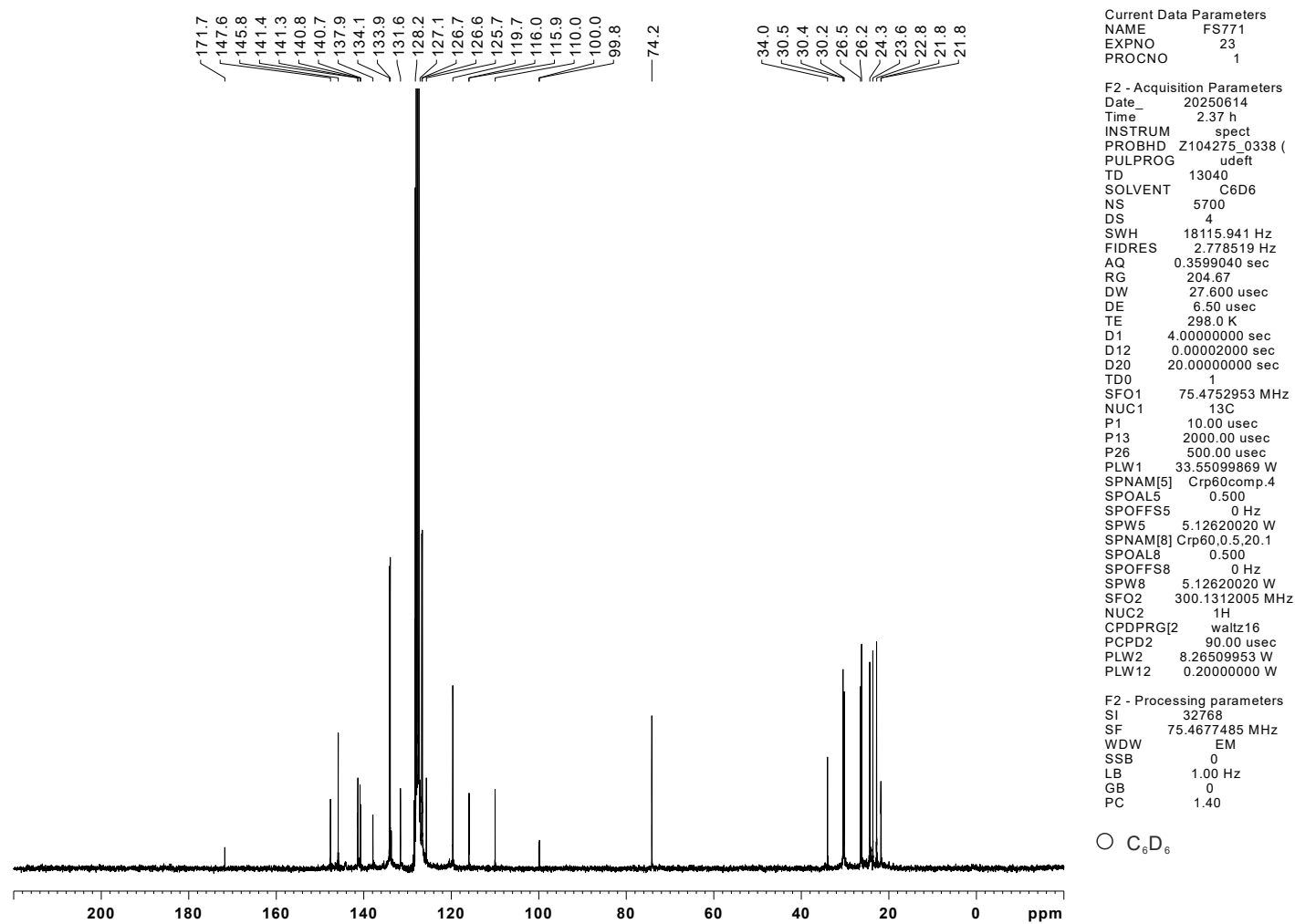
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 15.65 dB
PL2W 11.35402870 W
PL12W 0.21885175 W
SFO2 400.1120007 MHz

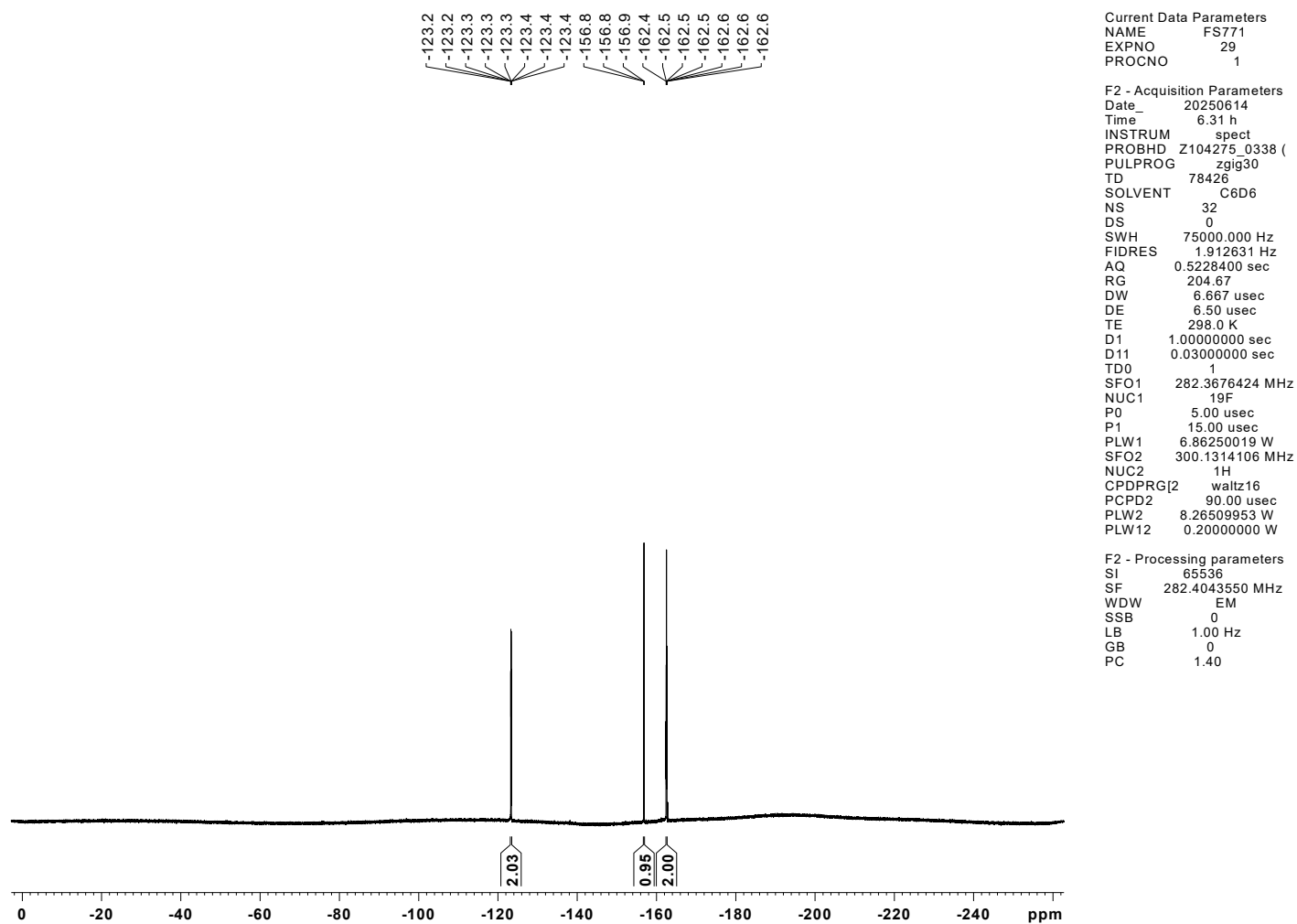
F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

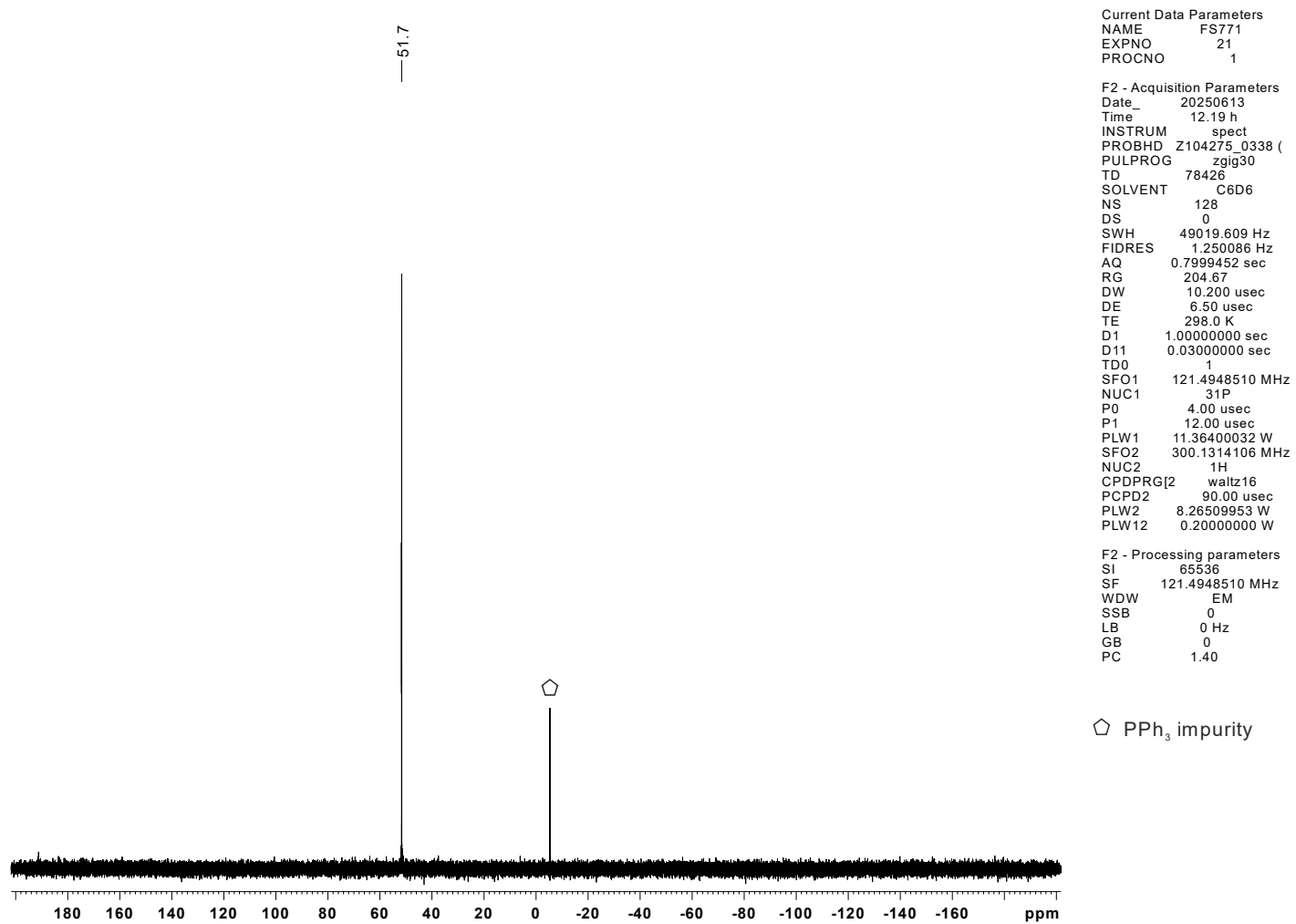
Figure S121. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 5.

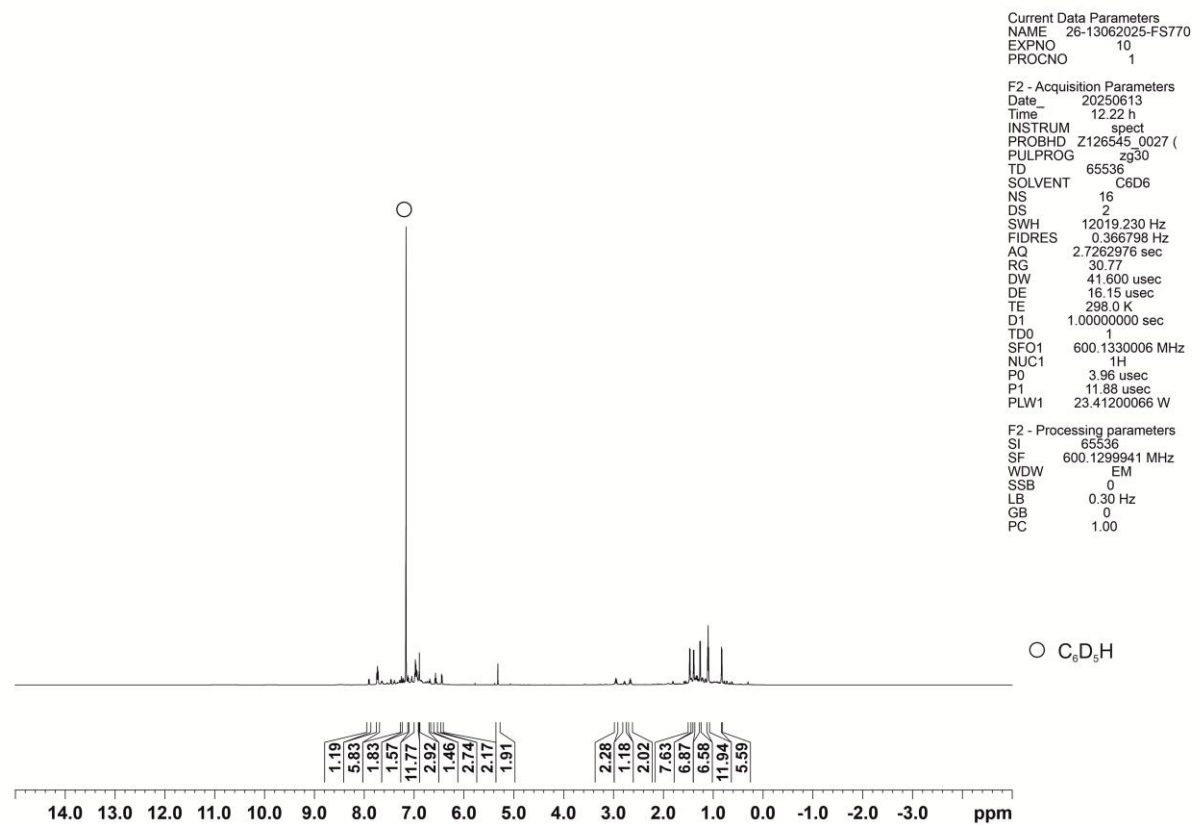
NMR spectra of compound **6**.Figure S122. ¹H NMR spectrum (–5 – 15 ppm) of compound **6**.

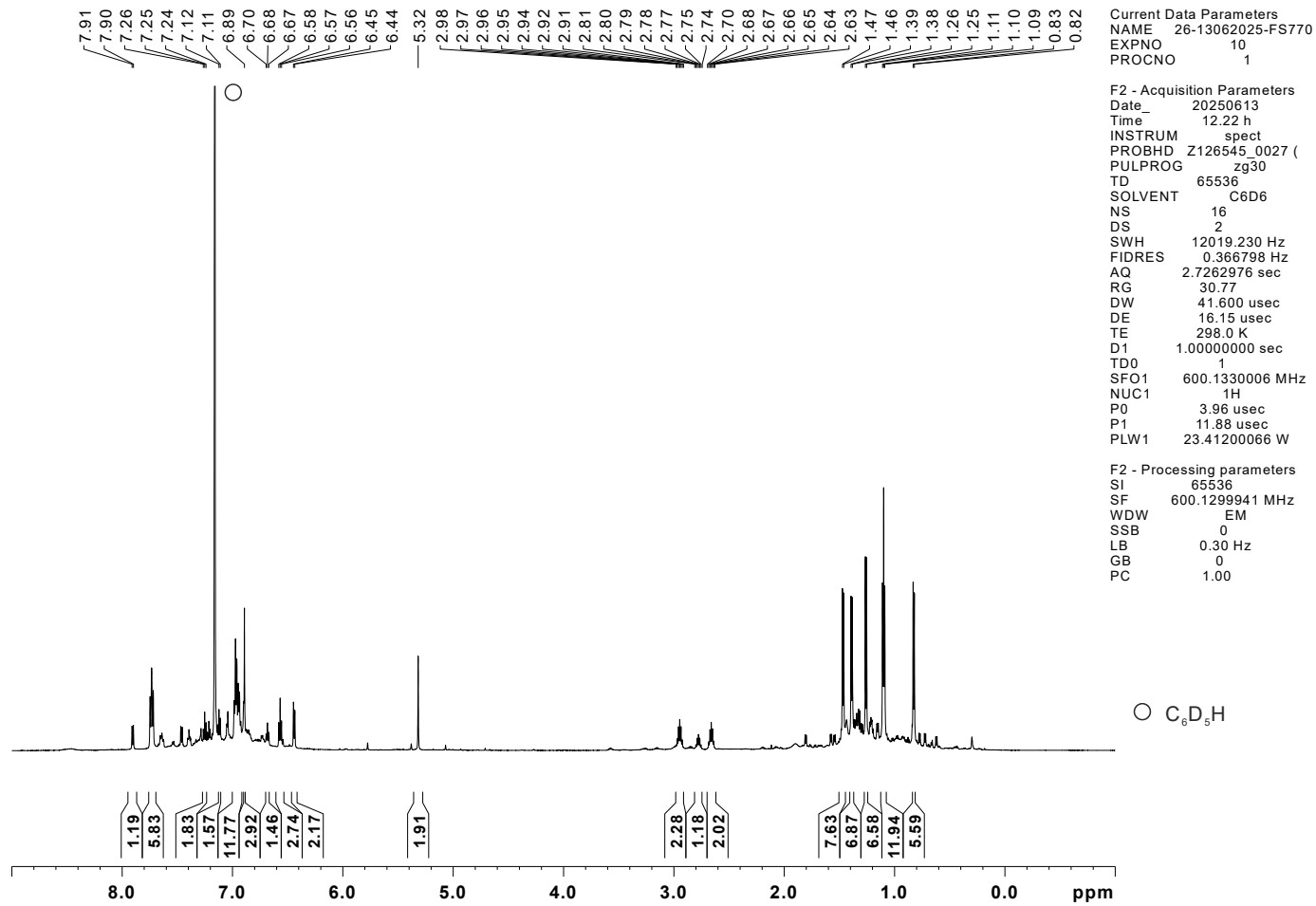
Figure S123. ¹H NMR spectrum of compound **6**.

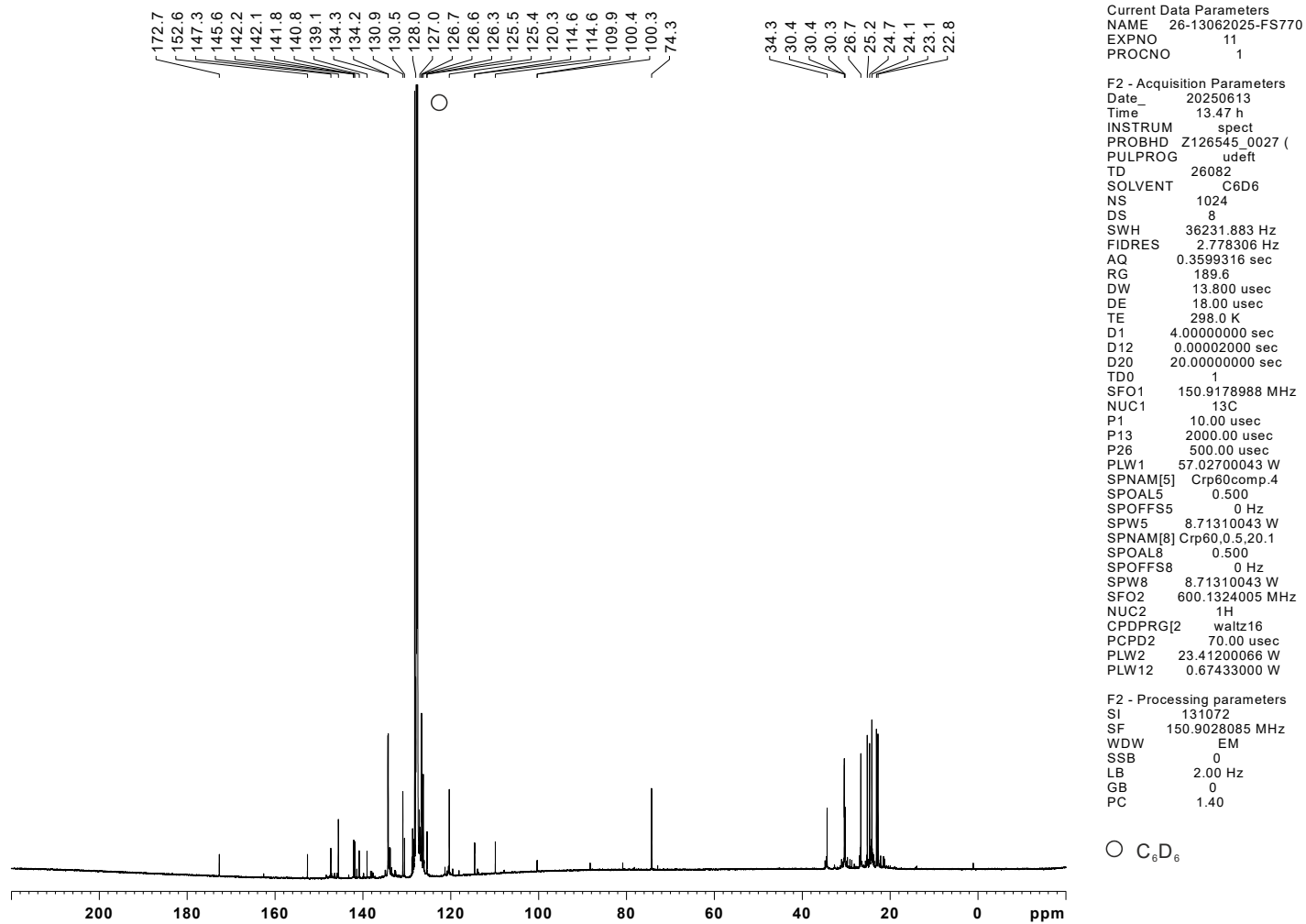
Figure S124. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6**.

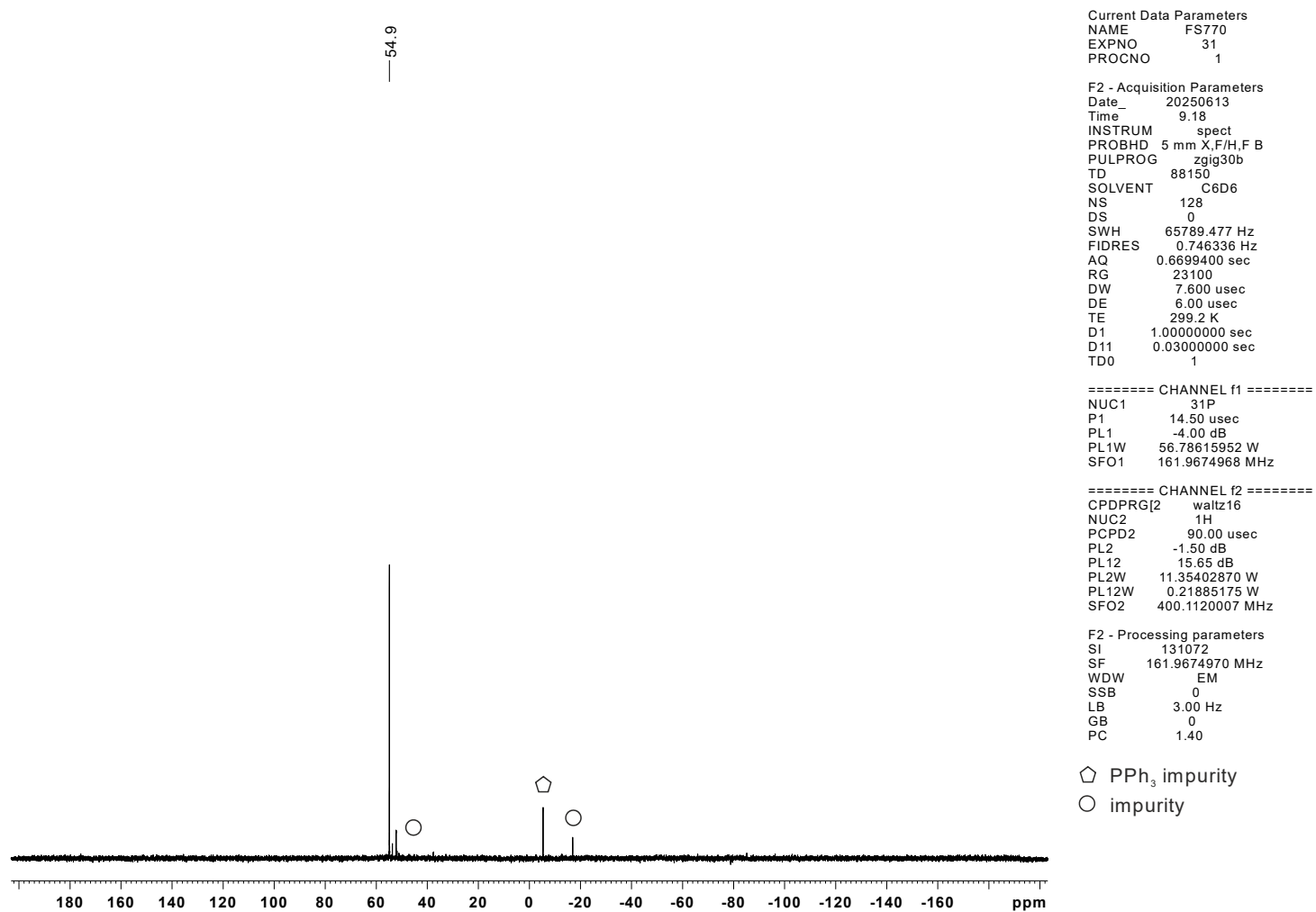
Figure S125. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of compound **6**.

Figure S126. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **6**.

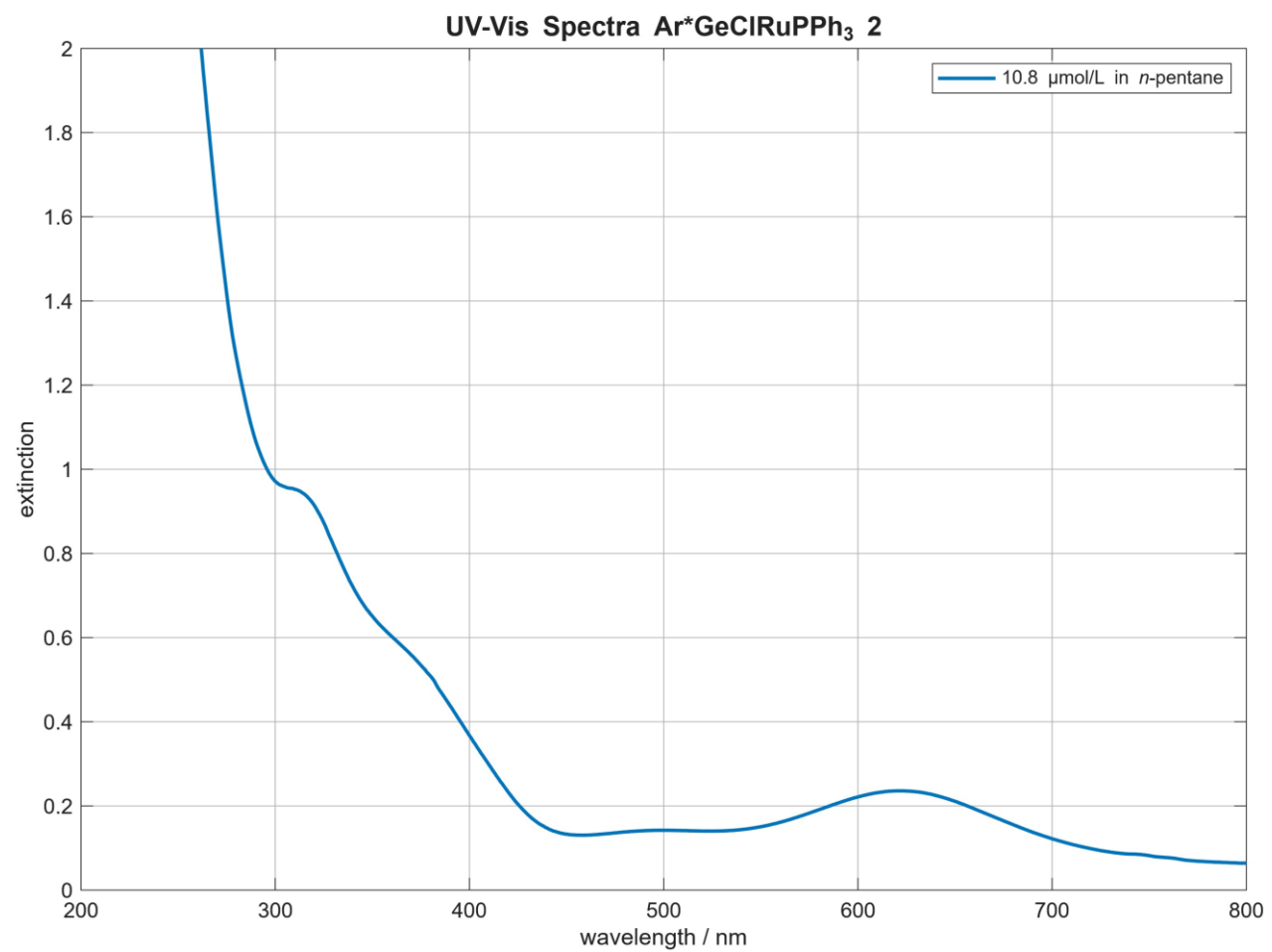
NMR spectra of compound **7**.Figure S127. ¹H NMR spectrum (–5 – 15 ppm) of compound **7**.

Figure S128. ¹H NMR spectrum of compound 7.

Figure SI29. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 7.

Figure S130. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 7.

UV-Vis spectroscopy

Figure S131. UV-Vis spectrum of compound **2**.

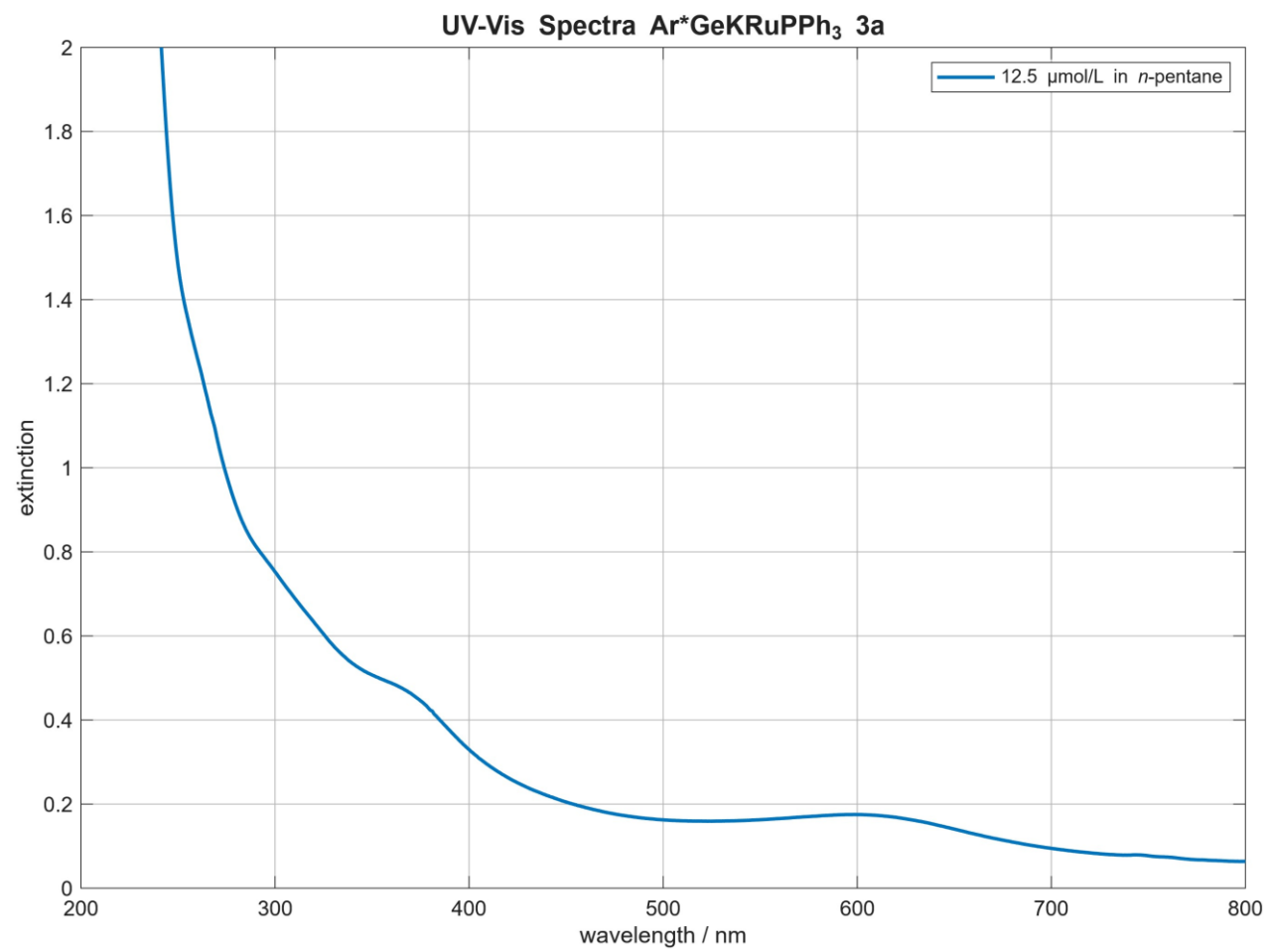


Figure SI32. UV-Vis spectrum of compound **3a**.

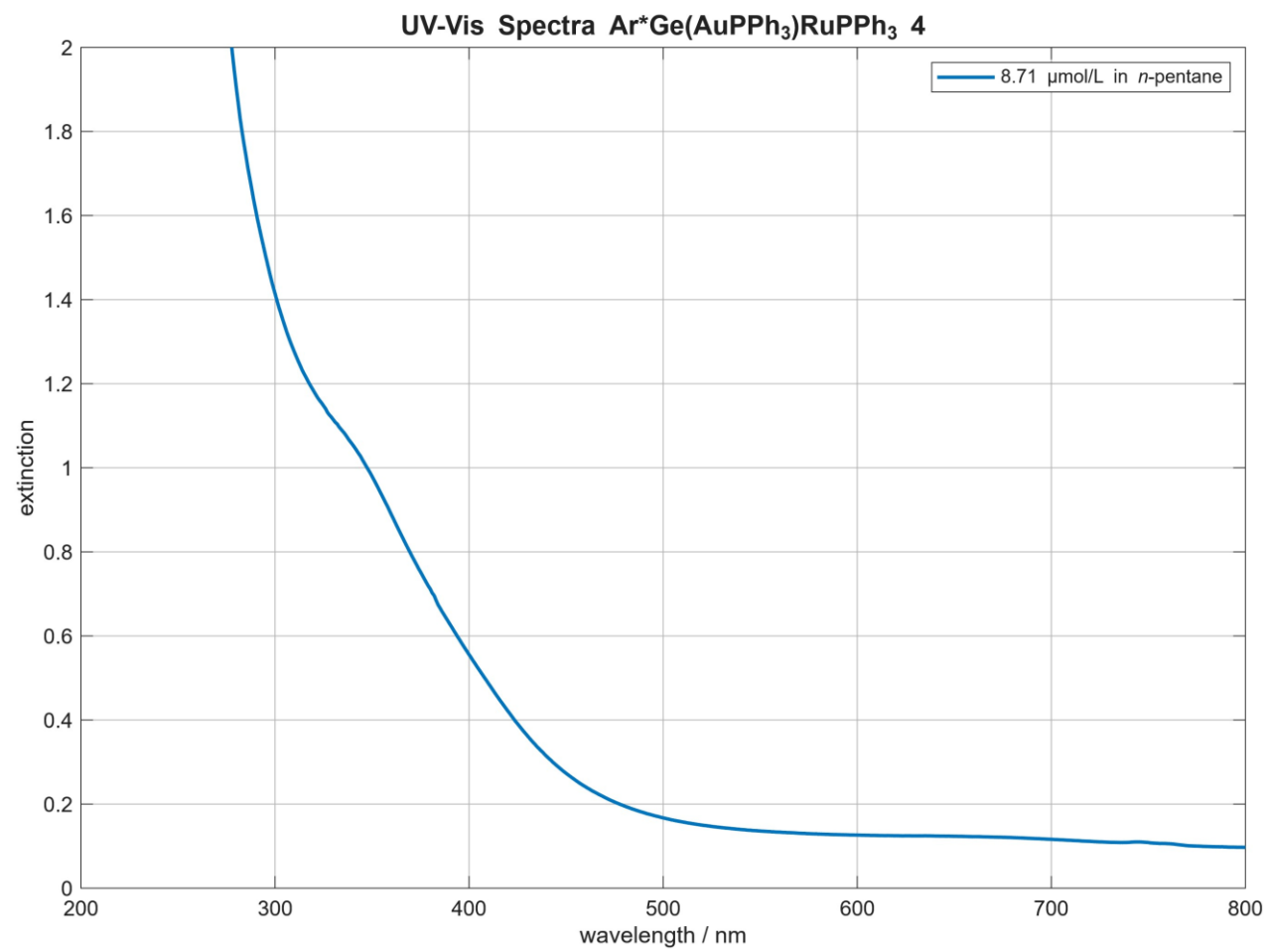


Figure SI33. UV-Vis spectrum of compound 4.

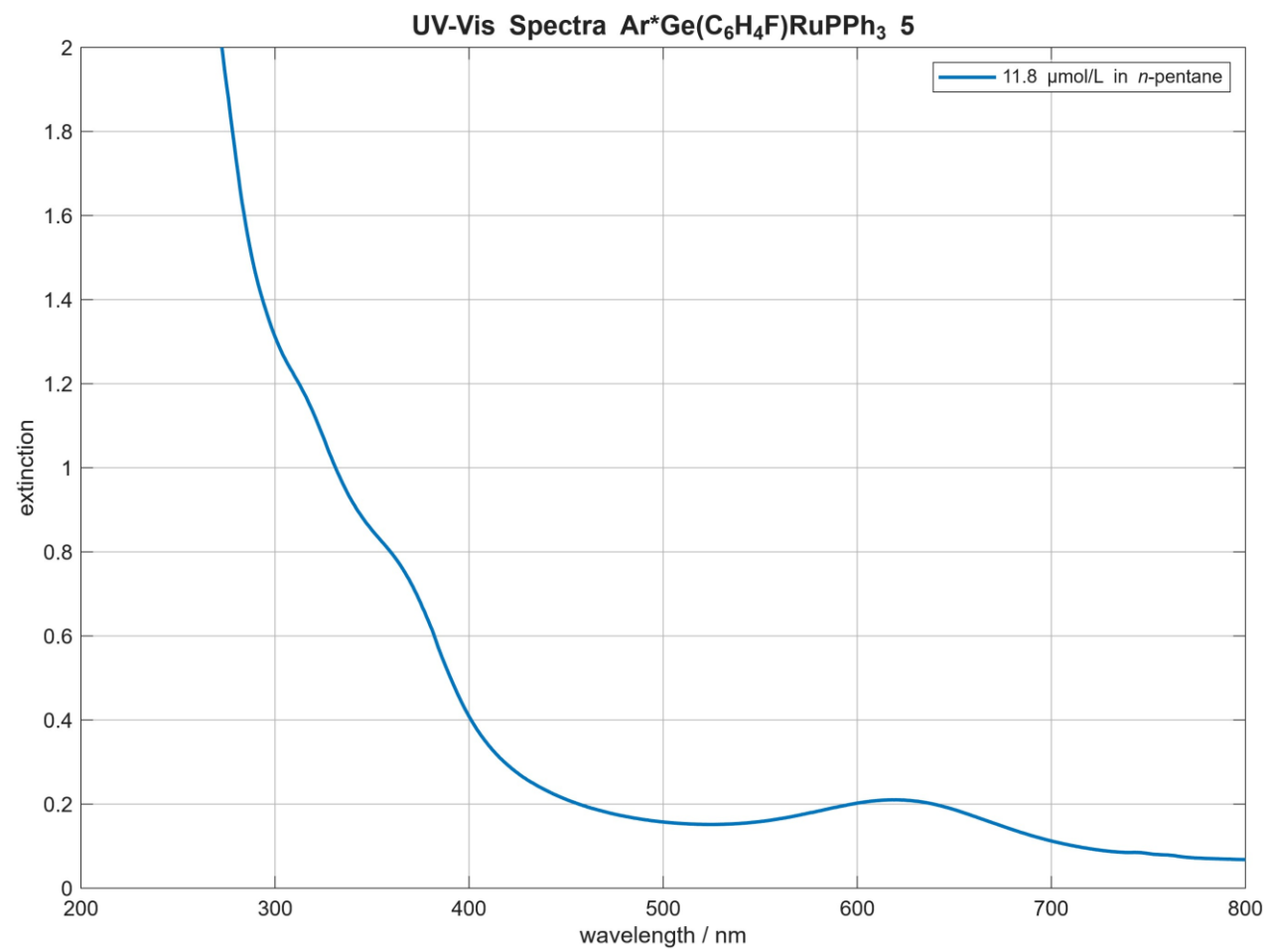


Figure SI34. UV-Vis spectrum of compound **5**.

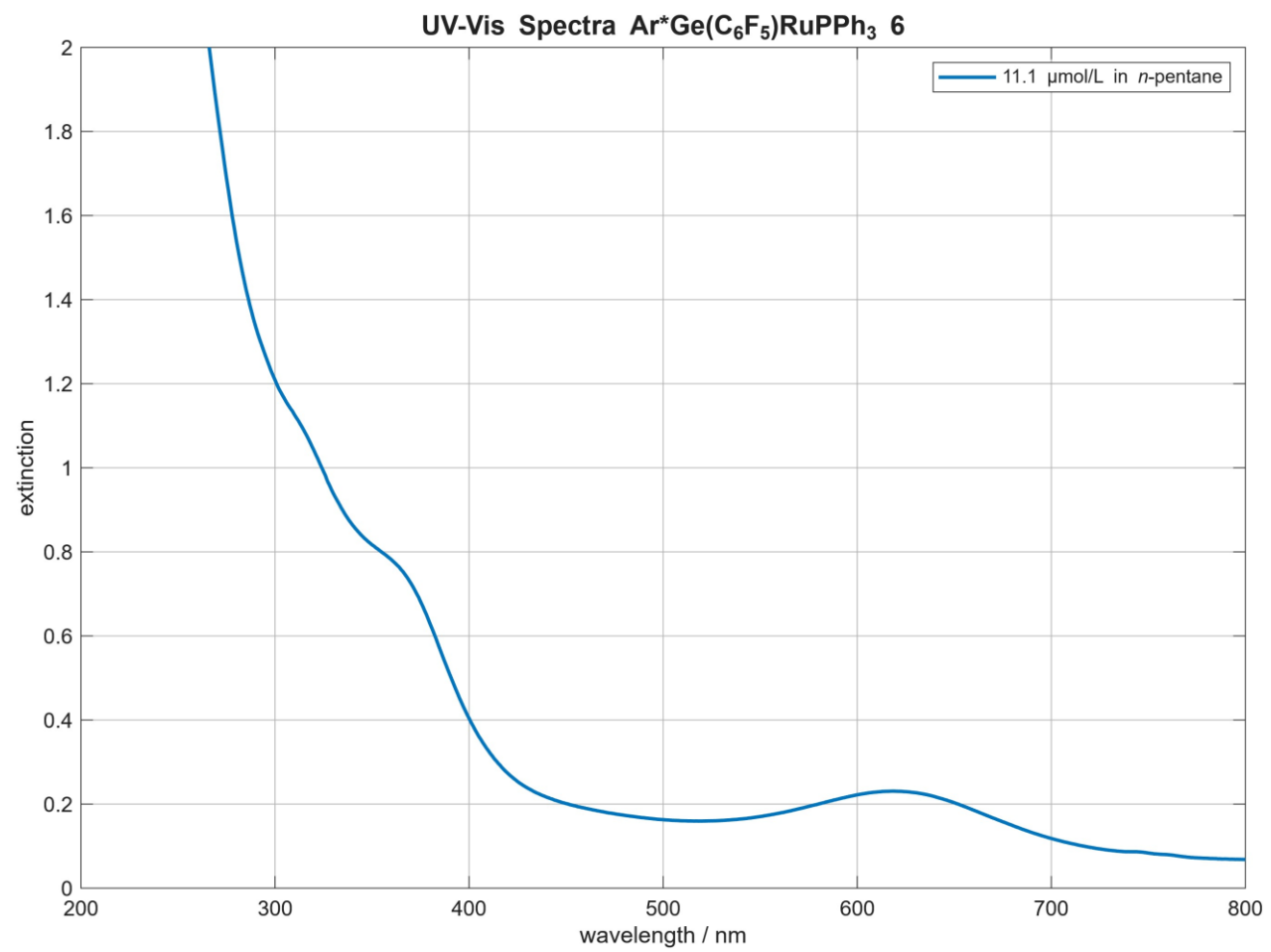


Figure SI35. UV-Vis spectrum of compound **6**.

Quantum chemical calculations

On the basis of the molecular structures of **3a**, **3b**, **4**, **5**, and **6** determined in the solid state, the structures of the complexes were optimized using the programme Orca5.0.3¹¹⁻¹³ along with BP86,^{14, 15} Grimme's dispersion correction and Becke-Johnson damping (D3BJ) with suitable RI approximations.¹⁶ The basis sets employed were def2-TZVP for Ge, Ru as implemented in ORCA5.0.3, and def2-SVP on all other elements.¹⁷⁻²⁰ For all calculations, tight or very tight convergence criteria were applied for optimisations and SCF convergence, respectively. A small imaginary frequency was obtained for **4** (-9.01 cm⁻¹). Analyses of the electronic structures were performed using NBO7, plots were generated using ChemCraft.^{21, 22}

Table SI2. Selected results of DFT calculations and NBO analyses.

	2	3a	3b	4	5	6
Ru-Ge [Å]	2.27271	2.34713	2.38133	2.30474	2.28834	2.27630
q [e] Ru, Ge	-0.47, 0.96	-0.47, 0.09	-0.51, 0.32	-0.43, 0.31	-0.45, 1.00	-0.45, 0.98
Wiberg/Löwdin	1.01/1.80	1.09/1.75	0.99/1.88	1.08/1.66	1.07/1.79	1.03/1.78
σ -bond occ.	1.8056	1.6821	1.3952	1.7537	1.7747	1.7780
Ru-Ge% (NLMO)	37, 58	55, 37	71, 23	46, 48	42, 52	41, 54
π -bond occ.	1.8652	1.8037	1.7936	1.8470	1.8553	1.8351
Ru-Ge% (NLMO)	71, 23	66, 24	71, 19	67, 26	69, 24	67, 25

[BP86-D3BJ, def2-SVP/TZVP(Ru, Ge, P, Cl, Au)]^{17, 18, 20}

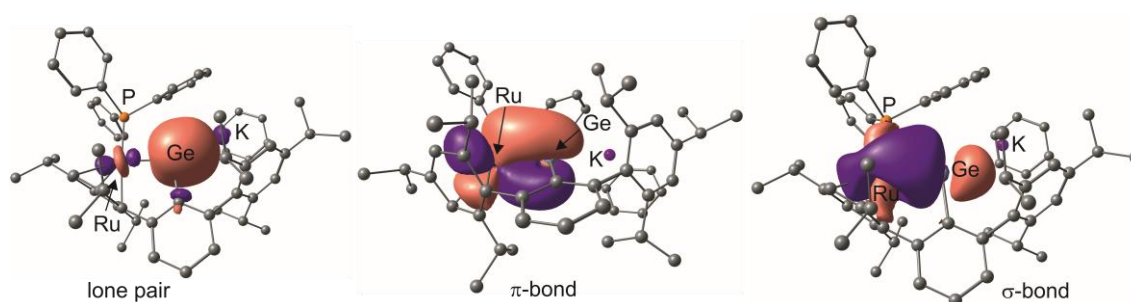


Figure SI36. NLMOs representing the Ru-Ge interactions in **3a** [lone pair: Ge 4s (78%) 4p (22%), π -bond: Ge 4p (100%), Ru 4d (100%), σ -bond: Ge 4s (16%), 4p (84%), Ru 5s(11%), 4d (89%) orbital].²¹

Calculation of Excited state spectra

Excited-state spectra of **3a** and **3b** were calculated using time-dependent density functional theory (TD-DFT) with the CAM-B3LYP functional, employing the def2-TZVP basis set and the RIJCOSX approximation as implemented in ORCA.^{17, 18, 23}

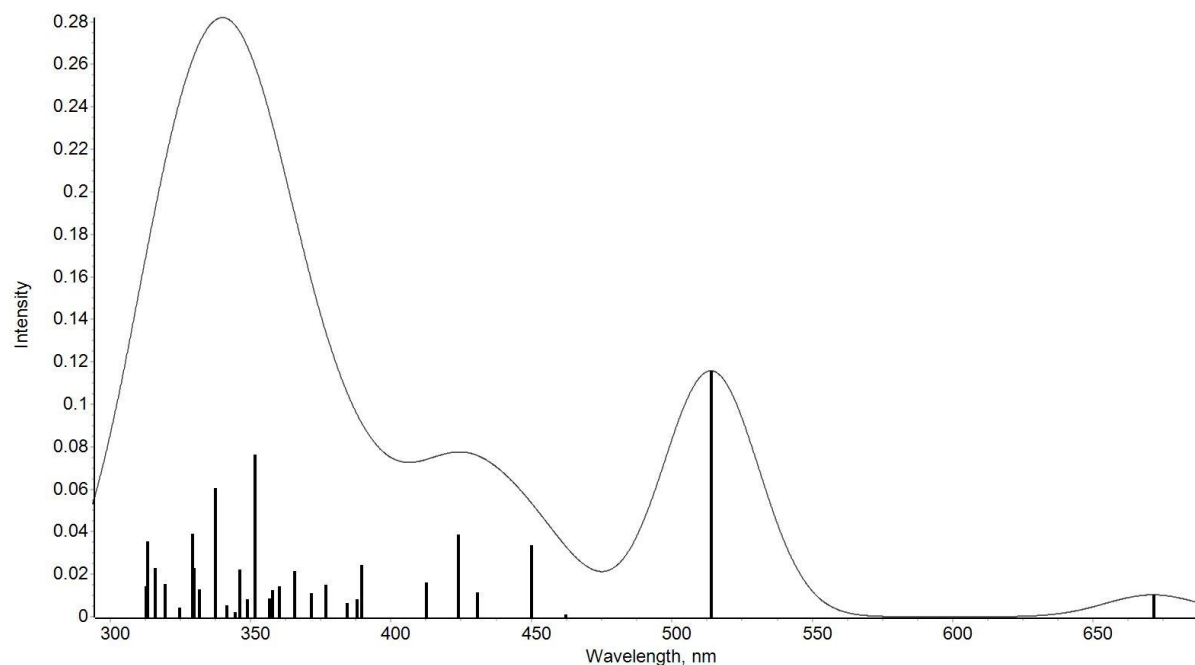


Figure SI37. Absorption spectrum computed at the TD-CAM-B3LYP/def2-TZVP level of theory of compound **3a**.

Table SI3. UV-VIS transitions (TD-CAM-B3LYP/def2TZVP) of **3a**.

State	energy (cm ⁻¹)	wavelength (nm)	fosc	Relevant Transitions
2	19457.4	513.9	0.12	HOMO → LUMO (c= 0.37849838) HOMO → LUMO⁺² (c= -0.34924516) HOMO → LUMO⁺³ (c= -0.10032208) HOMO → LUMO⁺⁸ (c= -0.10587851) HOMO⁻¹ → LUMO (c= 0.45022405) HOMO⁻¹ → LUMO⁺² (c= -0.53697752) HOMO⁻¹ → LUMO⁺⁴ (c= 0.15339810) HOMO⁻¹ → LUMO⁺⁹ (c= -0.14077980) HOMO⁻¹ → LUMO⁺²¹ (c= -0.10352862) HOMO⁻³ → LUMO⁺³ (c= 0.11319816)

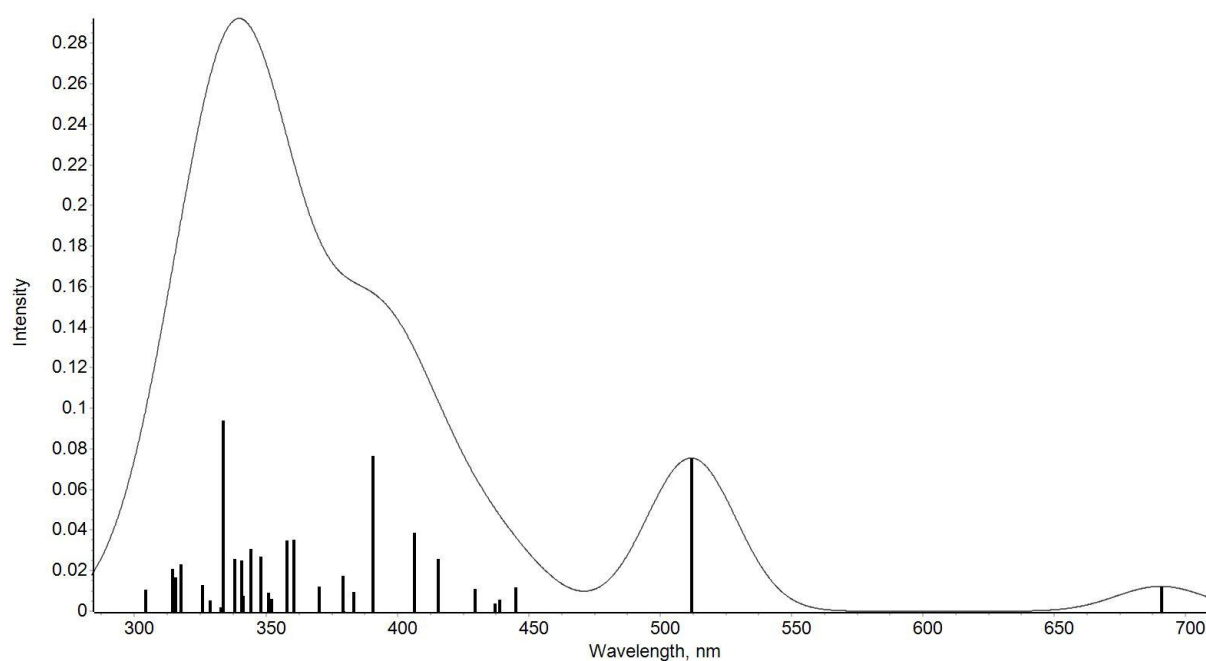


Figure SI38. Absorption spectrum computed at the TD-CAM-B3LYP/def2-TZVP level of theory of anion of compound **3b**.

Table SI4. UV-VIS transitions (TD-CAM-B3LYP/def2TZVP) of **3b**.

State	energy (cm ⁻¹)	wavelength (nm)	fosc	Relevant Transitions
2	19535.6	511.9	0.08	HOMO → LUMO ⁺⁴ (c= -0.11420294) HOMO ⁻¹ → LUMO (c= -0.70716904) HOMO ⁻¹ → LUMO ⁺¹ (c= -0.55456321) HOMO ⁻¹ → LUMO ⁺³ (c= -0.11345047) HOMO ⁻¹ → LUMO ⁺⁵ (c= -0.10180811) HOMO ⁻¹ → LUMO ⁺⁸ (c= 0.10280356) HOMO ⁻¹ → LUMO ⁺¹⁷ (c= 0.12787509)

Coordinates of optimized structures

Compound 2.

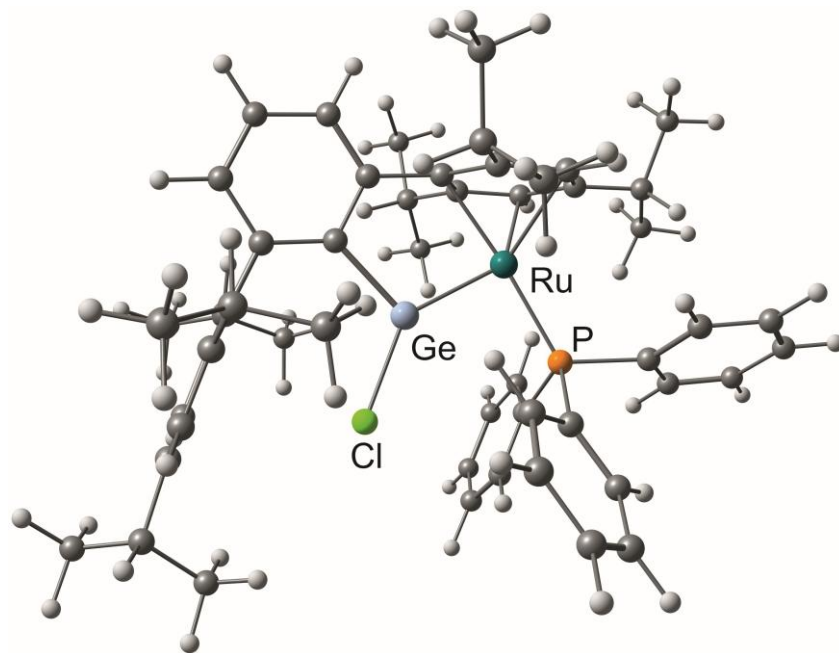


Figure SI39. Optimized structure of 2.

122
 Coordinates from ORCA-job bp86optfreq_hnumac E -5069.263510708493
 Ru 5.63793423910771 4.61351217296473 13.83545467280400
 Ge 5.19555914244482 6.54737155608290 13.03125205030311
 Cl 5.82744711285755 8.54323819393936 12.44074987537076
 C 3.56353026622735 5.47815700832933 13.87089245276632
 H 8.49748833000432 6.34750469234435 13.08349278970066
 O 9.52229395749364 7.25910457532677 12.74943303043546
 N 10.87070293927798 6.85994250830591 12.86961441265743
 S 11.66214631261994 7.5793950387863 12.60857769464669
 F 11.19900976790167 5.56907139612616 13.30520475992163
 Br 12.25391780109285 5.26669665135691 13.38939354480566
 I 10.1802770030892 6.6587803826500 13.63494101192265
 Ba 10.430654038686666 3.64171212332066 13.97348219297527
 La 8.83175847788884 5.04045191563517 13.53710156207095
 Ce 9.15778919352959 8.5251236089796 12.7303002473852
 Pr 8.89391078239281 8.83343987385664 10.8966689831332
 Nd 8.42292755835472 10.09022023796394 10.48480592129498
 Pm 1.924639872234 10.25043375663836 9.42038169862765
 Sm 8.21397599465014 11.13819515710817 11.39736236528104
 Eu 8.52289574409727 10.91568519044076 12.74892873355807
 Gd 8.36878391854462 11.73807684731257 13.46483003863442
 Tb 8.9328685360445 9.67433456276367 13.21017461065376
 Dy 9.06076085054242 7.70208085056942 9.88483849395881
 Ho 6.998296326969 6.927225969 10.360769189321
 Er 7.70955032494137 7.03920781573366 9.55667256045121
 Tm 7.83458684430349 6.22952490280854 8.80838155983735
 Yb 6.98443438391435 7.7716504330591 9.1569837616382
 Lu 7.24609099900340 6.58875339719531 10.45894005093801
 Sc 9.77812850971585 8.15979091465390 8.6031732396094
 Ti 9.98637748369758 7.29231379845890 9.843655729970
 V 10.74143817857528 8.65704748532247 8.83593553164906
 Cr 9.16284642539666 8.87466630689498 8.01839981317191
 Mn 7.51784601260895 12.4642018392076 10.961555608986
 Fe 7.66790303130059 13.15352042562037 11.81837166041883
 Co 6.13185104524414 12.28577303638475 10.57771513752579
 Ni 6.9659889608415 13.2569483845458 10.30831816824245
 Cu 5.56224852163265 11.84516512066766 11.42022061129413
 Zn 6.01969837062290 11.60216750325590 9.71031836377746
 Ga 6.4118863263683 13.1075619014232 9.786749757547
 Ge 7.99236560723543 14.10051359933991 9.53255119935785
 As 8.37752055011884 12.48084283333792 8.88091687398025
 Se 9.4777343208386 10.0695497685885 10.0695497685885
 Br 9.25614789614444 9.44275534029241 14.69701689206697
 Kr 9.97737232831285 8.60175281481157 14.77289176152708
 Rb 9.97207589748759 10.00417459812079 15.2298929406062
 Sr 8.15949130564615 8.87344645923078 16.51569605770246
 Y 7.58408034891136 8.03790251015487 15.03834417194514
 Zr 7.16313634974466 7.8509813163926 15.28669693202852
 Nb 9.8938859020989 10.65743459603905 15.39082974362477
 Mo 10.19369714777256 10.39836450474058 16.4269996382878
 Tc 9.18915433064163 11.51103647713784 15.46137538513391
 Ru 10.79448909541007 11.00819953622315 14.84751868769242
 Rh 7.7434807707910 4.06611175777809 13.8968738666541
 Pd 7.2189507968866 4.0347470450582 16.607951445036
 Ag 6.10097177831989 3.17902120829942 15.52215697504640
 Cd 5.67916823599902 3.14239997649838 16.53628145047532
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 At 8.8351208353205 5.41291447812103 17.3719706059202
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 Fr 6.41859929796296 4.62226322135049 17.99683848423480
 Ra 6.072098994994 3.93493876377711 17.99683848423480
 Ac 8.95925281483374 3.97614136607265 17.05569572633488
 Th 4.8869116851491 4.55836724321792 17.83765984547161
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 Bk 4.48745401782629 0.431535307288 16.3890498696941
 Cf 5.48151766658097 -0.36982423186474 14.78876883817375
 Es 3.9055947370310 1.1669286927945 13.67211553078887
 Fm 2.476121265541 0.6551918329896 14.03188935615382
 Md 3.87958383364573 0.49517565559617 12.93587741619716
 No 3.07354443508346 2.08896727597324 13.14823842960735
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 Rf 8.2562687007865 4.26364810597258 11.32760133287910
 Ta 6.5646574812250 3.38247532723517 10.34937167790216
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 Ir 8.6240037890893 1.4578909014925 11.035702424122
 Pt 9.08028772951389 2.17975112833204 10.19988501108941
 Au 8.08791343789487 1.17871409879796 11.31219349466243
 Hg 4.4498049211694 4.470785077961 11.9563277892957
 Tl 2.1036428429885 4.42046927730862 14.52261148159181
 Pb 2.29598995311299 4.06568790360262 15.88625935795196
 Bi 3.13734937734857 4.447048077961 16.8636129348577
 Po 1.32254360901572 3.24563129391762 16.47223083170408
 At 1.39783010116773 2.98020659939783 17.53806787901804
 Rn 0.25296138530849 2.76034720447918 16.63779010244327

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H	2.31233835614171	7.51092537994783	10.46435724933246
H	2.03784900048684	8.53767804454987	10.17763212993085
H	2.60919302986330	7.22362838332110	11.80810169836048
H	2.569560538910	8.02429837342434	12.55872980600046
H	3.20316051393808	6.99689475110480	14.85425887916152
H	1.87216209437426	7.43906278205661	15.01434247560105
H	1.04835187100816	6.87038437219289	14.55714782307159
H	1.59401731019494	8.59636841877094	15.75487200177056
H	0.55282456744304	8.93523086606050	15.87002296689526
H	2.64163923150791	9.31985866113505	16.35350489418338
H	4.2129644732986	10.22672877000120	16.83765284408181
H	3.96563572433662	8.87762753045809	16.20947457240239
H	4.79240268684959	9.43245017220731	16.67841939262328
H	4.24004859868917	7.72054803016510	15.96401041566187
H	5.27164447363468	7.35564022541614	15.34712536859867

Compound 3a.

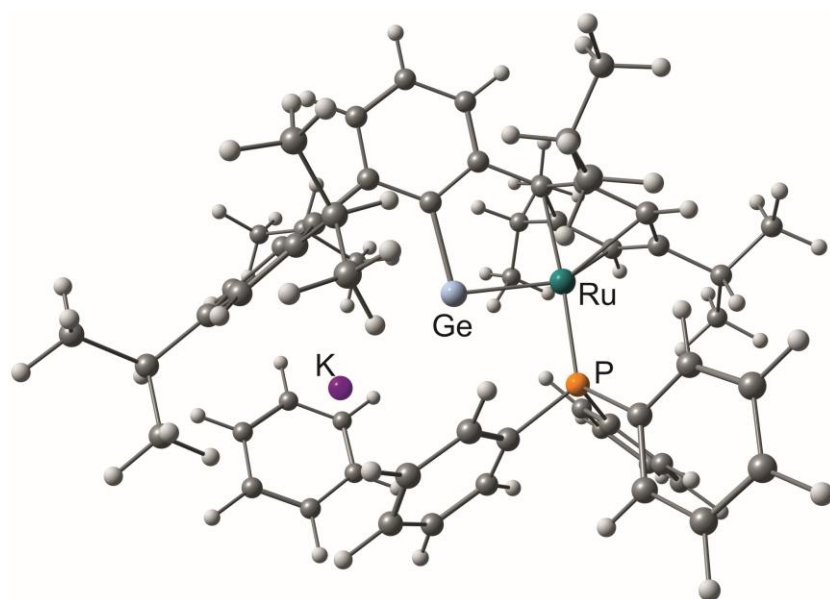
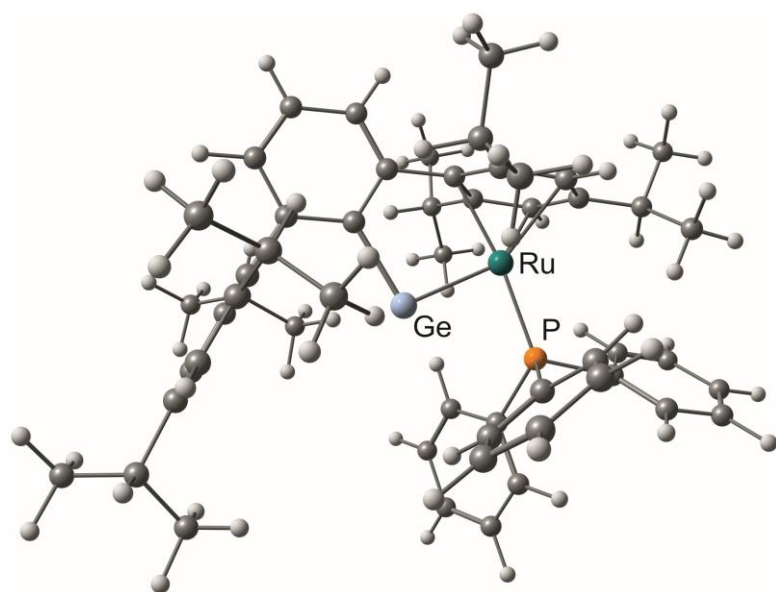


Figure SI40. Optimized structure of 3a.

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Coordinates from ORCA-job bp86optfreq_hnumac E -5441.084698086705

C	11.05300925325856	5.0718715969851	7.4785532954454
C	9.71192513452261	4.72536643581687	7.72253128185195
H	9.04771008630187	5.43311705387211	8.23937530675321
C	9.22189977084847	3.47556137324460	7.30031581165559
H	8.17539060368102	3.20016328126834	7.49568954016436
C	10.06800876238860	2.57741265638714	6.6263703261706
H	9.6848126243777	1.59893663103416	6.30060984921108
C	11.40777679538331	2.92699271977374	6.37707754097329
H	12.07139281462997	2.22413584677678	5.8521793055807
C	11.90071125444092	4.17038170055964	6.80828245935506
H	12.94918833025286	4.44107659068910	6.61765548338440
Ge	9.60719865914719	8.29184330812574	3.43055519937414
K	9.6860083941533	5.31411307263086	4.47647087635077
P	9.62650188175496	9.51620189461836	4.70633228069530
C	11.25281013231997	8.84619663912840	2.33327213032681
C	11.49654959278775	10.22824437757641	2.13736981893124
C	12.60309475946369	10.66985623528308	1.39103188254145
H	12.78344050740740	11.74918256292208	1.26265557428445
C	13.46648373361772	9.73111084641264	0.78743692933137
H	14.32351087706134	10.07286893301973	0.19685084483716
C	13.22955127721436	8.35680205346235	0.96213407602615
H	13.89760118495557	7.61994393485631	0.48636587539088
C	12.13631499454634	7.91370730431464	1.73705898190588
C	10.51086202901649	11.18210967241074	2.74121483222894
H	10.61482038557655	11.5234569404374	4.14363250285442
C	9.5770992382012	12.31691839813752	4.74568786392884
H	9.65255795703102	12.56477113098983	5.81195397125634
C	8.46436534231659	12.79033069613083	3.99063062895760
Ru	8.73641398674608	10.44404314418064	3.77521827718166
C	8.35457797770512	12.39343665579070	2.62195093681721
H	7.48422692909426	12.73208986286334	2.03869094273681
C	9.33165665629154	11.55827413401827	1.98461165614399
C	11.85211703792709	11.13859792232950	4.94619667758180
H	12.38556032659520	10.36688561746178	4.35488276115229
C	12.78508670562011	12.35778506448260	5.06994715860613
H	13.72982689779875	12.08942677918305	5.58715426323127
H	13.04413592085266	12.76210637650469	4.07059378457194
H	12.29948865091239	13.17365258503408	5.64600139671200
C	11.52679014933141	10.51755751556934	6.31029531330327
H	12.45791413731743	10.21708865303358	6.83395894677736
H	10.98351371715022	11.22224461019402	6.97393165937416
H	10.88678385571250	9.62331307575834	6.16788041684900
H	7.3650662692695	13.65083202977469	4.6029519390089
H	6.39776656593439	13.21085390729759	4.27157495371130
C	7.44535399794396	15.08605123547606	4.04407932732111
H	8.39995714374797	15.56671288575264	4.34516576843656
H	7.40103579671539	15.09747414002991	2.93642178317130
H	6.61142566298067	15.71046179532908	4.42760708893373
C	7.39393066300249	13.6604171137668	1.1351800247656
H	8.26167831498504	14.17465306537108	6.53864455954183
H	6.47594370531056	14.20323678775443	6.51726862800633
H	7.33827102585453	12.63538970402190	6.55011490780315
C	9.18642331009055	11.16647344969628	0.51986946797839
H	9.87520461857656	10.31172981594475	0.35816648664821
C	7.77247524390775	10.68399705764086	0.16982255749844
H	7.02234397963635	11.49998681247889	0.23195468087395
H	7.74078284336319	10.29056733680027	-0.86742742029138
H	7.46348370128621	9.88507530801614	0.8737848923116
C	9.64929333195810	12.31982698752993	-0.38875351775415
H	10.63207639020623	12.61642456371764	-0.15731204682436
H	9.60521293578790	12.0286136534266	-1.45923857847667
H	9.00678022496953	13.21523800202868	-0.25077349869762
C	11.87975995416145	6.45275987800202	1.94293612899304
C	10.80481083849314	5.82213409283332	1.25618506806571
C	10.55618927007447	4.46545958996057	1.48082463731954
H	9.72998642692600	3.97173173101010	0.93961372208759
C	11.33476628079605	3.69286512463591	2.37435891773253
C	12.38596011874141	4.33873349522589	3.05151158561865
H	13.00158646841762	3.74949641045020	3.74713831689900
C	12.67303854454630	5.70671640415818	2.85509465712242
C	9.96951250270436	6.60392847521794	0.24890526071246
H	10.06676548851314	7.66666518176014	0.56217331374746
C	10.68970095461319	6.51473018150210	-1.14917883420352
H	11.65147042140657	6.89261273178453	-1.13350859161446
H	10.63164667485620	5.46506531620493	-1.51199547510181
H	10.03757852865825	7.12022374116434	-1.88276000766021
C	8.49157228662434	6.19441919516407	0.23518643450636
H	7.90739031714315	6.88910314749226	-0.40110386061175
H	8.33422681014009	6.17088539441109	-0.16645272181679
H	8.07312644430029	6.24242334909006	1.26073763100376
C	11.06977643925704	2.20536577171939	2.57354605315855
H	11.70941363623175	1.87469283237720	3.42153783087085
H	11.49275390547182	1.40109948609663	1.32896933870497
H	11.35949865777732	0.31125136289883	1.48087839606644
H	10.88442119346998	1.69059525802922	0.44704494353070

H	12.55567558018861	1.58745349341696	1.07712845803439
C	9.6058319232881	1.91320389246572	2.95021576281252
H	9.3060064607544	2.44193463912924	3.87909538892661
H	8.90814190416773	2.22334173460726	2.14542108301643
H	9.44786036483726	0.82911293513562	3.12419293421779
C	13.75673196223868	6.41157457794826	3.66888933120723
H	14.2201601024701	7.16194976586790	2.99620607688778
C	14.87249504397985	5.48230354201004	4.16389531925578
H	14.50911042873046	4.76139244828265	4.92693237336311
H	15.31842219635437	4.89576245952307	3.33511297713045
H	15.68132221006314	6.07265869702756	4.63977759088894
C	13.12448762672190	7.19894663791740	4.83466868107107
H	13.89074570154122	7.78655282855619	5.38034538624905
H	12.34655651392484	7.90048797242392	4.47325319728122
H	12.64411115320490	6.51153486084614	5.55986495595112
C	6.76993830899123	7.68598487723031	4.87506410741674
C	6.67916289265614	6.93589752293838	3.67566162771976
H	6.64922268604091	7.47186699132440	2.71605053802192
C	6.55748907766696	5.53515168457441	3.70973292799565
H	6.43412780742834	4.97354273044756	2.76796652674576
C	6.55826379334431	4.85472981173935	4.94198644417552
H	6.44194224524267	3.75977834733155	4.97243232661569
C	6.68301679826731	5.59109621800602	6.13641398316341
H	6.65352924491218	5.07473563202836	7.10761535493284
C	6.79024323872263	6.99485345184984	6.09976372823771
H	6.86426685335648	7.56104133126141	7.03981921424149
C	6.65344949310683	10.05535725048995	6.45548129607716
C	7.79110033978742	10.03970394631416	7.29254837781710
H	8.74529012264899	9.69539548678079	6.86418410991053
C	7.71655206002713	10.49813529090219	8.61431389755669
H	8.61340520145907	10.47700960461232	9.25325122519721
C	6.50545035425489	11.01392654398229	9.11282977810608
H	6.44909261156064	11.39916199673609	10.14270539581695
C	5.37403683465559	11.04844505040423	8.28343429980498
H	4.42611299574360	11.46216266523032	8.66179661513829
C	5.44312665185616	10.56250398672131	6.96547161494668
H	4.55040603584776	10.59848499429445	6.32522294271295
C	5.25680370244817	9.83410690310709	3.96763178488618
C	4.11596190210686	9.07513605224398	4.30534219217737
H	4.20201799422722	8.25533537729160	5.03465327892537
C	3.88875389005395	11.16008919725152	2.43879779678655
H	3.80676233191325	11.97477440049801	1.70243472053625
C	5.13060240791817	10.86853866742945	3.02480552175002
H	6.04045396054649	11.41967335680610	2.74686497030279
C	2.87432476749663	9.35626103965564	3.71429773177754
H	1.99148266746944	8.75415426330409	3.98100009568155
C	2.75676205635097	10.40215071911804	2.78173660769695
H	1.78256249834926	10.61985625349119	2.31692006635730
H	11.43709001967576	6.04904411308775	7.80759635562625

Compound **3b**.Figure SI41. Optimized structure of **3b**.

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Coordinates from ORCA-job bp86optfreq_hnumac E -4608.980404669230

Ge	8.00706436994255	10.31575954460087	14.65144526310092
P	9.23483365690400	7.62225002691244	13.90669165483991
C	5.27366053402061	10.97065272735291	13.54008404403383
C	4.11661373483372	11.73041649699659	13.29014561555395
H	3.31562240568905	11.31495641378525	12.65632929260379
C	7.28901791724815	13.19699014809554	17.11278063376538
C	8.39075595063139	13.64569142626541	17.85910416962596
H	8.38172185598910	13.51754413747928	18.95336212670054
C	9.51654116970397	14.22301568059035	17.24451022893525
C	9.51494962522572	14.35035425080285	15.84723402722095
H	10.400644827926912	14.78553809027687	15.35449110656670
C	8.43660014021202	13.90775923287367	15.06022627423402
C	6.14013141170431	12.46196789738451	17.79711075454188
H	5.28087216429457	12.48066965384306	17.09573901800849
C	6.51639624762531	10.98307321773359	18.01411723725353
H	5.658977854093751	10.40397649121372	18.41731654679996
H	7.36791647346887	10.89078876667084	18.72102007174018
H	6.83853056004538	10.51440529963205	17.05922703307450
C	5.68530358349787	13.12656277969335	19.10591330676483
H	4.78975163814925	12.61227280030633	19.51360280161305
H	5.42961613697071	14.19516808346228	18.95065627305013
H	6.470981890277990	13.0787910253587	19.88969763100364
C	7.31169018354375	13.33214666473773	15.70035447687948
Ru	7.25790858178597	8.45916726773439	13.36204266153663
C	6.32532893586144	11.48053352847174	14.34170810863910
C	6.18767081527066	12.78381698658674	14.87781959002463
C	5.02632888929999	13.54637635177059	14.62893729348324
C	4.94097744697909	14.559680010015	15.05564900066266
C	8.51697649443875	14.00835754763316	13.54000803394922
H	7.57391527691034	13.58653250945631	13.13753164068538
C	9.67009515321961	13.15462523287479	12.98298245156648
H	9.6586559774010	13.14257716924123	11.8735695572422
H	9.5892831484888	12.10477541060910	13.34043866315278
H	10.65017605711745	13.53805284777168	13.30292892901064
C	8.60342849013032	15.47178066854132	13.07229210232461
H	8.61256600518805	15.53171693267611	11.96319840877758
H	9.52969442232440	15.96267284858551	13.44072829662421
H	7.74046702229059	16.06266540377417	13.44298651359113
C	5.47130367728911	9.61281615976818	12.94239730564641
C	6.25100451963035	9.49440772399395	11.72279554222300
C	6.51131298943009	8.18306818828426	11.20073109499901
H	7.08541710465995	8.08868137286258	10.26953021026189
C	6.0541112991620	7.00623922005219	11.86403455114436
C	5.36712939745959	7.14100971633874	13.10877853115464
H	5.05576422761097	6.22909442631664	13.64098562702751
H	5.079019222372	4.42634177109838	13.67939729653141
C	6.68777051408752	10.73532033574475	10.95242461874800
H	6.67336969796006	11.57557858637223	11.67629493546407
C	5.66962497228024	11.05654133587622	9.84291653978516
H	5.94280634376520	11.98727341404723	9.30125664018268
H	4.65319057408041	11.19159400807470	10.26541245777130
H	5.6195949638156	10.23017897914770	9.10142806517832
C	8.11976559906918	10.62924929033963	10.41520275034714
H	8.43793709284560	11.58838232883959	9.95578402352810
H	8.21924409275409	9.84314141017778	9.63663774753854
H	8.81616953262214	10.37741120037542	11.23873015076633
C	6.29589027406595	5.6187276263013	11.28770094792811
H	6.40057438596332	4.9288608963404	12.15280510145440
C	5.06748649408405	5.16281952417683	10.4732187524909
H	5.19323509339135	4.12479658928737	10.09523392837570
H	4.91258420536242	5.83027282028669	9.59888458811588
H	4.14420712771728	5.19988492128854	11.08667575258099
H	7.5819364280240	5.50397462643379	14.68855463496062
H	7.78333626228897	4.44604722384932	10.19404479437476
H	8.45171375359947	5.88392165935023	11.02817456148363
H	7.50985949320765	6.07700886131649	9.51086088934417
C	4.28763826381929	8.55373521383319	14.97525124207537
H	4.51356678795704	9.56327757132548	15.37709172798890
C	2.77581124515126	8.4884918594293	16.16418708273970
H	2.18083081062449	8.62698120240799	15.61688792455803
H	2.50161188911951	7.50566912370588	14.24823615677679
H	2.47433751438959	9.27551936483425	13.96843989700470
C	4.71069836562344	7.53206746390586	16.03812594810728
H	4.22652013946911	7.75419336474069	17.01197409406715
H	5.8113186505321	7.55910761808785	16.16418708273970
H	4.42884833001099	6.49530298296462	15.75736124997296
C	9.60023842371957	5.87169579831560	13.41687455881958
H	10.74412873710598	5.42309127838225	12.72794319536910
C	11.53438840992055	6.14046378402276	12.46134204120937
C	10.87594801519615	4.0702828463989	12.36801583249948
H	11.76844127974725	3.73750765820090	11.81357256217657
C	9.87908517104306	3.14398567400532	12.77448782837152
H	9.98312858901349	2.08470290139468	12.4303752147260
C	8.74640689503866	3.57890443701760	13.42757347121305
H	7.96143908774974	2.85874484995756	13.70912246550250

C	8.60730804580949	4.93143050757732	13.76540160620555
H	7.70892558745181	5.29884824300566	14.28846545177413
C	9.83360811272075	7.47258568737285	15.66335162260602
C	11.12320469433772	6.98949497276049	15.96267220746959
H	11.81047211111786	6.73046137856830	15.14249308476584
C	11.53739763993314	6.83866309193874	17.29530914233345
H	12.54940269048413	6.46292377705588	17.51707441128562
C	10.66094748549846	7.16616036042053	18.34594218320758
H	10.98576277614552	7.04818752101587	19.39242035034724
C	9.37174045671920	7.64171767369701	18.05506700345993
H	8.67881156146546	7.90310897391982	18.87053354489645
C	8.96446788526106	7.79350543111322	16.71936242815285
H	7.96137261238749	8.16853693252562	16.45821186939558
C	10.6185488688179	8.56051631367860	13.144461066633576
C	11.35731063320678	9.51248565119487	13.88332057936205
H	11.22938058714108	9.57288183887465	14.97279967835972
C	12.22054696980030	10.40723084952744	13.22843704478516
H	12.76709537357851	11.16050343050867	13.81781035039707
C	12.38163425776415	10.35272896026070	11.83530365996663
H	13.05782548257914	11.05700992387846	11.32547896657252
C	11.65805770863252	9.39846725449261	11.09216562950887
H	11.76511202847056	9.35312845980940	9.99660441738004
C	10.77471830504325	8.52641710678748	11.74041962019314
H	10.15821158812248	7.83087505378178	11.14986254261088
C	3.99110555494932	13.01985677554231	13.83971097804736
H	3.08647183216670	13.61796627690435	13.64465784296050
C	11.41922490477768	13.43267389624905	18.70369197461780
H	12.34099279121375	13.73074119325607	19.24799901122180
H	11.69141001559392	12.68305133272226	17.93425949380978
H	10.74564265177189	12.82902630495629	19.42829994280532
C	10.72583186638180	14.65159384105646	18.065122306899609
H	11.44762346742757	15.11605593633449	17.35651410927564
C	10.36478154717358	15.71037296242185	19.12271290025524
H	11.26620210013089	16.04926772643035	19.67673794843063
H	9.64898332923664	15.30331519097819	19.86753105608257
H	9.89001303159169	16.59719073327699	18.65568851545813

Compound 4.

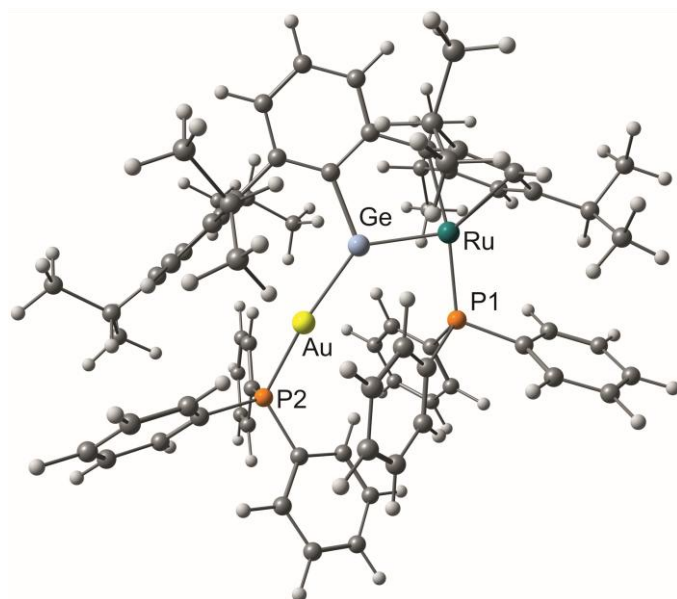


Figure SI42. Optimized structure of 4.

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Coordinates from ORCA-job bp86optfreq_hnumac E=-5780.929578887036

Au	10.93890550219480	6.29322969077136	6.18929274072640
Ru	11.09172249462762	3.28616810384839	3.04981060385656
Ge	11.93211681567550	4.66314081169910	4.69587492230781
P	9.05069826819675	4.11150243276375	3.50306263359391
C	13.90018846748675	4.47302723649629	4.46451915420702
P	9.7785933688787	7.99997641471030	7.27566087132815
C	14.90245399542960	5.14008026113206	5.20397353059966
C	16.26105043549380	4.85279903004309	4.95220400667830
H	17.03642462129497	5.36988384339421	5.53958155178010
C	16.62311694291178	3.92652289126252	3.96260332576201
H	17.68576060061581	3.71030195447822	3.77358402208151
C	15.62943321125339	3.27796719897562	3.20838469695828
H	15.90857899403354	2.55613847657285	2.42511777749867
C	14.27248213568619	3.54704868027124	3.45481103698091
C	14.52291016412110	6.16177863405435	6.22571696461619
C	14.62790708287859	7.54138445795667	5.91168201853924
C	14.30696429113272	8.48988251269558	6.90112875511116
H	14.40637257307377	9.55830469637086	6.66837439749904
C	13.86174378892150	8.10929010200020	8.17798208504705
C	13.70719990119270	6.73747168101576	8.44086503011032
H	13.33145666584628	6.43241338883327	9.42922248938692
C	14.02645886861431	5.75407544568406	7.49027085538382
C	15.01602497266784	7.97582036400603	4.49837479729482
H	15.77470335061265	7.25146104592587	4.13605808639104
C	13.81197842041729	7.86790000877937	3.53813055372438
H	14.11765665691142	8.08564211010235	2.49419928726351
H	13.01173650817425	8.58294032534933	3.81437792256887
H	13.36667272397720	6.85371749742053	3.55782468623099
C	15.64632093560457	9.37329882483304	4.42710496163457
H	16.00800503837272	9.58141931304528	3.39986771328999
H	16.50460191428854	9.47290205937193	5.12201192080415
H	14.91627928476490	10.17081987057241	4.68061054207751
C	13.61115743640521	9.11281393996629	9.29504065343693
H	12.76341529269820	8.71513089064961	9.89076059131487
C	13.22355782322759	10.51447791384221	8.80990649850843
H	14.06675940203791	11.01856840235488	8.29247928574456
H	12.93800050947544	11.15431795317104	9.66936799036374
H	12.36854287206782	10.48419571357196	8.10777631620298
C	14.83542606230482	9.17431529712097	10.23160024868982
H	15.72580708939346	9.55395815468371	9.68762524265078
H	15.08940895613837	8.17080335860542	10.62793465588272
H	14.64469495585451	9.84842560980318	11.09300672045567
C	13.88738208742123	4.27444721732817	7.83214961527609
H	13.81740940566329	3.72383772641280	6.87178291927478
C	12.60984007489513	3.95420001438909	8.62134785502229
H	11.71884946165158	4.34235206811877	8.08320698040328
H	12.62235153606028	4.39543294716781	9.64010370938653
H	12.49050818592116	2.85769254586294	8.73811003229403
C	15.15226142814876	3.77160008629626	8.55276144062795
H	16.05538463223909	3.94400907830104	7.93350222384860
H	15.08436190398266	2.68439925570532	8.76679183767955
H	15.29608966525536	4.30425699287414	9.51648523792399
C	13.18757337933178	2.86361647374856	2.67340742260374
C	12.58404235370386	1.66112390044618	3.21053618245018
C	11.46590902177870	1.08258864734129	2.52616541958490
H	11.00885647394957	0.17084779434923	2.92878045713291
C	10.93664816046103	1.66783511401969	1.33898264700190
C	11.51443866586475	2.87987886400468	0.84847780790604
H	11.07276415964754	3.35083493615909	-0.04147217425475
C	12.62420472605560	3.51082602911260	1.50052120635640
C	13.17874589601700	0.97941938965021	4.43720565696995
H	13.74697776778408	1.75655941926682	4.98865517960939
C	12.12181675533901	0.41681962589812	5.39502330956045
H	11.38800192211150	1.20281828955985	5.66028364854135

H	12.60022480948047	0.04649890984777	6.32445569453570
H	11.56228290459106	-0.43342030445294	4.95273673049148
C	14.17943469256839	-0.10232501598881	3.98916797979458
H	13.66663958736705	-0.89544645396115	3.40508015683571
H	14.66686746285683	-0.58110329745902	4.86350908085668
H	14.97410083783426	0.32810493706393	3.34780010216621
C	9.79886494300258	1.02044947225479	0.56691740422239
H	9.17975954172455	1.84822206971692	0.16205701421295
C	8.88386439026098	0.14220312678777	1.42684754620619
H	7.98996996814067	-0.16558261200613	0.84912637058405
H	8.53578616898554	0.68713959830240	2.32465263177062
H	9.39858561984462	-0.78412957167658	1.75775490159208
C	10.37238170524467	0.23161270561300	-0.62809508139897
H	9.55788215413497	-0.20042531844845	-1.24618126593092
H	11.01291000296568	-0.60331689614905	-0.27390023801607
H	10.9949005241453	0.87722925902414	-1.27996955991756
C	13.26269844719202	4.76912796797762	0.92913381937977
H	13.80012850399526	5.25670318910635	1.76834973259760
C	14.30684639975284	4.38925334397949	-0.13723454876822
H	13.82588044115089	3.86749348536189	-0.99143552014742
H	15.07862124052841	3.71216548070741	0.27999450709113
H	14.81983979078357	5.29089823186574	-0.53148417910343
C	12.23624173620746	5.77402956704259	0.39231248991430
H	12.73220931212094	6.72885252667473	0.12382039641199
H	11.45967807114465	5.97966592212083	1.15425285530126
H	11.72674584856426	5.40295166816843	-0.52155737126830
C	8.46459413297094	4.11164062430770	5.26674727756127
C	7.29837869567675	4.78786917505384	5.67330127713765
H	6.69160625037132	5.33124587822139	4.93784155027652
C	6.90828921416847	4.79895299414840	7.01975686817042
H	6.00480785194983	5.35017954601581	7.31750755932380
C	7.68393230290356	4.13800685164433	7.98585559441580
H	7.38717357085107	4.16732460204787	9.04568336778919
C	8.83176626179042	3.43404117453012	7.58911421122919
H	9.44092797424561	2.89664901417998	8.33179813035332
C	9.21062083732118	3.41701165878596	6.23782264766908
H	10.11079223500100	2.87799587745664	5.90660711788479
C	7.63630345851993	3.29714706768442	2.65996812074475
C	6.73658730703779	2.44405933455642	3.32855661603831
H	6.8252500995878	2.30609355233755	4.41599196932254
C	5.73013054711732	1.77114659075350	2.61627011506303
H	5.03537989531869	1.10582238162540	3.15200314069467
C	5.60688550409417	1.94667478155728	1.22860194779633
H	4.81557968738195	1.42194814400994	0.67163943131804
C	6.50036246616904	2.79773368368745	0.55382603504870
H	6.41047702208532	2.94135686880982	-0.53419625777434
C	5.71028904559415	3.46205569381918	1.26346840578142
H	8.21141594995875	4.12784818943235	0.73649311369087
C	6.88330533705585	5.89040919906008	3.05701916846372
C	7.38750825427435	6.33387071415792	2.71375385919648
H	6.56038726532830	5.61206154601788	2.65035535587196
C	7.14023020698828	7.68807335761207	2.43243747652373
H	6.12483425245084	8.00866410184568	2.15084719947906
C	8.17901570296239	8.63121956122323	2.51397269308065
H	7.98142402363107	9.69479579067913	2.31124664937873
C	9.47410703953439	8.20165019513432	2.84705524477972
H	10.30149867040452	8.92410798088691	2.91268309392482
C	9.72062370520276	6.84195076543190	3.09086271115680
H	10.74371598681664	6.49790014956345	3.30036601177192
C	7.96282779819709	7.98105152008222	7.22930816119937
C	7.16303541142363	7.96151781366573	8.38666837934612
H	7.63249241301167	7.93885256388685	9.38032652714612
C	5.76333219784246	7.97677242319189	8.26946296472106
H	5.14052190404423	7.96177445801328	9.17694304410884
C	5.16077321931560	8.01470192989204	7.00109523727756
H	4.06380654594810	8.03077461884213	6.91221243218616
C	5.96219386288228	8.02643832219418	5.84539738903680
H	5.50359262150863	8.04523249706917	4.84576686343641
C	7.35707330621897	7.99982576085967	5.95664310510164
H	7.98093921926574	7.99490552166797	5.05192544001341
C	10.16287585596453	9.59833828542519	6.49493301102989
C	11.36763317343988	9.70071084385694	5.77428190831297
H	12.02703185452903	8.82202935454526	5.71629428058548
C	11.71278787371348	10.90410785165261	5.14324023179762
H	12.65617227860958	10.97277933631141	4.58070074663720
C	10.85250982283092	12.01120795355702	5.22471434176799
H	11.11966573436895	12.95516447926788	4.72550718064904
C	9.64322507940665	11.91057777394284	5.93526792085368
H	8.96303426459061	12.77412898192481	5.99157742267251
C	9.29451862836452	10.70693523687775	6.56597366967666
H	8.33579444526389	10.62030778184574	7.09858098430453
C	10.16136606753689	8.17742553544663	9.04346328040501
C	10.10952341814109	9.41012046647304	9.72201014539839
H	9.87191602616460	10.33113577140808	9.17070128723170
C	10.38204305647572	9.46452107646053	11.09711750718408
H	10.35309784261677	10.43119228111829	11.62221747481672
C	10.70127872935238	8.28984235099895	11.80001373771165
H	10.92254737042155	8.33679990790043	12.87710068422637
C	10.74622198349788	7.05730163651177	11.12616983054168
H	11.00099059256308	6.13630594732887	11.67192473372952
C	10.48102014798277	7.00099023189442	9.75010362308089
H	10.53290032226396	6.04575043391390	9.20673134073157

Compound 5.

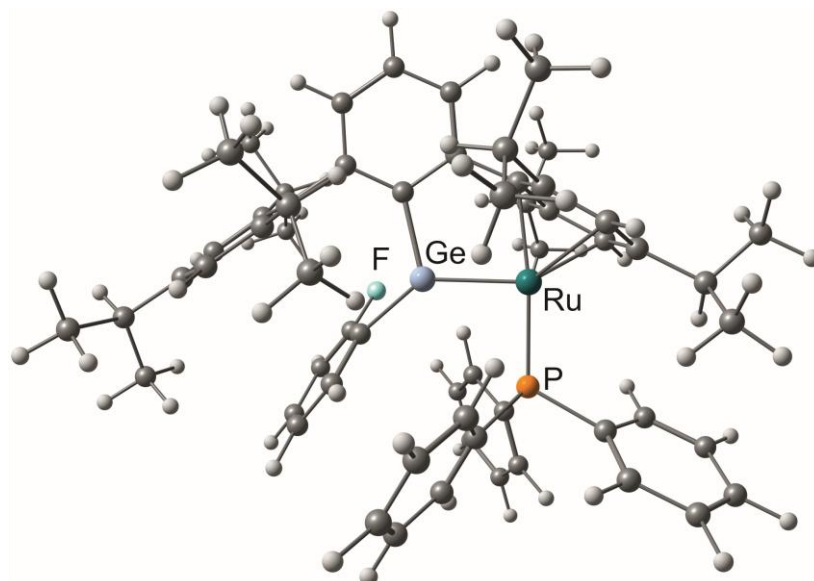


Figure SI43. Optimized structure of 5.

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Coordinates from ORCA-job bp86optfreq_hnumac E -4939.637810182548

Ru	5.54982084850912	2.17091256884478	8.00447620347388
Ge	3.86963807774423	3.65472077204142	8.46467819286517
P	6.03985970104469	3.25661213460371	6.09374781440579
F	4.41655268343535	6.39673174423899	9.60309446856605
C	3.28482275990124	3.22154364303926	10.30546394206210
C	2.18304490138123	3.74442446018908	11.02477039234881
C	1.90500785221711	3.24318765025456	12.31393659480609
H	1.03157255337007	3.62791583576989	12.86070776478958
C	2.7045833363404	2.24473682017434	12.88770380698715
H	2.47417447818810	1.86722418454370	13.89557994488828
C	3.77670037511659	1.70037818174811	12.16169484474305
H	4.38240984164284	0.88718234878379	12.59024410239303
C	4.06129530870020	2.17253868477523	10.86930915019910
C	1.27714313004232	4.73913776068688	10.37536957473981
C	1.24619631837911	6.09586853810811	10.80013964925605
C	0.39754897813438	6.99116924226643	10.13128026598599
H	0.36212473401838	8.04166946217939	10.46136914767071
C	-0.43255235176193	6.59462879093274	9.06696335487264
C	-0.38694346576180	5.25078399765752	8.67030210264704
H	-1.03649755010047	4.90652825022790	7.85266126209905
C	4.44557443385828	4.31238521093389	9.3077791817457
C	2.04552960590307	6.57372309999392	12.01051073441035
H	2.85336303566165	5.83347389365795	12.18593907224132
C	2.70873351344937	7.94731962684887	11.81583405002634
H	3.37392275107651	7.95103677919302	10.93435039989331
H	3.31937322512165	8.20473950810865	12.70570711172622
H	1.95863632044847	8.75601150724606	11.69338845163172
C	1.14328687265609	6.60091683457988	13.26222462446452
H	0.32570560087634	7.34133080677711	13.13521206599677
H	1.72387840072128	6.88403635485882	14.16500928409467
H	0.67030119583261	5.61825866548492	13.45353633502428
C	-1.34840359561941	7.62336220958800	8.41062282950191
H	-1.75739064931561	8.24521698783396	9.23942203956950
C	-0.55084044647599	8.56109830560777	7.48480154852204
H	-0.12834963901059	7.99269181703725	6.63235720267838
H	0.30173693179651	9.02752269289308	8.01675378570753
H	-1.19730110040478	9.36894208187719	7.08251811620567
C	-2.53959749515989	7.00743559019074	7.66479179426787
H	-3.22738490130510	7.80114363344332	7.30877444187590
H	-3.1175562453774	6.31629172482830	8.31104416856053
H	-2.20822680166195	6.43896209927208	6.77055451347749
C	0.33558466040341	2.84239473816076	8.90251512931807
H	1.10309251885274	2.27646897980257	9.46623670877524
C	0.60774125929620	2.60457399326363	7.40910493628983
H	-0.05173158229287	3.21475889002143	6.75855729477571
H	0.45128697087041	1.53918284926904	7.14641987378695
H	1.65877642359361	2.85227564884366	7.14778915135704
C	-1.03550286653586	2.27965007400027	9.32482822403213
H	-1.86404427885532	2.78589815952369	8.78684777550984
H	-1.20466559642571	2.42315800700480	10.41101092961546
H	-1.10160349259832	1.19352000715433	9.10487704739309
C	5.11881016991940	1.51036461425704	10.02969871132038
C	4.71031951530691	0.44914192519862	9.13012743094018
C	5.67216771410088	-0.11143330812631	8.22978450548814
H	5.36654486819430	-0.91785826700064	7.55298090522710
C	7.01632898960405	0.35951995544157	8.20017969771167
C	7.39925310878217	1.42368606956408	9.07765553666721
H	8.42771236019482	1.80612442063289	9.01930854363562
C	6.47609698327487	2.02952626173351	9.98998153179847
C	3.29398013193745	-0.11143841779737	9.18105375842175
H	2.65107176412283	0.67831780743669	9.61974293227616
C	2.72289439431716	-0.45237875235483	7.79966135919231
H	2.79673822684733	0.42330892842453	7.12658015749896
H	1.65610074318131	-0.74203783434318	7.88607357799890
H	3.25401432459907	-1.30128071605969	7.32152145479033

C	3.25781517830764	-1.32426667376910	10.12958622541302
H	2.22655572542571	-1.72182722267373	10.22513645828385
H	3.61432644559667	-1.05223171194638	11.14264435137459
H	3.90728985334308	-2.14095599729380	9.74996824022370
C	8.06226884967169	-0.27319186459996	7.29823935061013
H	8.73373069837457	0.54589913455899	6.96804091183952
C	8.90516176611704	-1.27264290258428	8.11652021146581
H	8.27433812589321	-2.10929547189140	8.48362610242569
H	9.36586027078637	-0.78765357619364	9.00075857157575
H	9.71846766970653	-1.70358862752012	7.49670855735421
C	7.48411875258516	-0.92804222295667	6.03908272569791
H	6.80435853331822	-0.23652806180998	5.50601010799917
H	6.92281059070986	-1.85529845749077	6.27919372237195
H	8.29857683541614	-1.20606445860281	5.34148106643911
C	6.91771982699674	3.11673500561850	10.95914478109817
H	6.02061321110634	3.73821488196648	11.16317385720496
C	8.00664642632188	4.03129998682040	10.38402006721161
H	8.98363470907625	3.51036388165449	10.30344858283200
H	8.16062427252888	4.90950619965946	11.04256195751886
H	7.72853035034327	4.39471705102007	9.37630745657303
C	7.36841778918325	2.48058776634989	12.28826003357197
H	8.24251914920015	1.81515456553050	12.12653670242656
H	6.56063077686447	1.87465517299195	12.74292941855305
H	7.66256398032546	3.26080863927189	13.02015074613768
C	4.61628797383322	3.50027318288587	4.94090212640829
C	4.45161342344762	4.62259824735246	4.10864562061414
H	5.19243310937085	5.43318230467388	4.12351660283730
C	3.31882911155266	4.73657629365188	3.28601827268497
C	3.19258539370675	5.63127028394097	2.65715820695243
C	2.34226003241106	3.72802961213731	3.27958793641473
H	1.45021263240897	3.82536235024878	2.64177956779432
C	2.50647849765639	2.59577081791425	4.09746170578403
H	1.74629509734996	1.79974675197620	4.10247064472168
C	3.63313592790339	2.48914160022489	4.92544696579513
H	3.75972340944460	1.63280821128505	5.60575500606512
C	7.27702491475134	2.48205142687904	4.97679680739464
C	6.9339553290732	1.85077829718822	3.76610021817453
H	5.88741141405579	1.85536842828956	3.42671832960575
C	7.91910642987506	1.22022989471270	2.98882997550096
H	7.63697772794768	0.72994578783528	2.04430354395632
C	9.25880207376981	1.21984473889353	3.40891675147018
H	10.03095516007715	0.72892018654393	2.79706320474118
C	9.61109281152567	1.85776419266301	4.61174492809203
H	10.66078536695379	1.86895989380844	4.94385677512214
C	8.62648618999565	2.48097637407585	5.39099945230272
H	8.90186619213786	2.98869822317490	6.32860517309800
C	6.75959760085891	4.95770939595708	6.18001583613783
C	7.44948177749873	5.53291281919900	5.08988328135508
H	7.61186702714522	4.94691495436780	4.17305420087763
C	7.93990074012232	6.84468471018127	5.17215296158319
H	8.47645697550107	7.28175209596950	4.31570783239197
C	7.75036528156414	7.59848490493014	6.34427726347008
H	8.13557239065675	8.62805477060945	6.40600546841665
C	7.08002950173822	7.02756745536539	7.43678281028168
H	6.93143546001553	7.59981546127741	8.36484190635385
C	6.59784098816445	5.7129594776568	7.35208068291915
H	6.09671384396357	5.24285286808359	8.21032112000838
C	3.2466908554893	5.39348943345653	7.79989445634098
C	2.55752668286893	5.57529860369899	6.58490991300967
H	2.19263141594540	4.69977497357178	6.03104007414806
C	2.3489595773492	6.85773386478576	6.05607887945329
H	1.82186284357591	6.96962185916266	5.09716186703961
C	2.82678706541015	7.98867656152291	6.73726108174963
H	2.67096397192384	8.99532226104526	6.32146559276711
C	3.50676196622240	7.84028026606137	7.95602856033297
H	3.90229432947628	8.70363522137224	8.50913410757487
C	3.69903381134564	6.54785236977768	8.44711784029283

Compound 6.

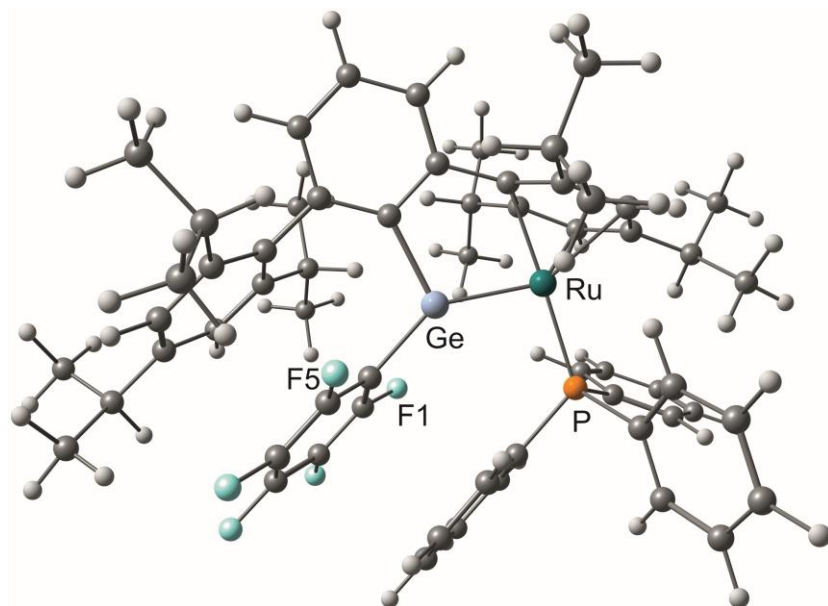


Figure SI44. Optimized structure of 6.

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Coordinates from ORCA-job bp86optfreq_hnumac E -5336.281969821012

Ru	12.52312808637063	10.04873762687408	3.81238254973482
Ge	12.93226364853443	7.82754979687568	4.09607194747880
P	14.62145708677344	10.74524974091367	4.25793171766898
F	15.30723040246345	7.13568883346401	2.12634153563904
C	11.20226643378918	6.90027956866577	3.75936467479872
F	17.29909287047239	5.29378055006428	2.37176688540031
C	10.88123795373032	5.52023055838216	3.73617595259441
F	17.48118078253935	3.76428878469718	4.63844526971168
C	9.53413933864007	5.13479400909100	3.54535245650019
H	9.29350017589261	4.06241377004548	3.51082390181509
F	15.67267675857333	4.09617734108979	6.67909130459716
C	8.52164120085282	6.08085835655533	3.34988049227949
H	7.48206172759388	5.75319256685938	3.19830074573991
F	13.66885844094083	5.95097076581703	6.41791267416989
C	8.84707963090715	7.44590158530351	3.30225339219123
H	8.07178853785202	8.19925856676632	3.09483617612129
C	10.17416308883206	7.85605003786509	3.50366967118872
C	11.93254201678128	4.45633664683952	3.80749956563280
C	12.80931092534605	4.26583804520691	2.69619778733803
C	13.79212458823163	3.26990395275396	2.78629938867857
H	14.48793634670773	3.12278806106864	1.94804316620459
C	13.94191642529648	2.45130521271178	3.92067090846664
C	13.05773431850016	2.64380843310245	4.98909979018950
H	13.15664172424232	2.02283250090525	5.88962902253076
C	12.05127374397945	3.62981366919008	4.95453264024217
C	12.691736033905410	5.10980768003126	1.42232735209258
H	12.66374976226721	6.17638961101605	1.73993179982169
C	11.38102477262649	4.82838369866047	0.65922351934692
H	11.32588731571716	5.45758466447282	-0.25325293828481
H	10.48361638705923	5.03815683477240	1.26827101675072
H	11.33953427802794	3.76527011156453	0.34268856161202
C	13.87178809806765	4.95297029757951	0.45261876725150
H	13.88342710949018	3.94335643186636	-0.00857975647800
H	14.85260616688496	5.12004777485188	0.93265650627028
H	13.77804909539937	5.68910954288399	-0.37047099192221
C	15.02778385034616	1.38184643551477	3.92006928451058
H	15.91643859764861	1.83922993240487	3.42969857821157
C	15.45840301906028	0.92581501790465	5.31984236472000
H	15.75337018950190	1.78350817607060	5.95332275001418
H	16.32218799352136	0.23410128066343	5.25161292388653
H	14.64330272976947	0.37972870388550	5.83940581706049
C	14.58765758590763	0.18080034261056	3.05761013596472
H	14.32033116779304	0.49540436355935	2.02890969781922
H	13.69399618842199	-0.30641921265301	3.50091238432150
H	15.39455002231228	-0.57817820012751	2.98793596085315
C	11.10256002262003	3.75932596017841	6.14501496817470
H	10.64305468136165	4.76858270857450	6.09235869415780
C	9.97197810026511	2.71291584814724	6.05337861517481
H	9.39736037308101	2.79781822885638	5.11153521167557
H	9.26092413151267	2.82359530158655	6.89852355796384
H	10.39261486814732	1.68623181391627	6.09393978355600
C	11.80664313255743	3.63234341209560	7.50868494312358
H	12.14456724169058	2.59211533545398	7.69820507338388
H	11.10477888050967	3.8954128330983	8.32640750230832
H	12.68875840587549	4.29307865169906	7.57816415034988
C	10.52900802611023	9.30986862309430	3.36636373413445
C	10.41627887059157	10.21287169996645	4.49500219790585
C	10.89220943894537	11.55664968276817	4.35156073043405
H	10.80331797904243	12.24898690430389	5.19871242148118
C	11.51097568448376	12.00380051068597	3.14123432672964
H	11.62935216693684	11.09208053974663	2.04518877551528
H	12.13131066406740	11.43522845857472	1.12946858728757
C	11.14764510797725	9.74716904165405	2.12526499449987

C	9.74219439672701	9.75398619511537	5.78082061055337
H	9.72344726559683	8.64516703822098	5.74681612056278
C	8.28360768646321	10.24934992383355	5.80293839460356
H	8.24239679418121	11.35864248810001	5.83021049953728
H	7.74750533965452	9.86531630330415	6.69493794025980
H	7.73052676838859	9.91604619812772	4.90213003540950
C	10.50530830627648	10.15838493284293	7.04810328848842
H	11.54527564165260	9.77928934596913	7.00659795883130
H	10.00987840984281	9.73889804815152	7.94706332777488
H	10.54256246310158	11.26010467110594	7.18061680237393
C	12.01397709220355	13.42679079710564	2.94350175054978
H	12.93606273693508	13.34931605437378	2.32882744742898
C	12.37950368258342	14.15627221541866	4.23892423148802
H	12.83936629952745	15.13763746122142	4.00778239841657
H	13.10287751815697	13.57823830708195	4.84330042960938
H	11.48675477131695	14.35289100545321	4.86900362093960
C	10.97189593386381	14.22288647819341	2.13118340065242
H	11.34201786052504	15.24519230878942	1.91075585584340
H	10.02119577793423	14.3168894719528	2.69684706233466
H	10.74129904200514	13.72609756827922	1.16744302849029
C	11.20895182847672	8.82608602280630	0.91345141104814
H	11.07594195565607	7.79187516673828	1.28785663297761
C	10.01898296535523	9.13599919702379	-0.01354951920977
H	10.08600536234237	10.16853989211765	-0.41649770795975
H	9.05685397182401	9.04697554674206	0.52981071491004
H	9.99360437881143	8.43326683656124	-0.87133569673684
C	12.550482289895740	8.86954515680623	0.17338547318266
H	12.55533511167434	8.13124523749338	-0.65356234186694
H	13.37936887164129	8.62501257261460	0.86647990821016
H	12.75287535663358	9.86463366773958	-0.27463414295743
C	14.91705096954699	11.68051610324572	5.82091773168700
C	13.83037334506006	11.94490305784653	6.67057423386490
H	12.83775610124051	11.58377440848296	6.36401889598569
C	14.01978318077230	12.62911429250003	7.88240929039698
H	13.16021075643961	12.82581423116257	8.54153486844895
C	15.30604611440382	13.05140797505350	8.25321238148822
H	15.46034356454112	13.58559696095407	9.20343923156442
C	16.40260440066003	12.77760558702080	7.41477515748934
H	17.41461725911413	13.09554033195353	7.70961612402045
C	16.21117713406023	12.08906286901468	6.20851435889224
H	17.07415991451458	11.85471395548120	5.56678670172367
C	15.19424417204277	11.91517413455651	2.95853551799656
C	15.61598979019952	13.23525829129724	3.20456187183100
H	15.71302171613424	13.59828147545879	4.23700164222138
C	15.88441421179760	14.10693631754789	2.13452537248484
H	16.19397627291892	15.14281331480338	2.34243457171251
C	15.75587301663207	13.66383301667723	0.80939688581790
H	15.96651250479723	14.34858579507507	-0.02632064558371
C	15.34922758804824	12.34099087145502	0.55490032975120
H	15.24412600511715	11.98345511945486	-0.48107383986649
C	15.05618099006705	11.48070607763093	1.62117684756748
H	14.67835440876635	10.46515436084249	1.43104080278129
C	16.01453162100095	9.55847401732679	4.41723886889691
C	16.99230718909412	9.36323016286537	3.42577869018479
H	16.95080248981813	9.93962312559841	2.49115682328334
C	18.02702524644285	8.43430711838669	3.62546978208146
H	18.77866741297425	8.27866083386535	2.83716739364093
C	18.10235442254551	7.70536888335244	4.82278394620067
H	18.91256677423145	6.97620776198942	4.97510726325436
C	17.1336422234813	7.90226871666247	5.82150494159787
H	17.18386403679116	7.3333885647436	6.76207879758173
C	16.09215302978057	8.81581795403423	5.61542750355090
H	15.32910302006781	8.96452302602201	6.39463365305106
C	14.40645367640596	6.53731130216867	4.24887266107285
C	15.36618209093709	6.38513408366866	3.24925380834311
C	16.40337380107175	5.45040174995607	3.35852120695286
C	16.49563962628573	4.66565833546613	4.51859802242113
C	15.56810264373229	4.83109532782810	5.55984159640556
C	14.54100400597741	5.76609961221905	5.40057615486629

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