

Supporting information for:

Stepwise Reduction of a Base-Stabilised Ferrocenyl Aluminium(III) Dihalide for the Synthesis of Structurally-Diverse Dialane Species

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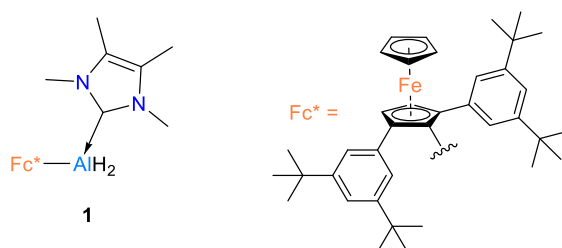
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Methods and materials

All manipulations were performed under an atmosphere of dry argon using glovebox or standard Schlenk line techniques. Deuterated solvents were dried over 4 Å molecular sieves and degassed by three freeze-pump-thaw cycles. All other solvents were dried by distillation from appropriate drying agents under an argon atmosphere and stored under argon over activated 4 Å molecular sieves. All NMR spectra were obtained from a Bruker Avance III HD 300 NMR spectrometer ($^{13}\text{C}\{^1\text{H}\}$: 75.5 MHz), from a Bruker Avance I 400 NMR spectrometer (^1H : 400.6 MHz, $^{13}\text{C}\{^1\text{H}\}$: 100.6 MHz) at 298 K unless otherwise stated. Chemical shifts (δ) are provided in ppm and internally referenced to the carbon nuclei ($^{13}\text{C}\{^1\text{H}\}$), residual protons (^1H) of the solvent. ^{27}Al NMR spectra were referenced to external $\text{Al}(\text{NO}_3)_3$. UV/vis absorption spectra were measured on a METTLER TOLEDO UV/VIS-Excellence UV5 spectrophotometer. Solid-state IR spectra were recorded on a Bruker FT-IR spectrometer ALPHA II inside a glovebox. Microanalyses (C, H, N, S) were performed on an Elementar vario MICRO cube elemental analyzer. High-resolution mass spectrometry (HRMS) data were obtained from a Thermo Scientific Exactive Plus spectrometer. Aluminum hydride *N,N*-dimethylethylamine complex solution was purchased from Sigma-Aldrich / Merck and used without further purification. Iodomethane was purchased commercially, dried over CaH_2 , and degassed via the freeze-pump-thaw method. NHC^{Me_4} (1,3,4,5-tetramethylimidazolin-2-ylidene) $^1\text{KC}_8$, $^2\text{Fc}^*\text{Li}^3$ and $\text{NHC}^{\text{Me}_4}\cdot\text{AlH}_3^4$ were synthesised according to the literature procedures.

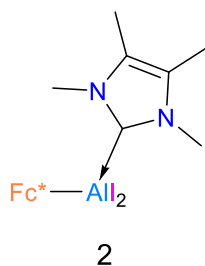
Synthetic procedures

Synthesis of **1**



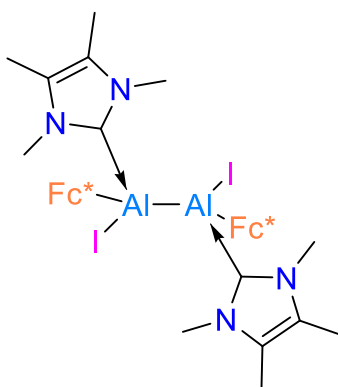
$\text{NHC}^{\text{Me}_4} \cdot \text{AlH}_3$ (0.542 g 3.51 mmol) and $\text{Fc}^* \text{Li}$ (2 g, 3.51 mmol) were added to a dry Schlenk flask and the flask was cooled to -78°C followed by addition of 50 mL of toluene. The reaction mixture was then warmed to room temperature over 3 h and then stirred for 12 h. After completion of the reaction (as confirmed by ^1H NMR spectroscopy) the volatiles were evaporated and solid was extracted with 150 mL of toluene. Toluene was then evaporated and solid was washed with 10 mL of cold (-35°C) hexane to obtain a pure orange powder (**1**). X-ray quality crystals were grown from a saturated hexane solution at room temperature overnight. Yield: 2.1 g (85%). ^1H NMR (400 MHz, C_6D_6 , 298 K): $\delta = 1.05$ (s, 6H, $\text{CH}_3\text{-C-C-CH}_3$, NHC^{Me_4}), 2.42 (s, 36H, CH_3 , *t*Bu), 2.97 (s, 6H, N- CH_3 , NHC^{Me_4}), 4.35 (s, 5H, C-*H*, Cp), 4.98 (s, 2H, C-*H*, Cp), 7.41 (s, 2H, Ar-*H*), 7.96 (d, $^4J = 1.6$ Hz, 4H, Ar-*H*) ppm. *The Al-H signal was not found due to quadrupolar broadening by the Al nucleus.* $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 298 K): $\delta = 7.9$ (2C, $\text{CH}_3\text{-C-C-CH}_3$, NHC^{Me_4}), 32.2 (CH_3 , *t*Bu), 33.4 (2C, N- CH_3 from NHC^{Me_4}), 35.3 (C- CH_3 , *t*Bu), 71.8 (5C, unsubstituted Cp ring), 72.7 (2C, unsubstituted Cp ring), 99.6 (2C, Cp- C_q), 119.8 (2C, Ar-*CH*), 124.9 (2C, $\text{CH}_3\text{-C-C-CH}_3$), 125.8 (1C, Ar- C_q), 128.3 (1C, Ar- C_q), 142.7 (1C, Ar- C_q), 149.5 (1C, Ar- C_q) ppm. *We did not observe the signals for the carbene carbon or quaternary carbon nucleus attached to aluminium due to quadrupolar broadening by the Al nucleus.* $^{27}\text{Al}\{^1\text{H}\}$ NMR (78.2 MHz, C_6D_6 , 298 K): $\delta = 112.4$ (br) ppm. UV/vis $\lambda_{\text{max}} = 303, 369$ nm. FT-IR (KBr, cm^{-1}): $\bar{\nu}$ (cm^{-1}) = 1818 (vw), 1744 (w), 1642 (w), 1591 (s), 1478 (m), 1454 (m), 1420 (w), 1393 (w), 1360 (s), 1308 (w), 14240 (s), 1194 (w), 1158 (w), 1102 (m), 1047 (mw), 1007 (w), 900 (m), 870 (s), 706 (vs), 678 (s). Elemental Analysis: Calcd. for ($\text{C}_{45}\text{H}_{63}\text{AlFeN}_2$): C, 75.61; H, 8.88; N, 3.92. Found: C, 75.47; H, 8.72; N, 3.87.

Synthesis of 2



1 (1.50 g, 2.10 mmol) was added to a dry Schlenk flask and dissolved in 200 mL toluene. The mixture was then cooled to 0 °C followed by addition of iodomethane (0.70 mL, 10.5 mmol). The flask was then fitted with an oil bubbler to allow release of byproduct methane and stirred for 12 h at room temperature. After completion of the reaction (confirmed by ^1H NMR spectroscopy) the volatiles were evaporated and the residue was washed with 15 mL of cold hexane to obtain a orange powder. Yield: 1.60 g (80 %). X-ray quality single crystals were grown from a saturated toluene solution at -30 °C overnight. ^1H NMR (400 MHz, C_6D_6 , 298 K): δ = 1.00 (s, 6H, $\text{CH}_3\text{-C-C-CH}_3$, NHC^{Me_4}), 2.41 (s, 36H, CH_3 , *t*Bu), 3.26 (s, 6H, N- CH_3 , NHC^{Me_4}), 4.46 (s, 5H, C-*H*, unsubstituted Cp), 4.86 (s, 2H, C-*H*, substituted Cp), 7.38 (s, 2H, Ar-*H*), 7.80 (s, 4H, Ar-*H*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 298 K): δ = 8.2 (2C, $\text{CH}_3\text{-C-C-CH}_3$, NHC^{Me_4}), 32.46 (12C, CH_3 , *t*Bu), 35.27 (2C, N- CH_3 from NHC^{Me_4}), 35.63 (C-(CH_3)₃ from *t*Bu), 72.76 (2C, C-*H*, Cp), 73.2 (5C, C-*H*, Cp), 100.0 (2C, Cp- C_q), 121.34 (2C, Ar-*CH*), 125.6 (3C, Ar-*CH*), 126.0 (2C, $\text{CH}_3\text{-C-C-CH}_3$), 128.5 (Ar- C_q), 128.7 (1C, Ar-*CH*), 128.9 (Ar- C_q), 141.7 (Ar- C_q), 150.2 (Ar- C_q) ppm. *We did not observe signals for the carbene carbon and quaternary carbon nuclei attached to aluminium due to quadrupolar broadening by the Al nucleus. Likewise, no signal was observed in the ^{27}Al NMR spectrum.* UV/vis (λ_{max}) = 459 nm. FT-IR (KBr, cm^{-1}): $\bar{\nu}$ (cm^{-1}) = 1651 (mw), 1597 (vs), 1454 (s), 1398 (s), 1360 (vs), 1552 (w), 1251 (s), 1200 (w), 1103 (mw), 1050 (mw), 996 (mw), 900 (mw), 870 (s), 843 (s), 830 (s), 818 (s), 714 (vs), 690 (w). Elemental Analysis: Calcd. for ($\text{C}_{45}\text{H}_{61}\text{AlI}_2\text{Fe}$): C, 55.92; H, 6.36; N, 2.90. Found: C, 55.58; H, 6.29; N, 2.85.

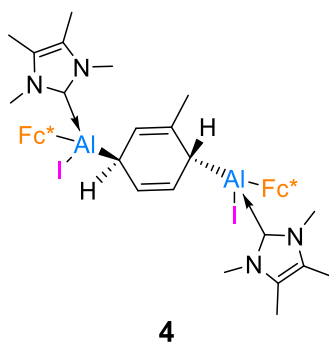
Synthesis of **3**



3

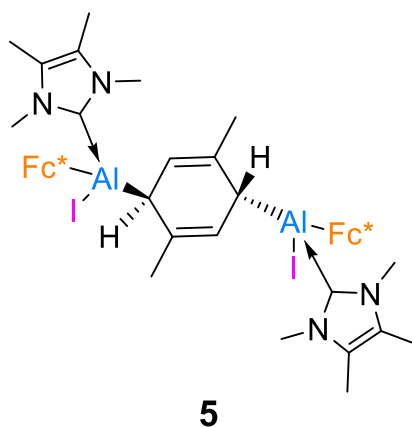
In a glovebox, dry hexane (10 mL) was added to a vial containing **2** (0.29 g, 0.30 mmol) and freshly prepared potassium graphite (0.06 g, 0.45 mmol) at room temperature. The reaction mixture was then stirred vigorously for 3 d at room temperature. A ^1H NMR spectrum of the resulting mixture showed consumption of all starting materials **2**. The solution was filtered and the filtrate evaporated to obtain an orange residue, which was extracted with *n*-hexane (7 mL). The resulting hexane solution was then kept at room temperature overnight (ca. 24 h), during which time orange crystals grew, which were filtered and dried under vacuum. Yield: 145 mg (58%). ^1H NMR (400 MHz, C_6D_6 , 297 K): δ = 1.33 (br, 36H, 30H from CH_3 of *t*Bu and 6H from hexane), 1.49 (12H, $\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 1.56 (s, 42H, CH_3 of *t*Bu), 2.33 (s, 6H, N- CH_3 of NHC^{Me_4}), 4.06 (s, 6H, N- CH_3 of NHC^{Me_4}), 4.38 (s, 10H, unsubstituted CH of Cp), 4.43 (d, $^3J = 2.2$, 2H, CH substituted Cp), 4.49 (d, $^3J = 2.2$, 2H, CH substituted Cp), 7.10 (t, $^4J = 1.85$ Hz, 2H, Ar-*H*), 7.16 (br, s, 8H, Ar-*H*), 7.40 (t, $^4J = 1.85$ Hz, 2H, Ar-*H*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 297 K) (selected) δ = 8.9 (2C, $\text{CH}_3\text{-C-C-CH}_3$, of NHC^{Me_4}), 9.45 (2C, $\text{CH}_3\text{-C-C-CH}_3$, of NHC^{Me_4}), 32.1 (CH_3 of *t*Bu), 32.2 (CH_3 of *t*Bu), 32.3 (CH_3 of *t*Bu), 32.87 (CH_3 of *t*Bu), 34.8 (1C, N- CH_3 of NHC^{Me_4}), 35.3 (1C, N- CH_3 of NHC^{Me_4}), 35.7 (2C, N- CH_3 of NHC^{Me_4}), 71.9 (CH of substituted Cp), 72.0 (CH , substituted Cp), 72.5 (CH , unsubstituted Cp), 119.6 (Ar- CH), 121.0 (Ar- CH), 125.4 (2C, $\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 125.5 (2C, $\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 128.3 (Ar- CH), 128.47 (Ar- CH), 128.52 (Ar- CH), 128.75 (Ar- CH), 128.93 (Ar- CH), 142.09 (C_q), 143.86 (C_q), 148.29 (C_q), 151.25 (C_q), 165.26 (C_q) (carbene carbon, confirmed by HMBC) ppm. No signal was observed in the ^{27}Al NMR spectrum. UV/vis $\lambda_{\text{max}} = 470$ nm. FT-IR (KBr, cm^{-1}): $\bar{\nu}$ (cm^{-1}) = 1660 (mw), 1591 (s), 1398 (m), 1360 (s), 1251 (s), 1211 (w), 1109 (m), 1058 (w), 996 (w), 899 (w), 877 (m), 809 (s), 740 (w), 713 (s), 500 (m). Elemental analysis for $[\text{C}_{90}\text{H}_{122}\text{Al}_2\text{Fe}_2\text{I}_2\text{N}_4]$ ($M_w = 1679.46$): calcd. C 64.37, H 7.32, N 3.34; found C 64.11, H 7.76, N 3.10.

Synthesis of 4



In a glovebox, dry toluene (5 mL) was added to a vial containing **2** (0.20 g, 0.21 mmol) and freshly prepared potassium graphite (0.04 g, 0.31 mmol) at $-35\text{ }^{\circ}\text{C}$ (cooled inside glovebox freezer). The reaction mixture was then stirred vigorously for 30 h at room temperature. A ^1H NMR spectrum of the resulting mixture showed consumption of all of the starting material **2**. The solution was filtered and evaporated to obtain an orange residue, which was extracted with *n*-hexane (5 mL). The resulting hexane solution was then kept at room temperature overnight (ca. 24 h), during which time orange crystals grew, which were filtered and dried under vacuum. Yield: 35 mg (20%). ^1H NMR (300 MHz, toluene- d_8 , 297 K): δ = 1.06 (br, 1H, Al-CH), 1.08 (br, 1H, CH, Al-CH), 1.34 (s, 36H, *t*Bu), 1.35 (s, 36H, *t*Bu), 1.40 (s, 3H, CH_3 of toluene unit), 1.48 (s, 12H, $\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 1.50 (s, 3H, N- CH_3 of NHC^{Me_4}), 1.58 (s, 3H, N- CH_3 of NHC^{Me_4}), 2.81 (s, 3H, N- CH_3 of NHC^{Me_4}), 3.72 (s, 3H, N- CH_3 of NHC^{Me_4}), 4.12 (s, 10H, CH-Cp), 4.16 (d, $^3J=3.7$, 1H, CH-Cp), 4.37 (br, 2H, CH-Cp), 4.78 (d, $^3J=2.2$ Hz., 1H, CH-Cp), 4.83 (br, 3H, C-H, vinyl), 7.10 (t, $^4J=2$ Hz, 2H, Ar-CH), 7.15 (t, $^4J=2$ Hz, 2H, Ar-CH), 7.7 (br, 4H), 7.8 (br, 4H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, toluene- d_8 , 297 K) selected signals: δ = 22.8 (CH_3 of toluene), 31.7 (CH_3 of *t*Bu), 31.8 (N- CH_3 , NHC^{Me_4}), 31.9 (CH_3 of *t*Bu), 32.0 (CH_3 of *t*Bu), 32.1 (CH_3 of of *t*Bu), 34.9 (N- CH_3 , NHC^{Me_4}), 68.1 (1C, CH of substituted Cp), 72.7 (10C, CH of Cp, unsubstituted), 72.9 (2C, CH of substituted Cp), 98.6 (C_q , of substituted Cp), 120.5, 121.8 (CH of Ar-H) ppm. UV/Vis $\lambda_{\text{max}} = 303, 369$ nm. FT-IR (KBr, cm^{-1}): $\bar{\nu}$ (cm^{-1}) = 2958 (vs), 2861 (s), 1653 (w), 1597 (vs), 1478 (s), 1450 (s), 1393 (m), 1364 (s), 1251 (s), 1200 (w), 1115 (m), 1063 (m), 995 (m), 877 (s), 809 (s), 718 (s). Elemental analysis for $[\text{C}_{97}\text{H}_{130}\text{Al}_2\text{Fe}_2\text{I}_2\text{N}_4]$ ($M_w = 1771.60$): calcd. C 65.76, H 7.40, N 3.16, found C 65.30, H 7.44, N 3.18. *Comments: Compound 4 is not soluble enough to obtain ^{13}C NMR data of sufficient quality, and moreover it is unstable in toluene and benzene. Consequently, we present only selected signals that we could assign unambiguously using 2D spectra.*

Synthesis of **5**



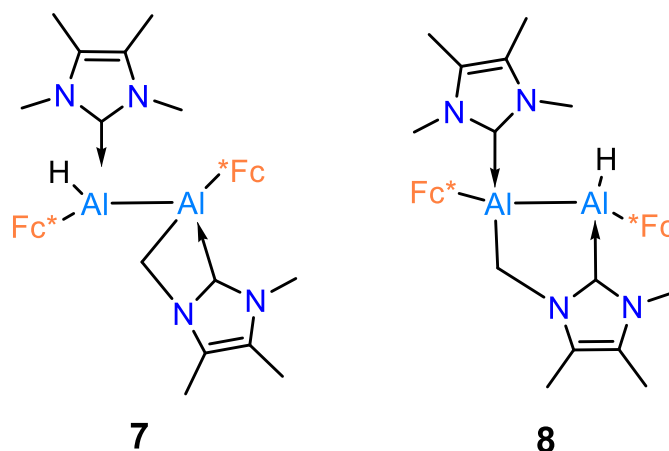
In a glovebox, dry *p*-xylene (5 mL) was added to a vial containing **2** (0.17 g, 0.17 mmol) and freshly prepared potassium graphite (0.03 g, 0.26 mmol) at room temperature. The reaction mixture was then stirred vigorously for 30 h at room temperature. A ^1H NMR spectrum of the resulting mixture showed consumption of all of the starting material **2**. The solution was filtered and evaporated to obtain an orange residue, which was extracted with *n*-pentane (5 mL). The resulting pentane solution was then kept at room temperature overnight (ca. 24 h), resulting in orange crystals that were separated (20 mg (14%)) from the mother liquor. Attempts to obtain further crops of crystals from the mother liquor provided only mixtures of **5** and **3**.

*Comments: The NMR data were recorded using toluene solutions, however, the crystalline compound is poorly soluble in benzene or toluene. After recording the ^{13}C NMR data, the ^1H NMR spectrum showed a significant amount of decomposition product. ^1H NMR experiments have shown that decomposition is noted after an hour in benzene or toluene, and complete decomposition was observed within 24 h, leading to Fc^*H . Compound **5** immediately decomposed in THF and CH_2Cl_2 into an unidentified product. This instability rationalises the low yield and the microanalysis data. Nevertheless, the stability of **5** is sufficient to obtain relatively clean ^1H NMR data. However, we present only selected ^{13}C NMR signals that we could assign unambiguously using 2D spectra.*

^1H NMR (400 MHz, toluene- d_8 , 297 K): δ = 0.66 (s, 2H, CH of Al-C-H), 1.32 (s, 18H, CH_3 of *t*Bu), 1.36 (s, 18H, CH_3 of *t*Bu), 1.40 (s, 36H, CH_3 of *t*Bu), 1.51 (s, 12H, from $\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 1.55 (br, 3H, CH_3 from xylene unit), 1.84 (s, 3H, CH_3 from xylene unit), 2.76 (s, 3H, N- CH_3 of NHC^{Me_4}), 2.90 (br, 3H, 3H, N- CH_3 of NHC^{Me_4}), 3.73 (br, 3H, 3H, N- CH_3 of NHC^{Me_4}), 3.92 (s, 3H, 3H, N- CH_3 of NHC^{Me_4}), 4.00 (br, 1H, vinylic C-H), 4.12 (s, 5H, unsubstituted Cp ring), 4.13 (s, 5H, unsubstituted Cp ring), 4.62 (dd, 3J = 2 Hz, 2H, substituted Cp ring, two coincident doublets appear as a triplet), 4.72 (d, 3J = 2 Hz, 1H, substituted Cp ring), 4.75 (d, 3J = 2 Hz, 1H, substituted Cp ring), 5.23 (br, 1H, vinylic C-H), 7.07-7.09 (m, 3H, Ar-H), 7.18 (t,

$^3J = 2.0$ Hz, 1H Ar-*H*), 7.63-8.02 (m, 8H, Ar-*H*) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, C_6D_6 , 297 K) (selected) $\delta = 8.5$ ($\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 9.3 ($\text{CH}_3\text{-C-C-CH}_3$ of NHC^{Me_4}), 27.5 (C- CH_3 , from xylene unit), 31.7 (CH_3 , from *t*Bu), 31.9 (CH_3 , from *t*Bu), 32.0 (CH_3 from *t*Bu), 32.0 (C- CH_3 , xylene unit), 35.0 (N- CH_3 of NHC^{Me_4}), 35.1 (N- CH_3 , NHC^{Me_4}), 70.3 (C-H, substituted Cp ring), 71.5 (C-H, substituted CP ring), 72.8 (C-H, unsubstituted CP ring), 72.8 (C-H, unsubstituted Cp ring), 119.8 (vinylic-C-H), 121.7 (CH, Ar-CH), 125.5 (Ar-CH), 128.3 (Ar-CH), 129.3 (Ar-CH) ppm.

Synthesis of 7 and 8



Path a: In a glovebox, dry hexane (10 mL) was added to a vial containing **2** (0.20 g, 0.21 mmol) and freshly prepared potassium graphite (0.14 g, 1.05 mmol) at room temperature. The reaction mixture was then stirred vigorously for 10 d at room temperature. A ^1H NMR spectrum of the resulting mixture showed consumption of all of the starting material **2**. The solution was filtered and the filtrate evaporated to obtain an orange residue, which was extracted with *n*-hexane (5 mL). The resulting hexane solution was then kept at room temperature overnight (ca. 20 h), during which time orange crystals of **8** grew, which were filtered and dried under vacuum. Yield of **8**: 45 mg (30%).

Path b: In a glovebox, dry hexane (5 mL) was added to a vial containing **3** (0.10 g, 0.06 mmol) and freshly prepared potassium graphite (0.02 g, 0.18 mmol) at room temperature. The reaction mixture was then stirred vigorously for 5 d at room temperature. A ^1H NMR spectrum of the resulting mixture showed consumption of all of the starting material **3**. The solution was filtered and the filtrate evaporated to obtain an orange residue, which was extracted with *n*-hexane (3 mL). The resulting hexane solution was then kept at room temperature overnight, during which time orange crystals of **8** grew, which were filtered and dried under vacuum. Yield of **8**: 43 mg (50%).

Comments: When the reaction in path a and path b was stopped after 5 days and 1 day respectively, we obtained mostly 8 and a few crystals of 7. Several attempts were made to obtain 7 exclusively by recrystallisation and varying the reaction time and temperature, but we were unable to isolate pure 7. We have characterised 7 only by single-crystal molecular structure determination.

¹H NMR (400 MHz, C₆D₆, 297 K) for **8**: δ = 1.14 (s, 18H, CH₃ of *t*Bu), 1.19 (s, 6H, CH₃-C-CCH₃ of NHC^{Me4}), 1.27 (s, 21H, CH₃ of *t*Bu), 1.38 (s, 18H, CH₃ of *t*Bu), 1.54 (br, 9H, 3H from CH₃ of *t*Bu, 6H from CH₃-C-C-CH₃ of NHC^{Me4}), 1.56 (br, 12H, CH₃ of *t*Bu), 2.20 (d, ²J_{HH} = 12 Hz, 1H, N-CH₂-Al), 2.44 (d, ²J_{HH} = 12 Hz, 1H, N-CH₂-Al), 2.94 (s, 6H, N-CH₃ of NHC^{Me4}), 3.64 (s, 3H, N-CH₃ of activated NHC^{Me4}), 4.20 (s, 5H, CH of unsubstituted Cp), 4.26 (s, 5H, CH of unsubstituted Cp), 4.64 (d, ²J_{HH} = 2 Hz., 1H, CH of substituted Cp ring), 4.68 (d, ²J_{HH} = 2 Hz., 1H, CH of substituted Cp), 4.77 (d, ²J_{HH} = 2 Hz, 1H, CH of substituted Cp), 5.08 (br, s, CH of substituted Cp ring), 7.11 (s, 1H, Ar-H), 7.16 (Ar-H, 1H coincidental with the benzene signal), 7.33 (t, 1H, ³J = 1.8 Hz), 7.43 (br, s, 5H, Ar-H), 7.79 (s, 2H, Ar-H), 8.35 (br, 2H, Ar-H) ppm. ¹³C {¹H} NMR (100 MHz, C₆D₆, 297 K) δ = 8.6 (CH₃-C-C-CH₃, of NHC^{Me4}), 9.0 (CH₃-C-C-CH₃, of NHC^{Me4}), 9.8 (CH₃-C-C-CH₃, of NHC^{Me4}), 32.0 (CH₃ of *t*Bu), 32.2 (CH₃ of *t*Bu), 32.3 (CH₃ of *t*Bu), 32.4 (CH₃ of *t*Bu), 32.6 (CH₃ of *t*Bu), 34.9 (C_q-CH₃ of *t*Bu), 35.0 (C, N-CH₃, NHC^{Me4}), 35.3 (N-CH₃, NHC^{Me4}), 35.6 (C_q-CH₃ of *t*Bu), 71.9 (CH, from Cp), 72.4 (CH from Cp), 99.7 (C_q, from CP), 99.8 (C_q, from Cp), 119.9 (Ar-CH), 120.0 (Ar-CH), 120.2 (Ar-CH), 123.4 (CH₃-C-C-CH₃, NHC^{Me4}), 124.0 (Ar-CH), 124.5 (Ar-CH), 125.5 (Ar-CH), 128.3 (Ar-CH), 128.5 (Ar-CH), 128.7 (C_q), 128.9 (C_q), 144.1 (C_q), 144.7 (C_q), 148.7 (C_q), 149.0 (C_q), 149.83 (C_q), 149.8 (C_q) ppm. *The signals for the carbon nuclei bound to aluminium were not observed due to high quadrupole moment of aluminium. No signal was observed in the ²⁷Al NMR spectrum.* UV/Vis λ_{max} = 401, 334 nm. FT-IR (KBr, cm⁻¹): $\bar{\nu}$ (cm⁻¹) = 1769 (w), 1654 (w), 1590 (s), 1477 (m), 1438 (s), 1395 (m), 1358 (s), 1385 (w), 1246 (s), 1203 (w), 1107 (w), 1054 (w), 1005 (w), 973 (w), 899 (w), 837 (s), 836 (m), 816 (vs), 742 (m), 709 (s). Elemental analysis for [C₉₀H₁₂₂Al₂Fe₂N₄] (M_w = 1425.65): calcd. C 75.82, H 8.63, N 3.93, found C 75.83, H 8.68, N 3.81.

Oxidation of 3 by iodine

3 (0.030 g, 0.02 mmol, in 1 mL hexane) was added to a dry Schlenk tube. The tube was then cooled to $-78\text{ }^{\circ}\text{C}$, followed by the addition of a toluene solution of iodine (0.02 mmol, 4.5 mL of a 0.004 M solution). The mixture was then allowed to warm to room temperature overnight. After completion of the reaction (confirmed by ^1H NMR spectroscopy) the volatiles were evaporated. ^1H NMR of the crude reaction mixture showed the presence of Fc*H and an unidentified mixture of products.

Oxidation of 8 by iodine

8 (0.020 g, 0.01 mmol, 2 mL hexane) was added to a dry Schlenk tube. The tube was then cooled to $-78\text{ }^{\circ}\text{C}$, followed by the addition of a toluene solution of iodine (0.03 mmol, 7.1 mL of 0.004 M solution). The mixture was then allowed to warm to room temperature overnight. After completion of the reaction (confirmed by ^1H NMR spectroscopy) the volatiles were evaporated. ^1H NMR of the crude reaction mixture showed the presence of **2**, Fc*H and Fc*I (33:43:23 relative product ratio as noted from ^1H NMR data).

NMR spectra

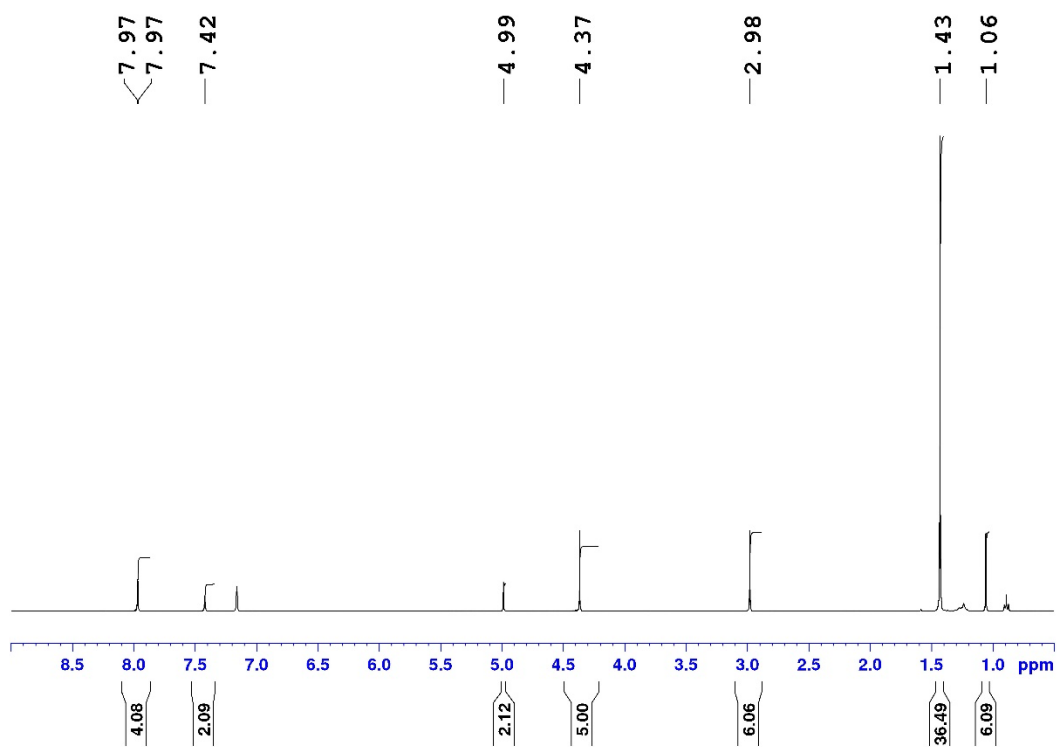


Figure S1. ^1H NMR spectrum of **1** in C_6D_6 at RT.

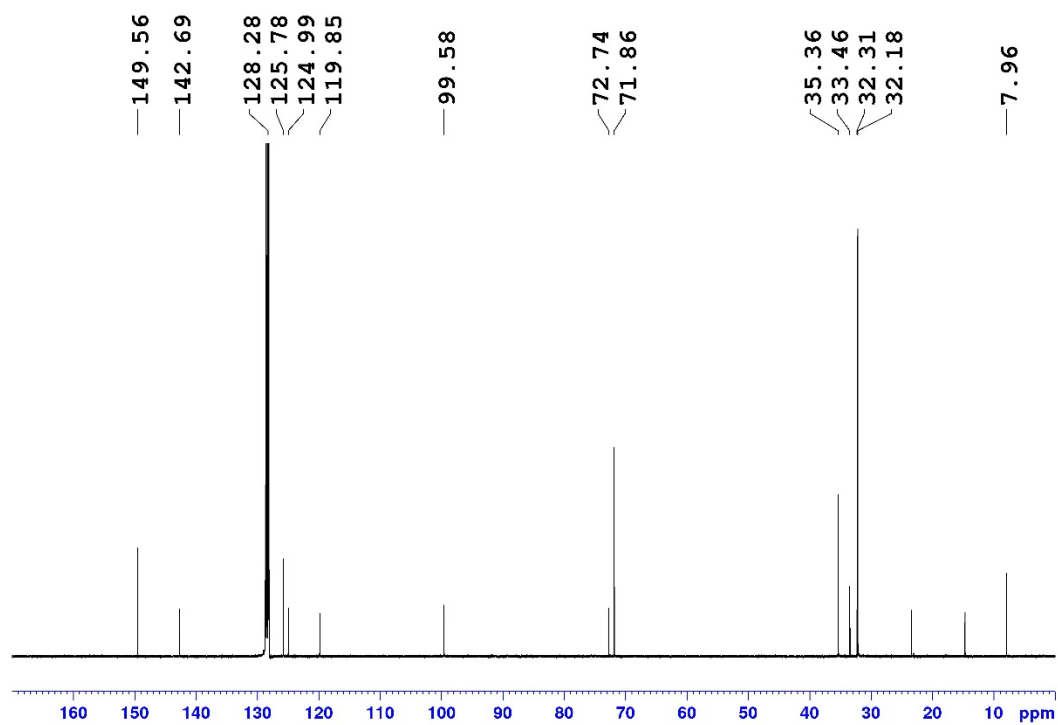


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** in C_6D_6 at RT.

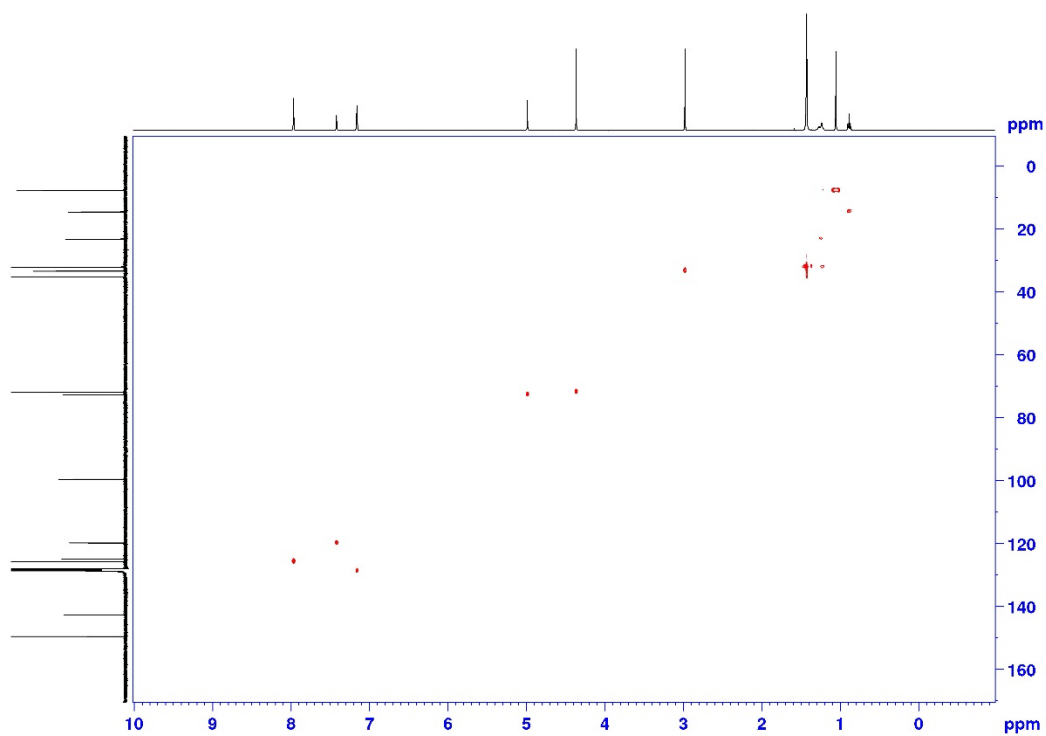


Figure S3. ^{13}C - ^1H HSQC NMR spectrum of **2** in C_6D_6 at RT

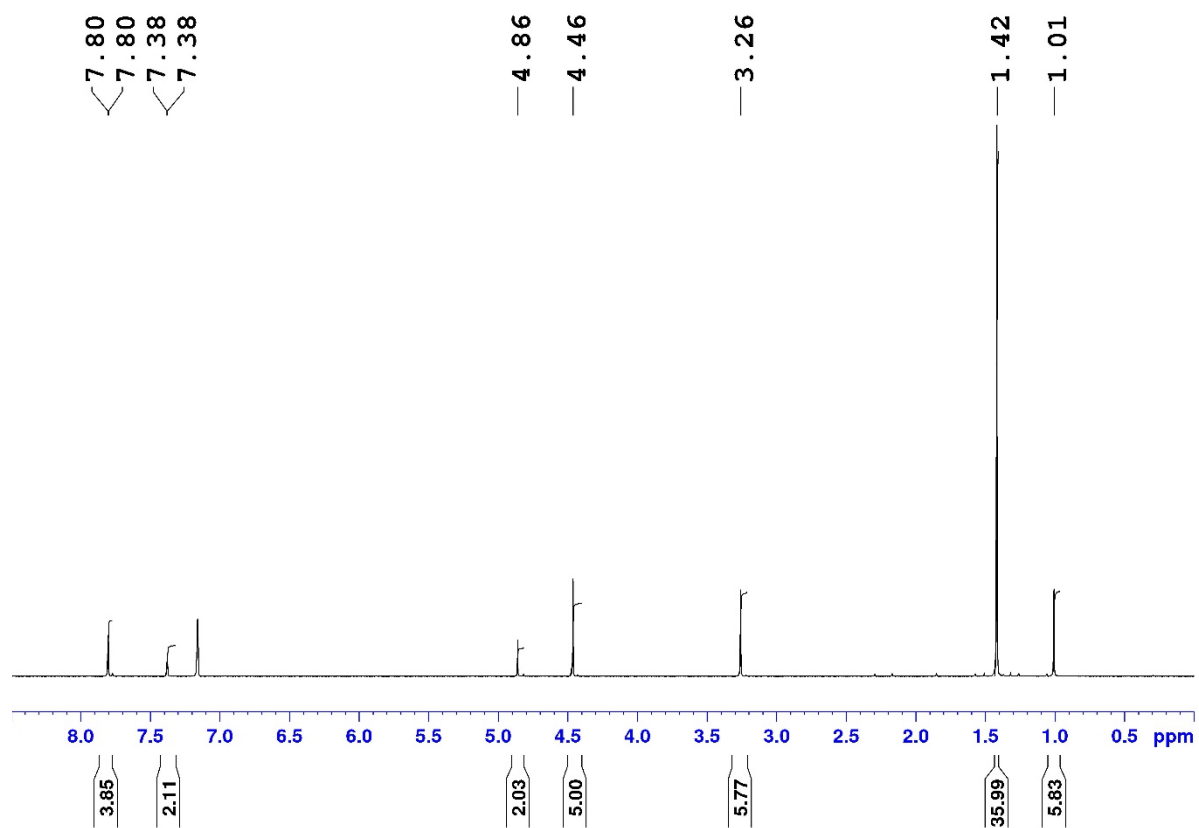


Figure S4. ^1H NMR spectrum of **2** in C_6D_6 at RT.

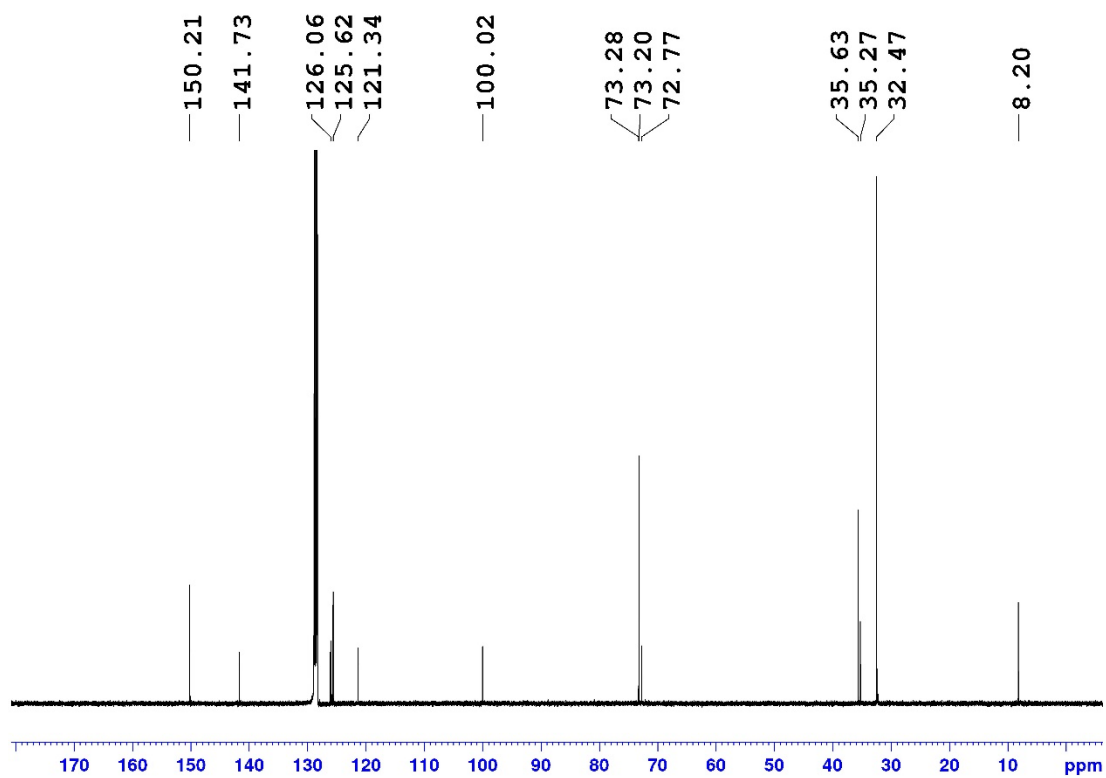


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 at RT.

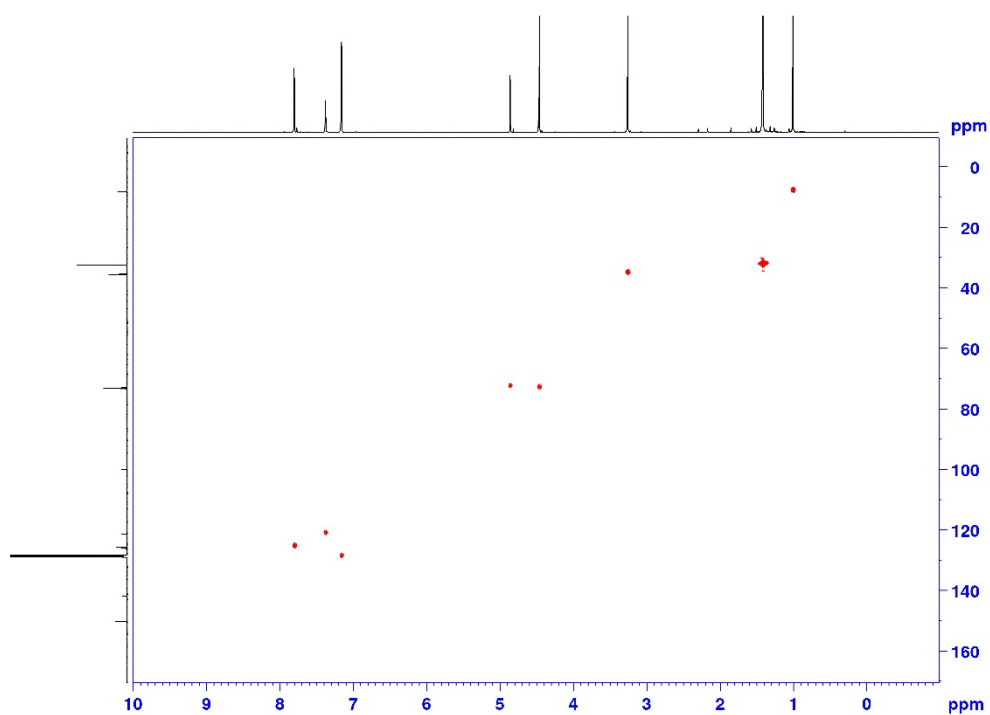


Figure S6. $^{13}\text{C}-^1\text{H}$ HSQC NMR spectrum of **2** in C_6D_6 at RT.

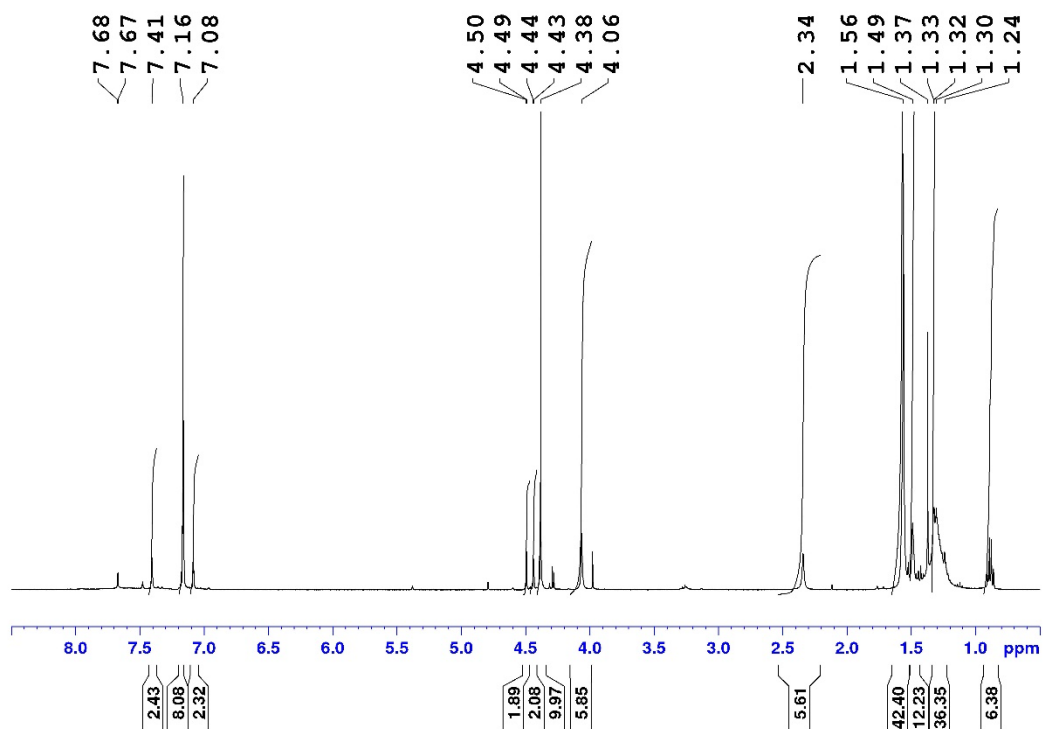


Figure S7. ^1H NMR spectrum of **3** in C_6D_6 at RT.

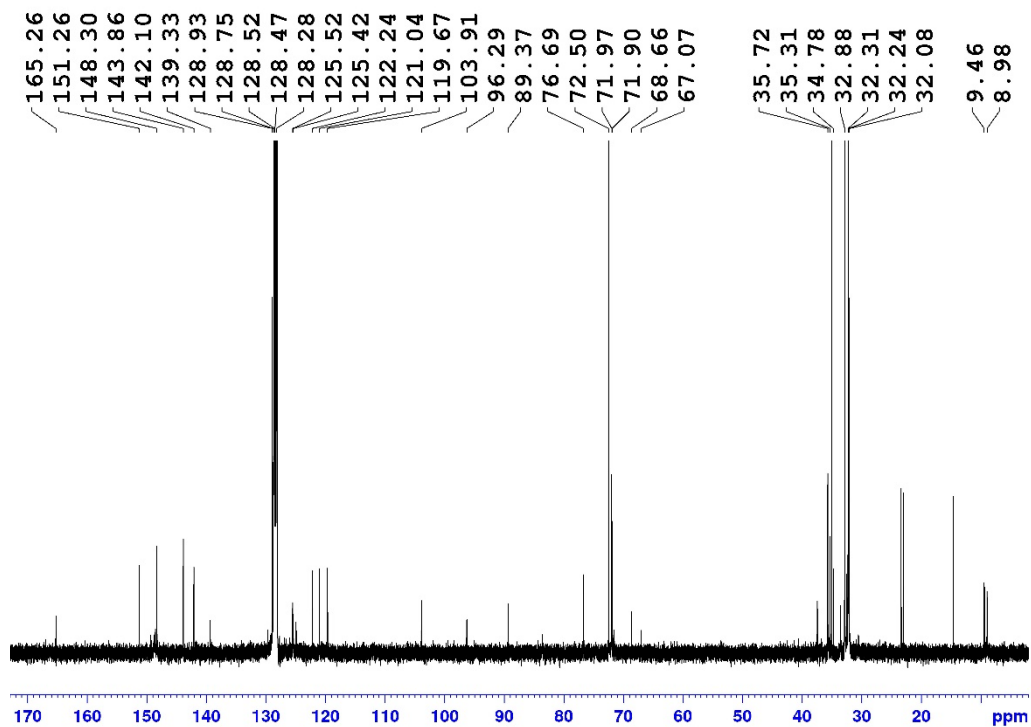


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 at RT.

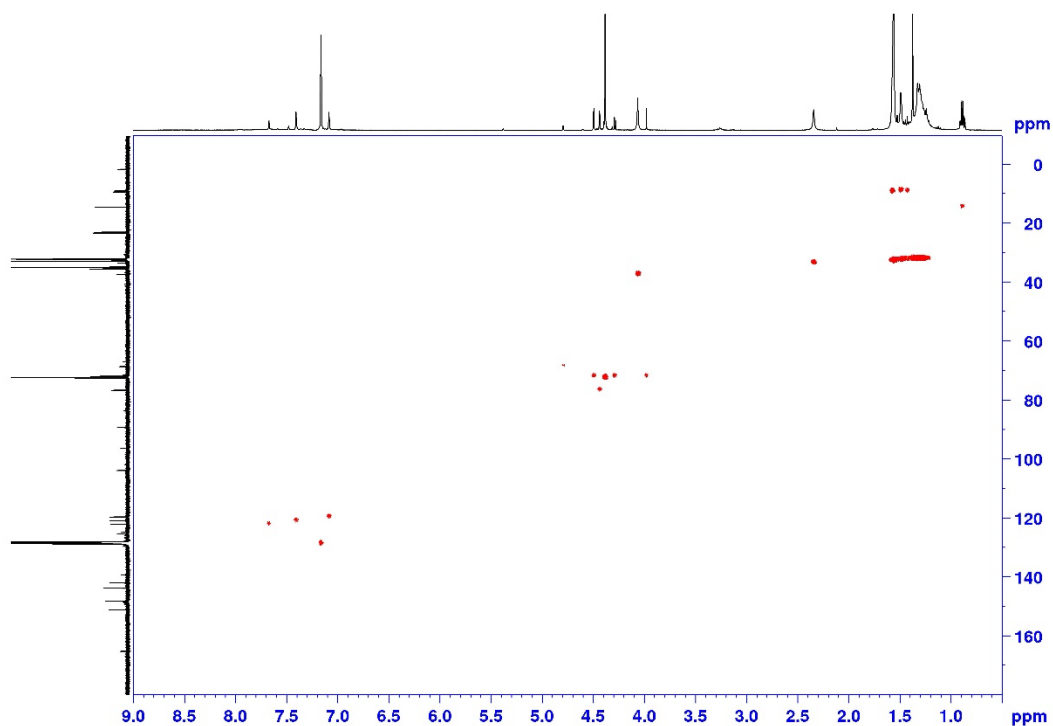


Figure S9. ^{13}C - ^1H HSQC NMR spectrum of **3** in C_6D_6 at RT.

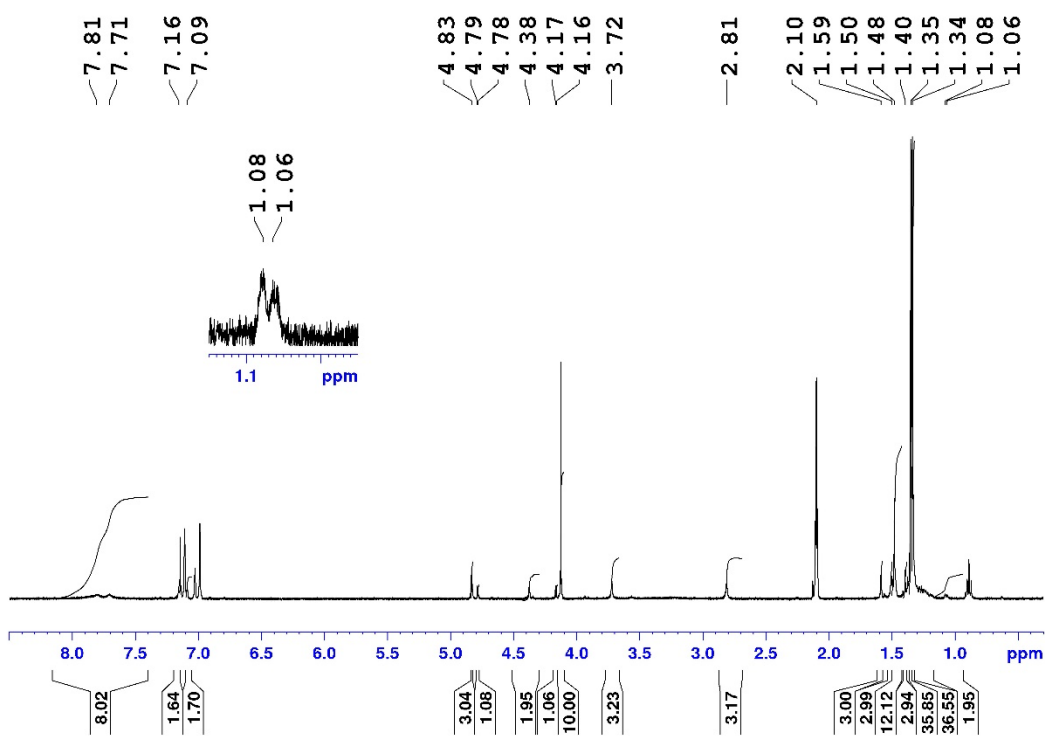


Figure S10. $^1\text{H}\{^{27}\text{Al}\}$ NMR spectrum of **4** in toluene- d_8 at RT.

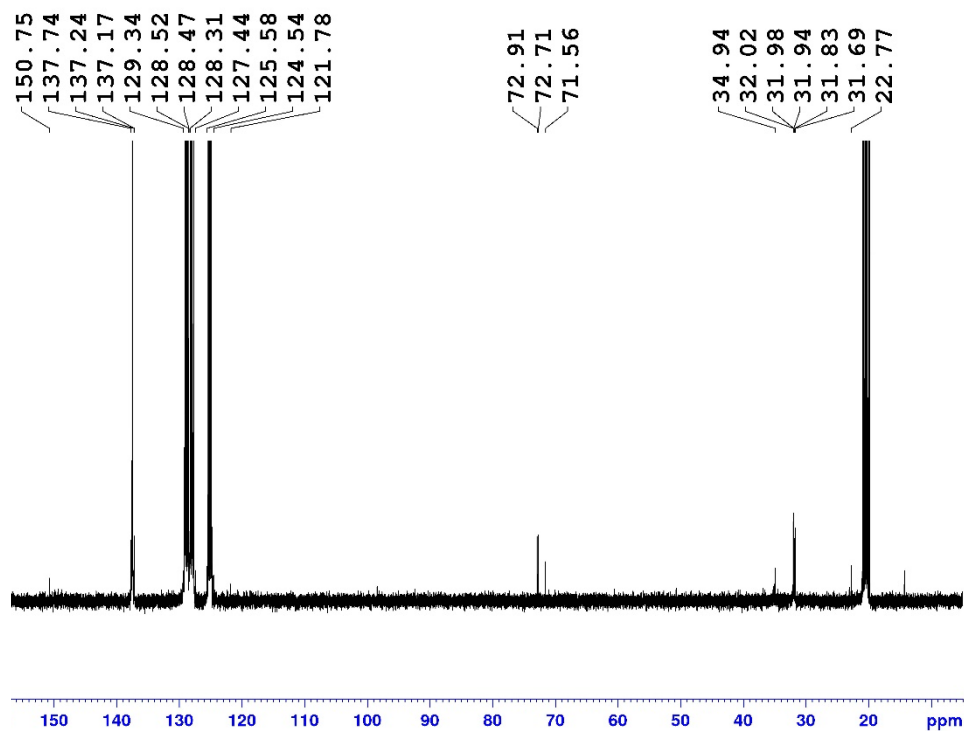


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** in toluene- d_8 at RT.

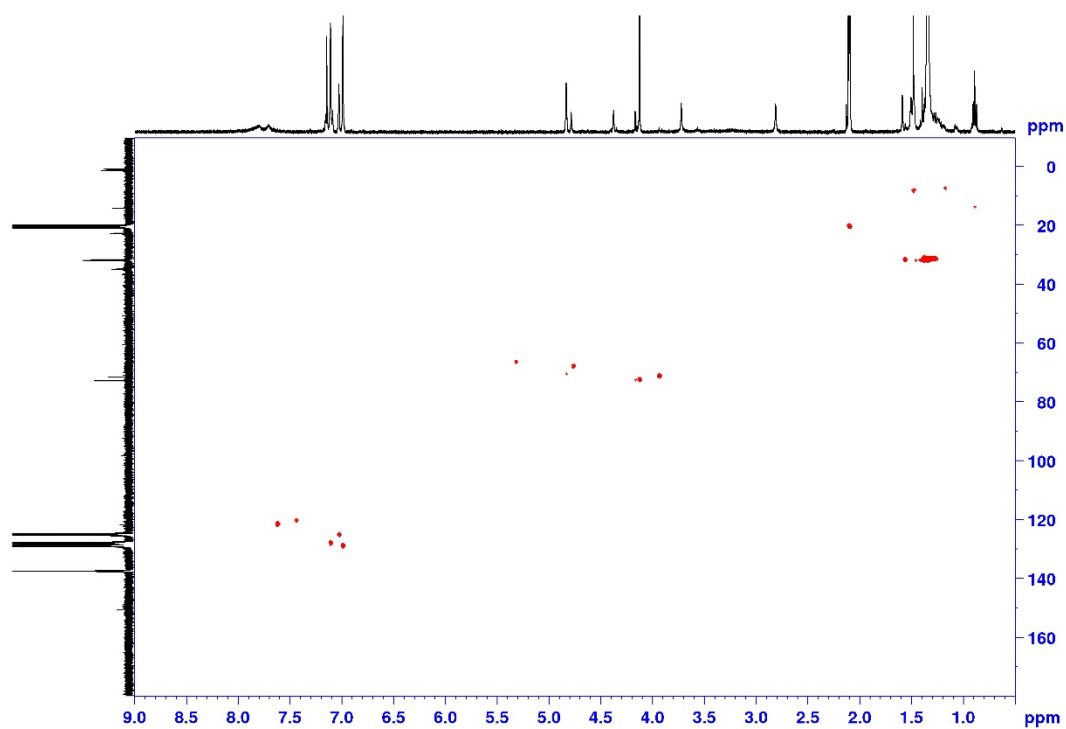


Figure S12. $^{13}\text{C}-^1\text{H}$ HSQC NMR spectrum of **4** in toluene- d_8 at RT.

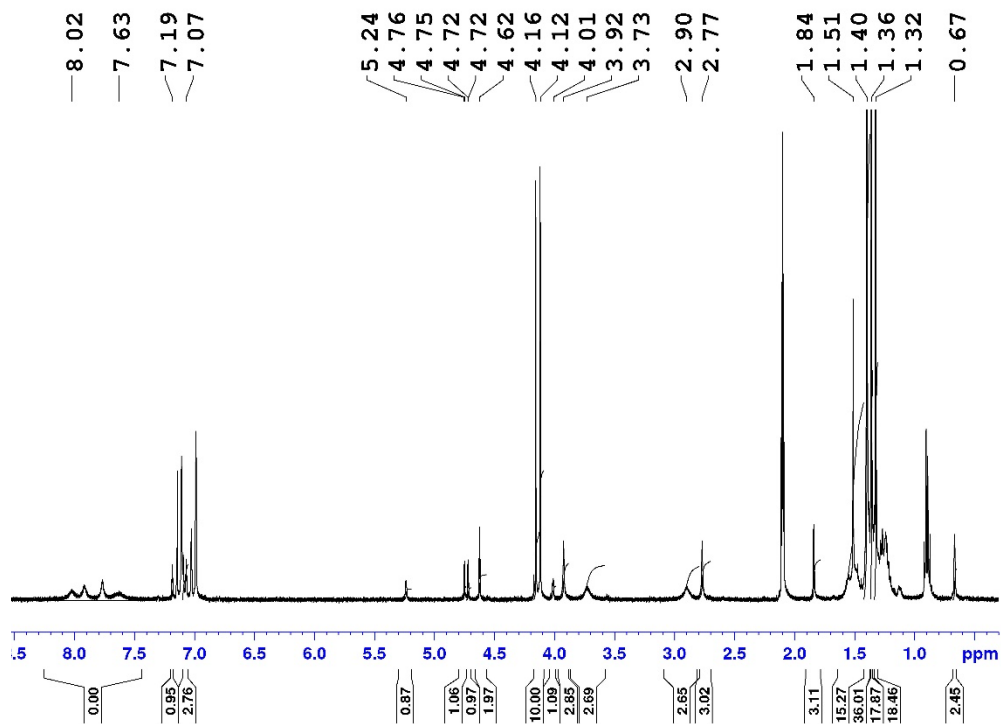


Figure S23. $^1\text{H}\{^{27}\text{Al}\}$ NMR spectrum of **5** in toluene- d_8 at RT.

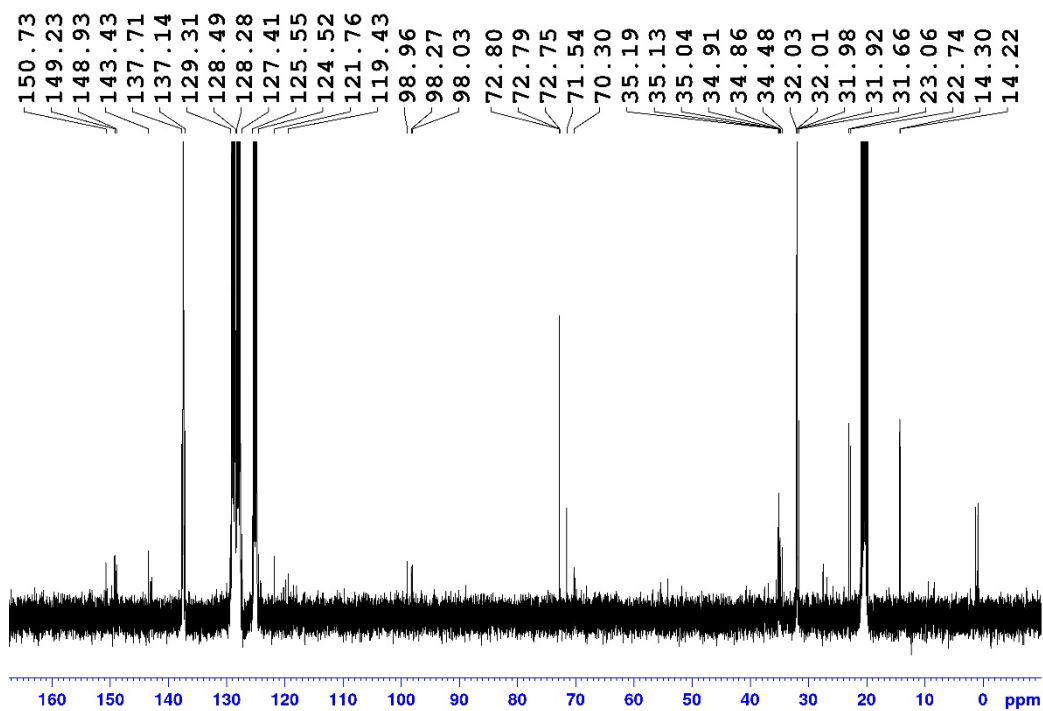


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** in toluene- d_8 at RT.

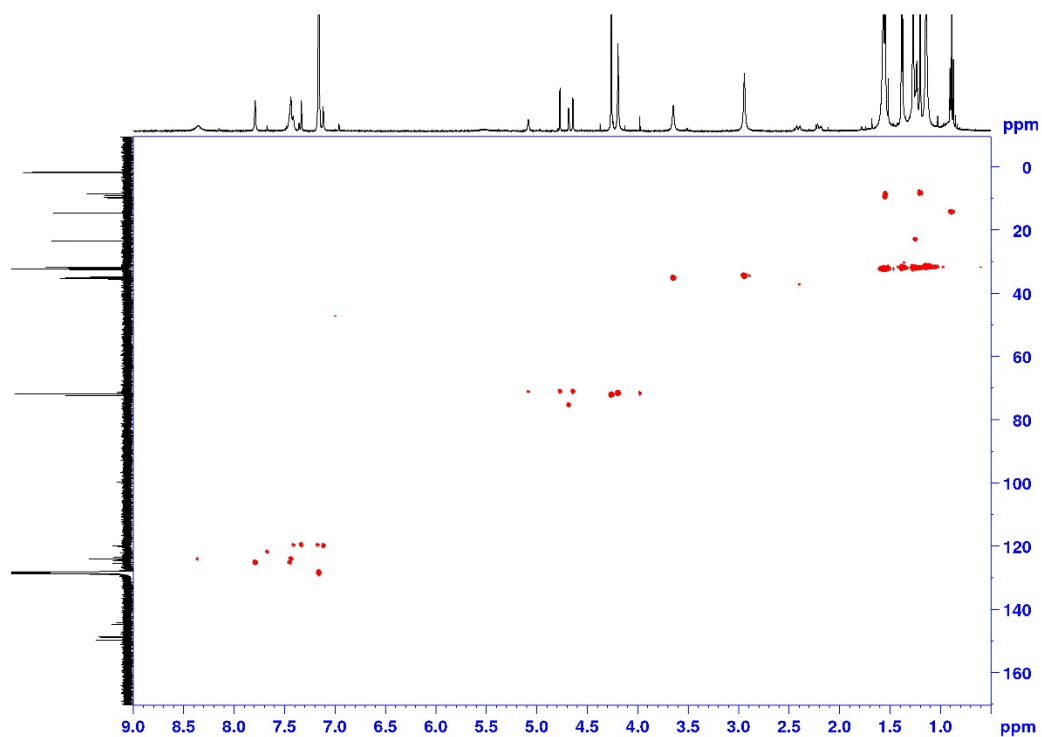


Figure S15. ^{13}C - ^1H HSQC NMR spectrum of **5** in toluene- d_8 at RT.

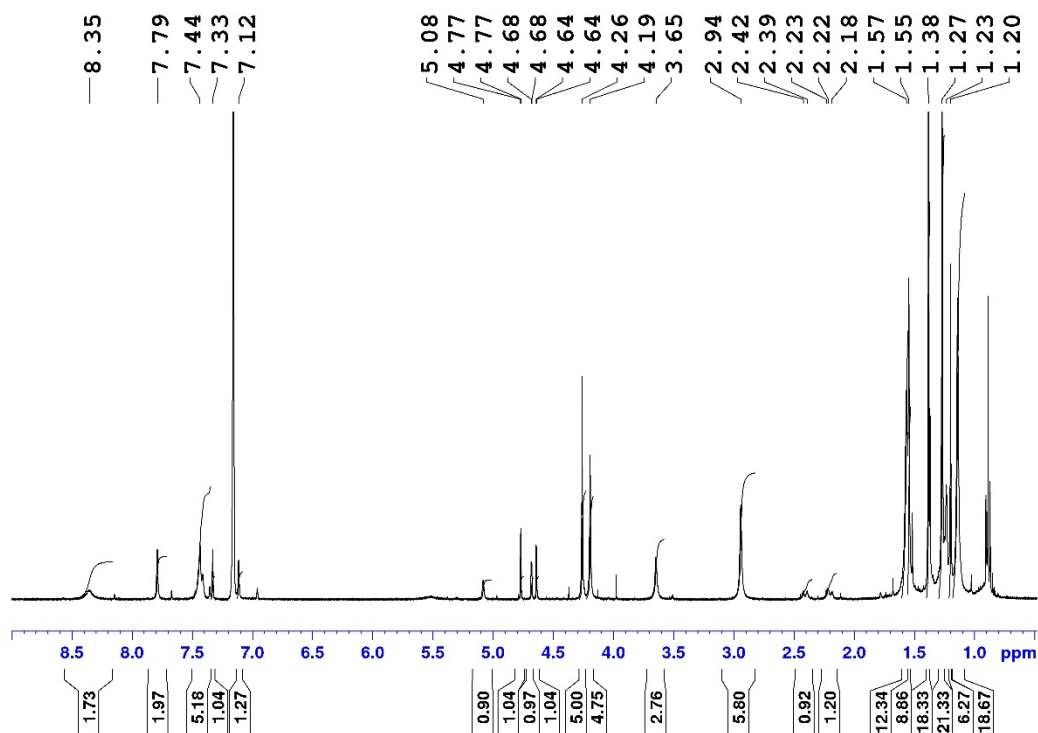


Figure S36. ^1H NMR spectrum of **8** in C_6D_6 at RT.

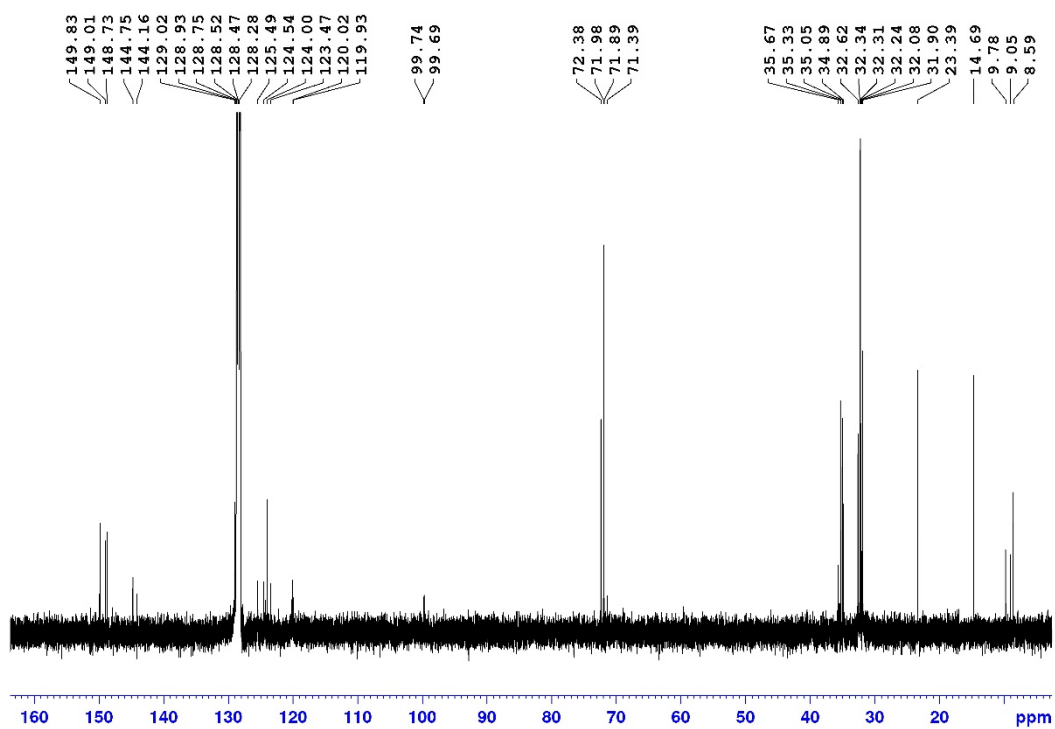


Figure S17. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** in C_6D_6 at RT

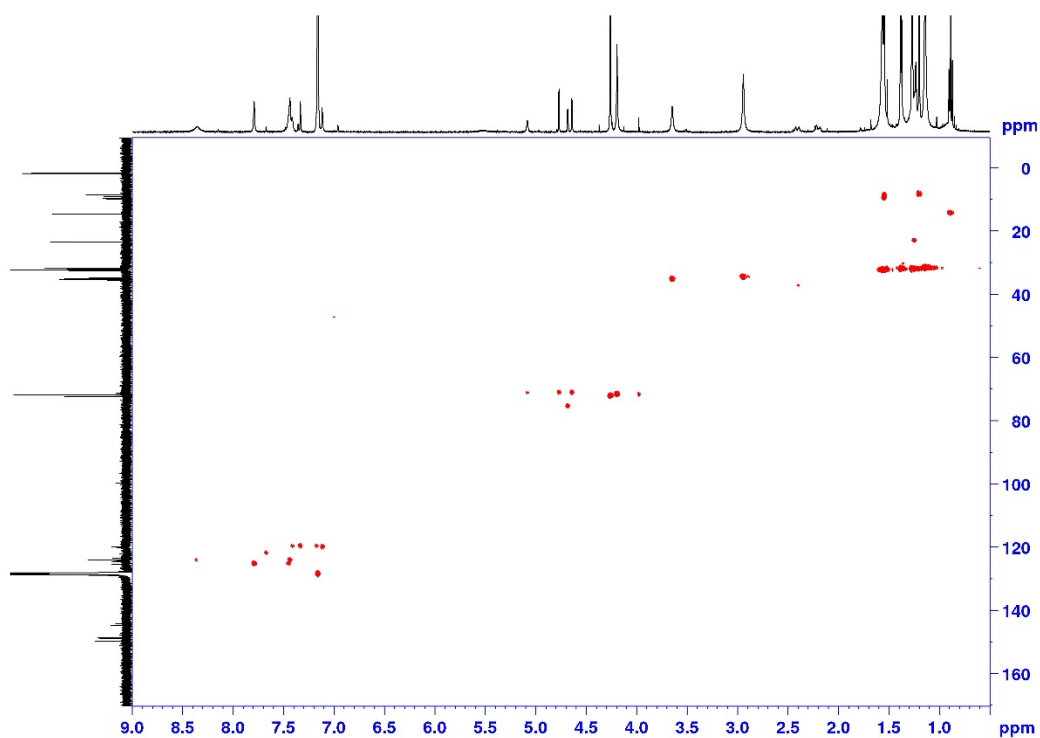


Figure S18. $^{13}\text{C}\text{-}^1\text{H}$ HSQC NMR spectrum of **8** in C_6D_6 at RT.

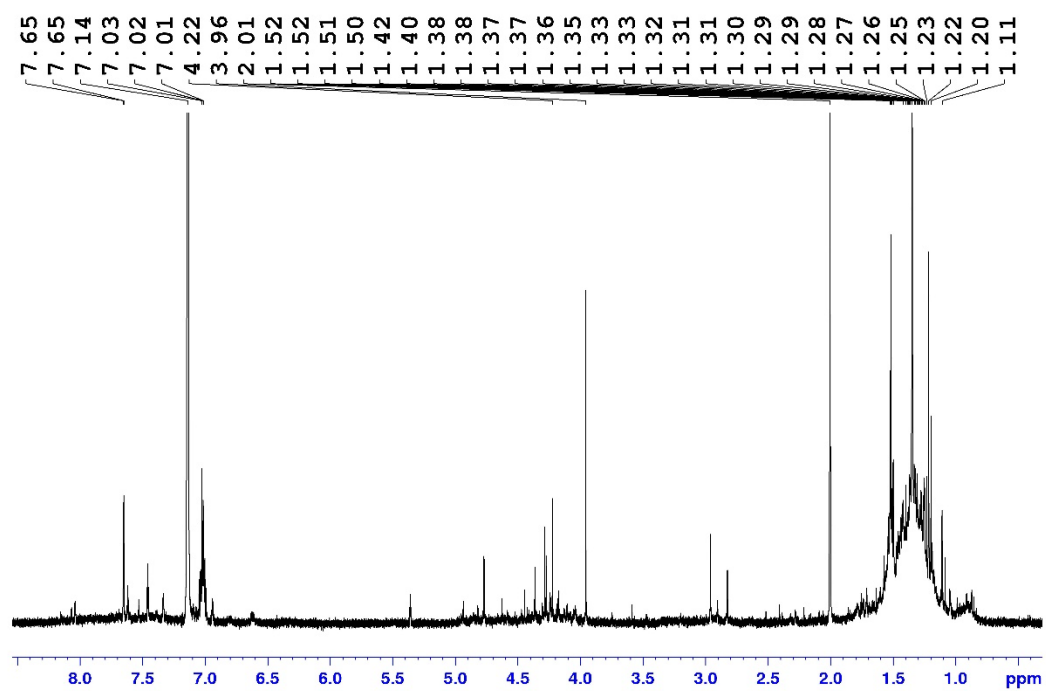


Figure S19. ^1H NMR spectrum of the crude reaction mixture of reduction of **2** in *o*-xylene in C_6D_6 at RT.

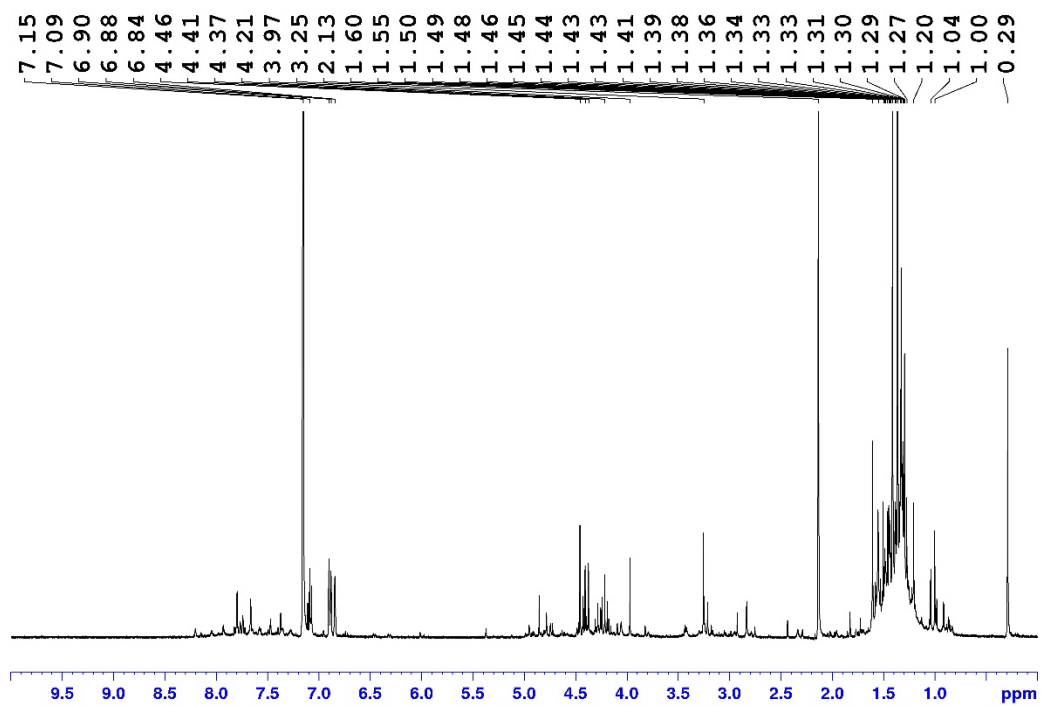


Figure S20. ^1H NMR spectrum of the crude reaction mixture of reduction of **2** in *m*-xylene in C_6D_6 at RT.

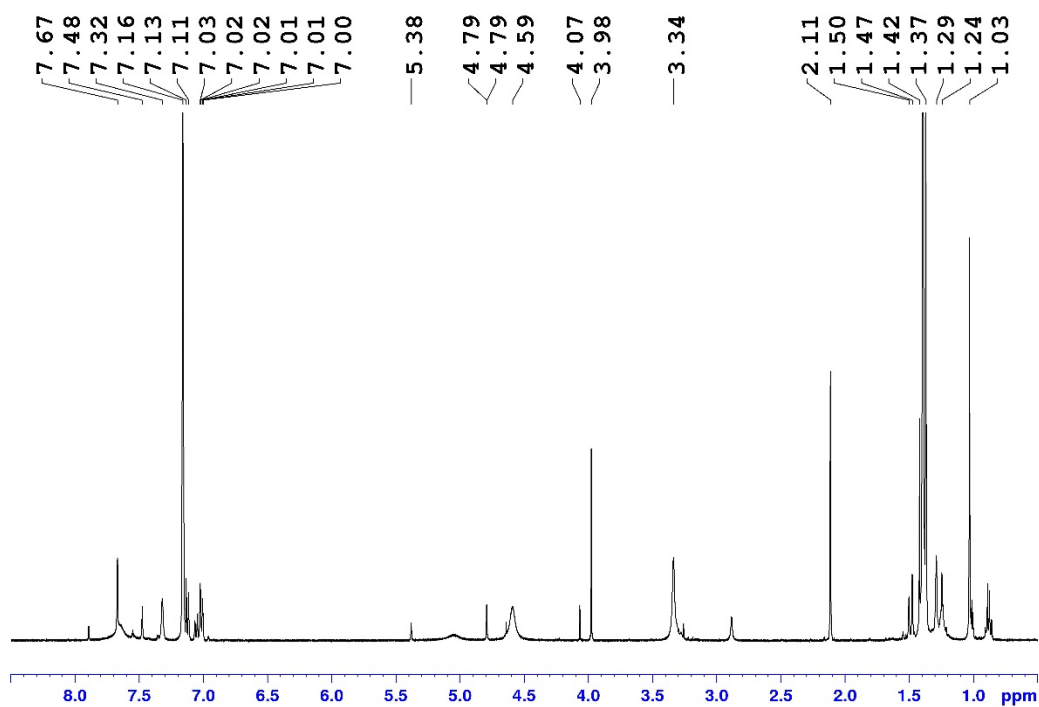


Figure S21. ^1H NMR spectrum of the crude reaction mixture of oxidation of **3** with iodine in C_6D_6 at RT.

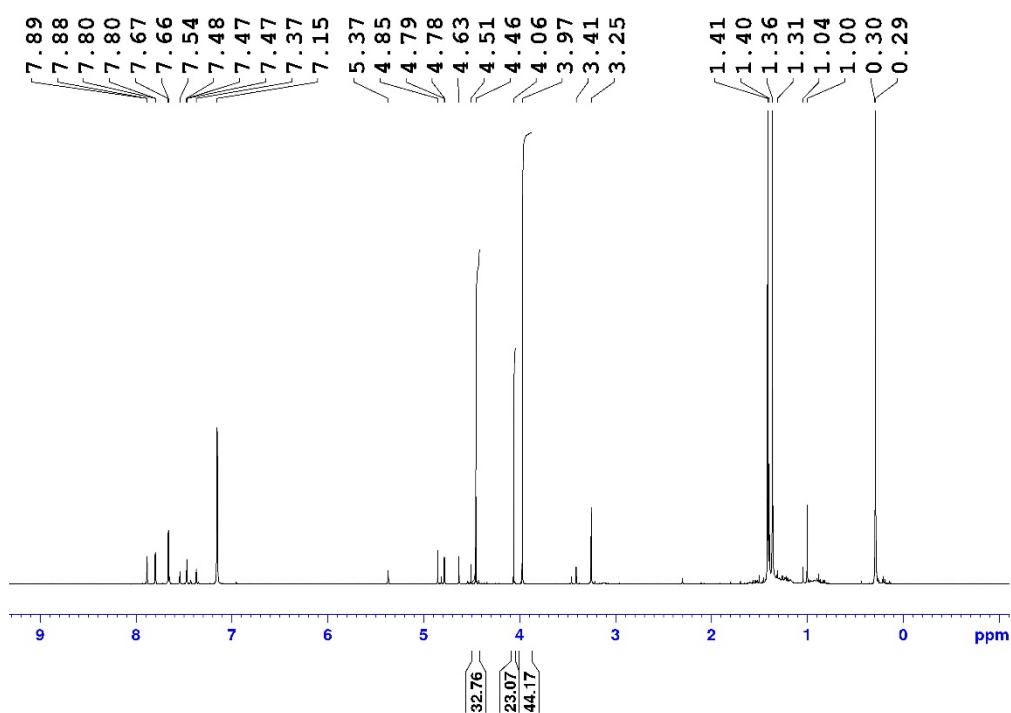


Figure S22. ^1H NMR spectrum of the reaction mixture of oxidation of **8** with iodine in C_6D_6 at RT.

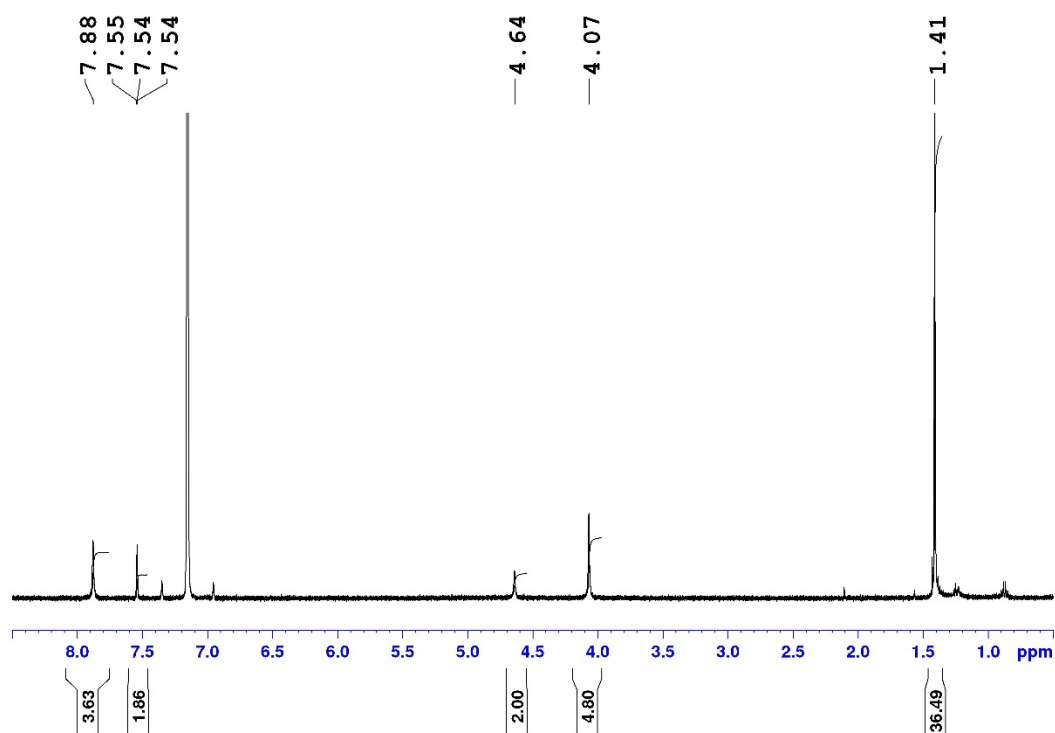


Figure S23. ^1H NMR spectrum of Fc^*I in C_6D_6 at RT.

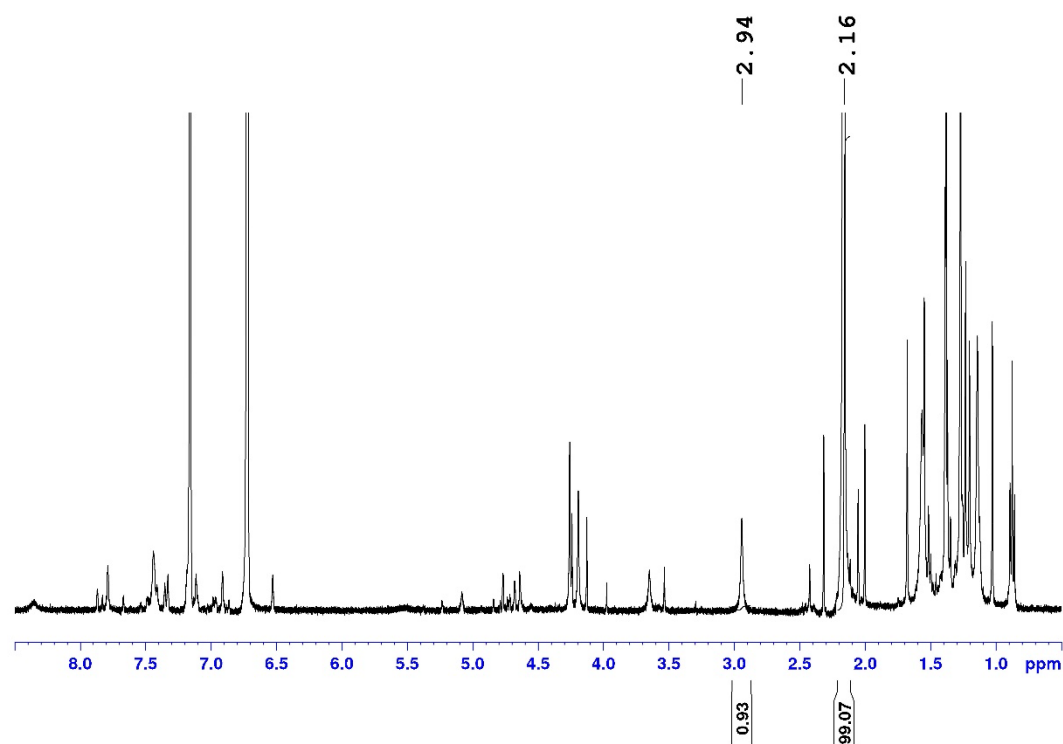


Figure S24. ^1H NMR spectrum of crude mixture of oxidation of **7** and **8** with mesitylene as internal standard in C_6D_6 at RT after 30 mints of dissolving the crude.

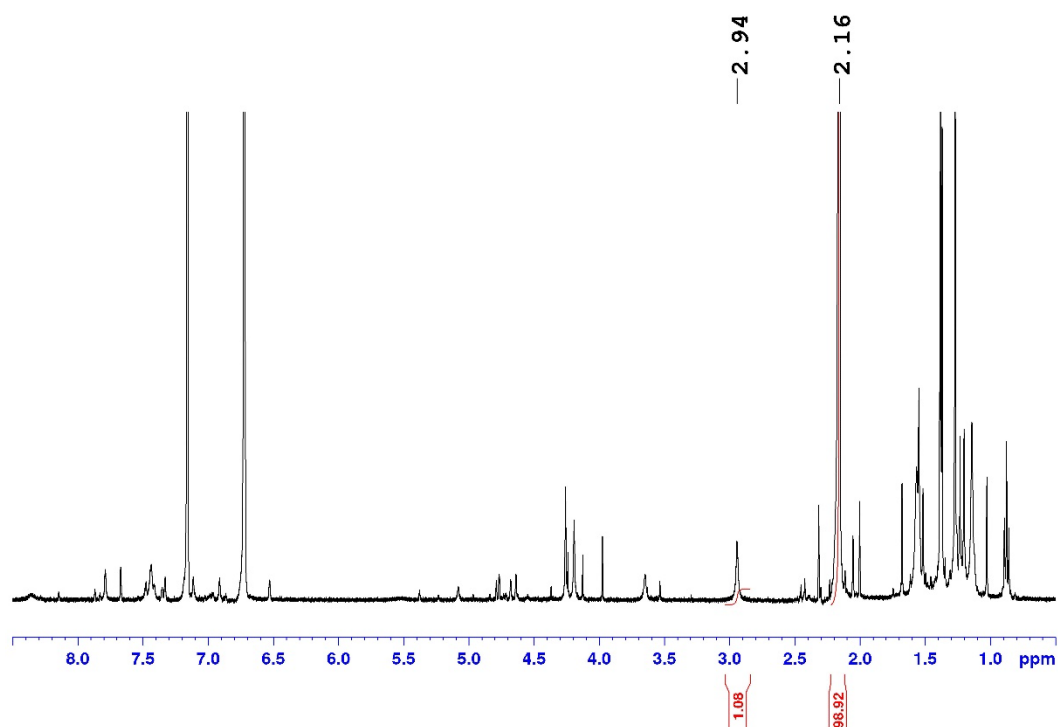


Figure S25. ^1H NMR spectrum of a crude mixture of oxidation of 7 and 8 with mesitylene as internal standard in C_6D_6 at RT after 12 h of dissolving the crude.

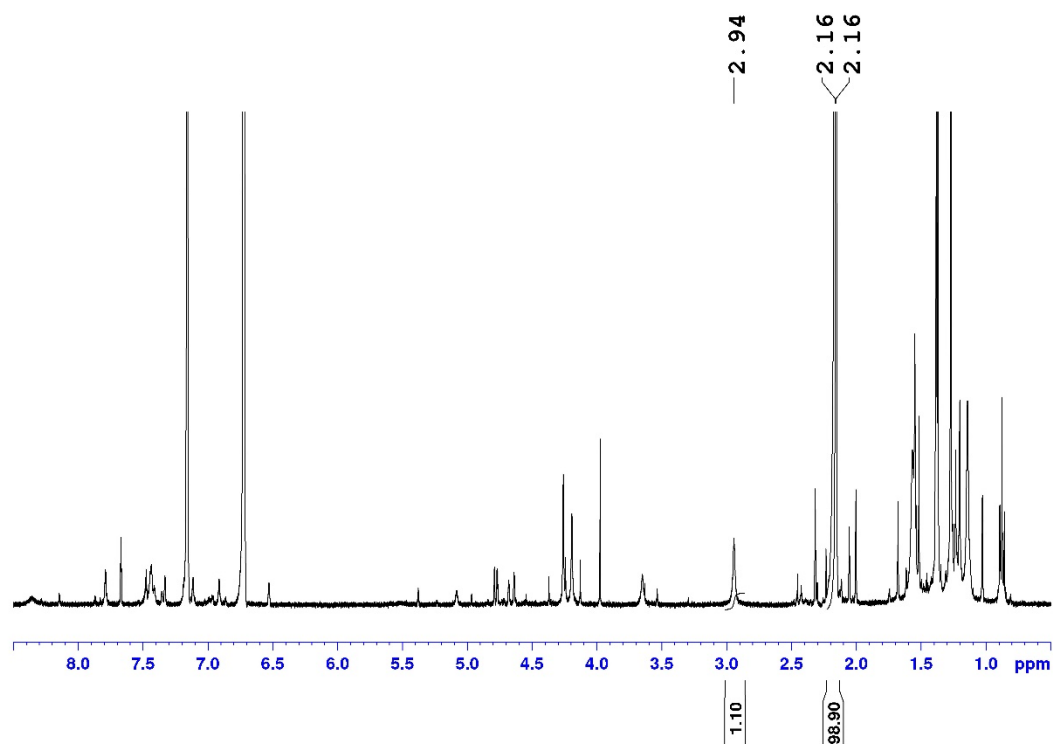


Figure S26. ^1H NMR spectrum of a crude mixture of oxidation of 7 and 8 with mesitylene as internal standard in C_6D_6 at RT after 24 h of dissolving the crude.

Cyclic voltammetry

Cyclic voltammetry experiments were performed using a Gamry Instruments Reference 600 potentiostat. A standard three-electrode cell configuration was employed using a platinum disk working electrode, a platinum wire counter electrode, and a silver wire, separated by a *Vycor* tip, serving as the reference electrode. Formal redox potentials are referenced to the ferrocene/ferrocenium ($[\text{Cp}_2\text{Fe}]^{+/0}$) redox couple by using ferrocene as an internal standard. Tetra-*n*-butylammonium hexafluorophosphate ($[\text{nBu}_4\text{N}][\text{PF}_6]$) was employed as the supporting electrolyte. Compensation for resistive losses (iR drop) was employed for all measurements.

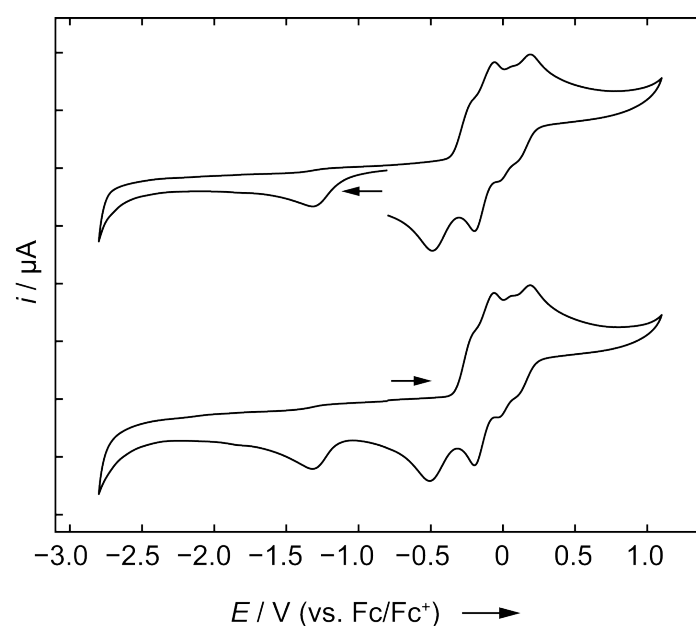


Figure S27. Cyclic voltammograms of **2** in 1,2-difluorobenzene/0.1 M $[\text{nBu}_4\text{N}][\text{PF}_6]$ measured at 250 mV s^{-1} . The voltammetric response for the positive and negative scan direction is shown. Formal potentials: $E_{\text{pc}} = -1.33 \text{ V}$, $E_{\text{pa}}(\text{onset}) = -0.34 \text{ V}$ (oxidation of the ferrocene unit at ca. $E_{1/2} = -0.15 \text{ V}$; relative to the Fc/Fc^+ couple).

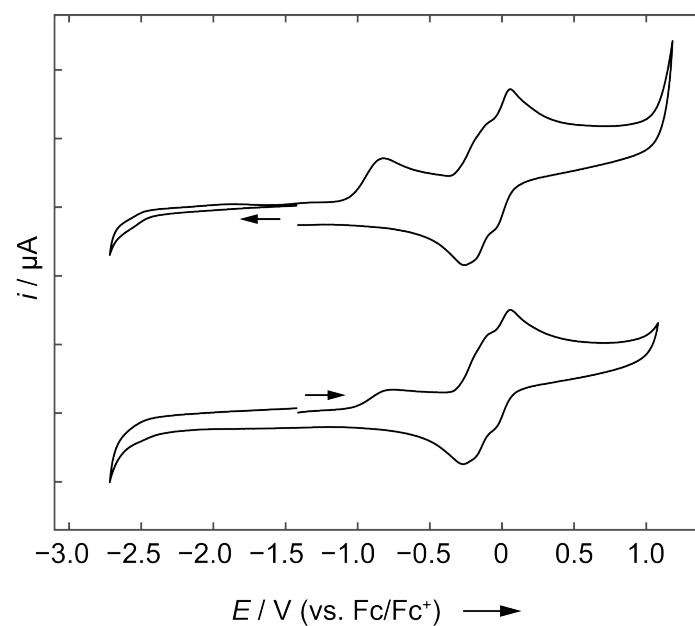


Figure S28. Cyclic voltammograms of **8** in 1,2-difluorobenzene/0.1 M [*n*Bu₄N][PF₆] measured at 250 mV s⁻¹. The voltammetric response for the positive and negative scan direction is shown. Formal potentials: $E_{\text{pa}}(\text{onset}) = -0.82$ V (oxidation of the ferrocene units between ca. $E_{1/2} = -0.2$ and 0.0 V; relative to the Fc/Fc⁺ couple).

UV-Vis spectra

The UV-vis absorption spectra of **2**, **3**, and **8** were measured on a METTLER TOLEDO UV-VIS Excellence UV5 spectrophotometer.

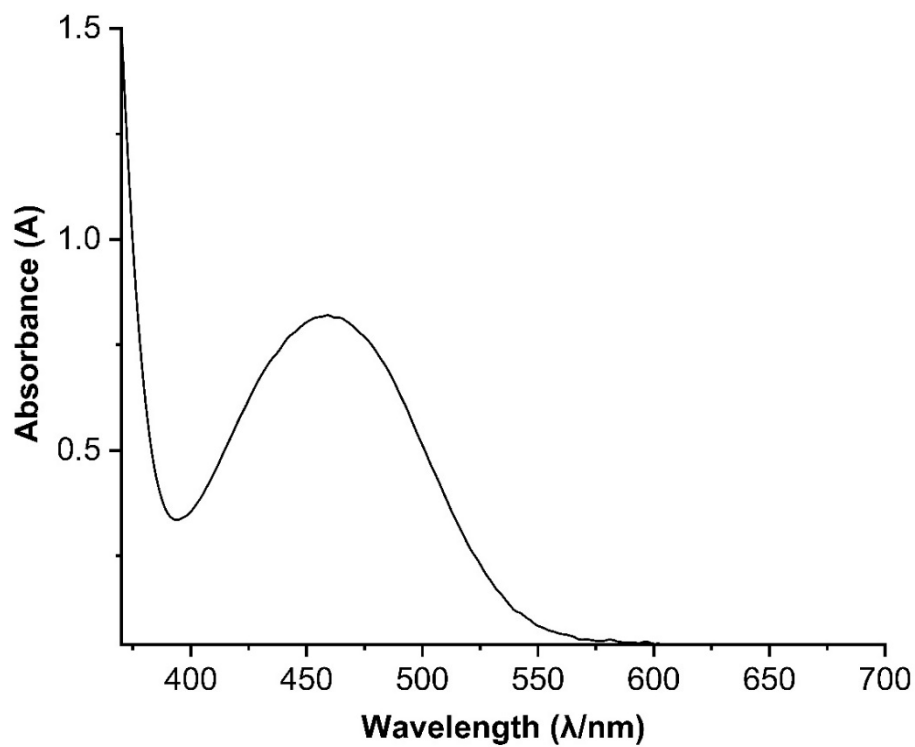


Figure S29. UV/Vis spectrum of compound **2** in hexane at RT.

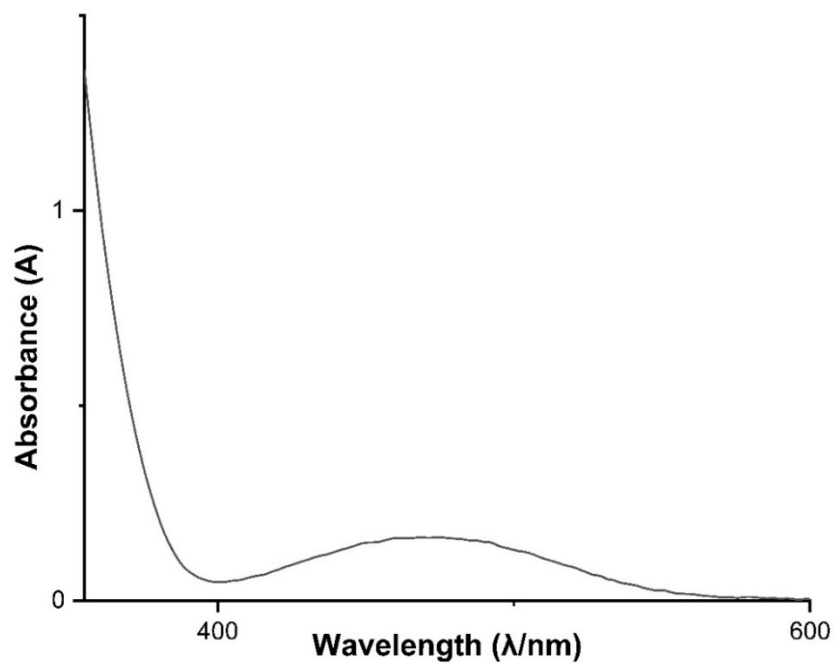


Figure S30. UV/Vis spectrum of compound **3** in hexane at RT.

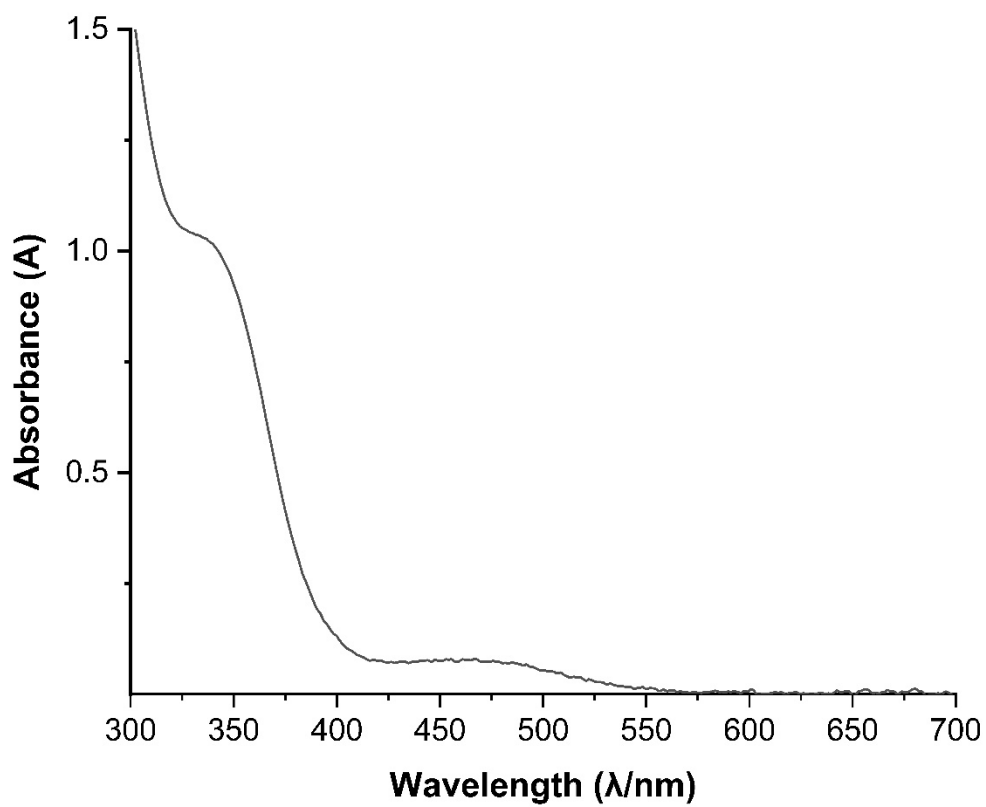


Figure S31. UV/Vis spectrum of compound **8** in hexane at RT.

X-ray crystallographic data

The crystal data of **1**, **3**, **4**, and **5** were collected on an XTALAB SYNERGY, DUALFLEX, HYPIX diffractometer with a hybrid pixel array detector and multi-layer mirror monochromated MoK α radiation. The crystal data of **2** was collected on a BRUKER X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated MoK α radiation. The crystal data of **8** were collected on a BRUKER D8 QUEST diffractometer with a CMOS area detector and multi-layer mirror monochromated MoK α radiation. The structures were solved using the intrinsic phasing method,⁵ refined with the SHELXL program⁶ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions unless otherwise stated.

Crystal data for 1 (CCDC: 2166939)

Identification code	test2_a
Empirical formula	C ₄₈ H ₇₀ N ₂ AlFe
Formula weight	757.89
Temperature/K	99(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	16.196(6)
b/Å	12.016(4)
c/Å	23.162(10)
α/°	90
β/°	93.907(14)
γ/°	90
Volume/Å ³	4497(3)
Z	4
ρ _{calc} /cm ³	1.119
μ/mm ⁻¹	0.387
F(000)	1644.0
Crystal size/mm ³	0.343 × 0.176 × 0.108
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	2.976 to 50.904
Index ranges	-19 ≤ h ≤ 19, -14 ≤ k ≤ 14, -27 ≤ l ≤ 27
Reflections collected	51189
Independent reflections	8308 [R _{int} = 0.0976, R _{sigma} = 0.0682]
Data/restraints/parameters	8308/360/548
Goodness-of-fit on F ²	1.031
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0434, wR ₂ = 0.0961
Final R indexes [all data]	R ₁ = 0.0718, wR ₂ = 0.1084
Largest diff. peak/hole / e Å ⁻³	0.38/-0.40

Refinement details: The methyl groups of the *t*Bu group C1 > C4 were modeled as twofold rotationally disordered (RESI 11, RES 111, RES 6, RES 16 TBU). ADPs (anisotropic displacement parameters) were restrained with the similarity restraint SIMU and the rigid bond restraint RIGU. After applying necessary restraints some of the ellipsoids were not properly shaped so equivalent atomic displacement parameters (EADP constraint) has been applied to those atoms (C1_11 to C4_111) that share the same site to ensure they have the same anisotropic displacement parameters (ADPs).

Crystal data for 2 (CCDC: 2166948)

Empirical formula	C ₄₅ H ₆₁ AlFeI ₂ N ₂
Formula weight (g·mol ⁻¹)	966.58
Temperature (K)	296(2)
Radiation, λ (Å)	MoK α , 0.71073
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	16.6116(8)
<i>b</i> (Å)	14.2020(7)
<i>c</i> (Å)	20.0432(11)
α (°)	90
β (°)	103.503(3)
γ (°)	90
Volume (Å ³)	4597.8(4)
<i>Z</i>	4
Calculated density (Mg·m ⁻³)	1.396
Absorption coefficient (mm ⁻¹)	1.720
<i>F</i> (000)	1960
Theta range for collection	2.681 to 24.998°
Reflections collected	39832
Independent reflections	8068
Minimum/maximum transmission	0.6163/0.7454
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	8068 / 486 / 0
Goodness-of-fit on <i>F</i> ²	1.034
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	R ₁ = 0.0466, wR ₂ = 0.0943
R indices (all data)	R ₁ = 0.0894, wR ₂ = 0.1200
Maximum/minimum residual electron density (e·Å ⁻³)	0.687 / -0.436

Crystal data for 3 (CCDC: 2166949)

Empirical formula	C ₉₆ H ₁₃₆ Al ₂ Fe ₂ I ₂ N ₄
Formula weight (g·mol ⁻¹)	1765.54
Temperature (K)	99.99(10)
Radiation, λ (Å)	Cu _{Kα} 1.54184
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	15.8692(2)
<i>b</i> (Å)	16.9522(3)
<i>c</i> (Å)	18.67859(19)
α (°)	112.0886(13)
β (°)	93.6385(11)
γ (°)	100.4721(13)
Volume (Å ³)	4530.36(11)
<i>Z</i>	2
Calculated density (Mg·m ⁻³)	1.294
Absorption coefficient (mm ⁻¹)	8.408
<i>F</i> (000)	1848
Theta range for collection	2.5801 to 77.4246°
Reflections collected	61135
Independent reflections	18481
Minimum/Maximum transmission	0.53386/1.00000
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	18481 / 1029 / 150
Goodness-of-fit on <i>F</i> ²	1.044
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	R ₁ = 0.0597, ωR ² = 0.1499
R indices (all data)	R ₁ = 0.0743, ωR ² = 0.1592
Maximum/minimum residual electron density (e·Å ⁻³)	2.702 / -1.350
Flack parameter	not applicable

Refinement details: The displacement parameters of atoms C8 to C14 of the residues 6 and 16 were restrained to the same value with similarity restraint SIMU. The atomic displacement parameters of atoms C8 to C14 of the disordered *tert*-butyl group (residues 6 and 16) were

restrained with RIGU keyword in ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.003 for both parameters s1 and s2 were used). The 1-2 and 1-3 distances in residues 6 and 16 were restrained to the same values with SAME due to disorder on the *tert*-butyl group attached to the ring.

Crystal data for 4 (CCDC:2166951)

Empirical formula	C ₉₇ H ₁₃₀ Al ₂ Fe ₂ I ₂ N ₄
Formula weight (g·mol ⁻¹)	1771.50
Temperature (K)	99.9(7)
Radiation, λ (Å)	CuKα1.54184
Crystal system	
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	22.1651(2)
<i>b</i> (Å)	19.7884(2)
<i>c</i> (Å)	23.3393(2)
α (°)	90
β (°)	113.1360(10)
γ (°)	90
Volume (Å ³)	9413.59(16)
<i>Z</i>	4
Calculated density (Mg·m ⁻³)	1.250
Absorbtion coefficient (mm ⁻¹)	8.130
<i>F</i> (000)	3696
Theta range for collection	2.330 to 77.762°
Reflections collected	121360
Independent reflections	19848
Minimum/maximum transmission	0.40140/1.00000
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	19848 / 1182 / 1191
Goodness-of-fit on <i>F</i> ²	1.059
Final R indices [<i>I</i> >2σ(<i>I</i>)]	R ₁ = 0.0438, wR ₂ = 0.1097
R indices (all data)	R ₁ = 0.0533, wR ₂ = 0.1148
Maximum/minimum residual electron density (e·Å ⁻³)	1.407 / -1.761

Refinement details: The displacement parameters of atoms C1 of residues 5 and 105 (Fc) were constrained to the same value with EADP keyword, as were those of the atoms C1 of the residues 18 and 118 (TBU). The coordinates of atoms C1 to C7 of residues 2 and 102 (toluene) were constrained to the same value. The atomic displacement parameters of disordered atoms were restrained with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.004 for both parameters s1 and s2 were used), as were those of the atoms C1 to C11 of residues 5 and 105 (Fc) and for the atoms C1 to C4 of the residues 18 and 118 (*t*Bu).

The displacement parameters of atoms C1 to C7 of residues 2 and 102 (toluene) were restrained to the same value with similarity restraint SIMU, as were those of the atoms C1 to C11 of

residues 5 and 105 (Fc) and those of the atoms C1 to C4 of the residues 18 and 118 (*t*Bu). The distances between atoms C2 of residues 5 and 105 (Fc) and C1 of residue 6 (Ar) were restrained during refinement to the same value, as were those of the atoms C5 of the residues 5 and 105 (Fc) and C1 of residue 9. The 1-2 and 1-3 distances in residues 5 and 105 (Fc) were restrained to the same values with SAME.

Crystal data for 5 (CCDC: 2166952)

Empirical formula	C ₁₀₄ H ₁₄₆ Al ₂ Fe ₂ I ₂ N ₄
Formula weight (g·mol ⁻¹)	1871.70
Temperature (K)	100(2)
Radiation, λ (Å)	MoK α 0.71073
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	16.797(3)
<i>b</i> (Å)	16.275(4)
<i>c</i> (Å)	19.697(6)
α (°)	90
β (°)	112.357(12)
γ (°)	90
Volume (Å ³)	4980(2)
<i>Z</i>	2
Calculated density (Mg·m ⁻³)	1.248
Absorbtion coefficient (mm ⁻¹)	0.974
<i>F</i> (000)	1964
Theta range for collection	2.461 to 29.831°
Reflections collected	62023
Independent reflections	14170
Minimum/maximum transmission	0.6405/0.7459
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	14170 / 732 / 1003
Goodness-of-fit on <i>F</i> ²	1.019
Final R indices [<i>I</i> >2 σ (<i>I</i>)]	R ₁ = 0.0717, wR ² = 0.1686
R indices (all data)	R ₁ = 0.1144, wR ² = 0.2007
Maximum/minimum residual electron density (e·Å ⁻³)	2.950 / -1.525

Refinement details: The structure has disordered *tert*-butyl, carbene and xylene moieties, thus necessary restraints and constraints were applied to all these disordered atoms. More specifically, the similarity restraint SIMU and the rigid bond restraint RIGU were applied, assuming that the atoms in these moieties move similarly both in direction and magnitude. The same distances restraint SAME was used to enforce similar geometries of all disordered residues within their own class. After applying necessary restraints some of the ellipsoids were not properly shaped, so equivalent atomic displacement parameters (EADP constraints) were applied to those atoms to ensure they have the same anisotropic displacement parameters (ADPs).

Crystal data for 7 (CCDC: 2166953)

Empirical formula	C ₉₀ H ₁₂₂ Al ₂ Fe ₂ N ₄
Formula weight (g·mol ⁻¹)	1425.57
Temperature (K)	100(2)
Radiation, λ (Å)	MoK α , 0.71073
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	19.856(8)
<i>b</i> (Å)	14.800(4)
<i>c</i> (Å)	29.131(10)
α (°)	90
β (°)	105.079(12)
γ (°)	90
Volume (Å ³)	8266(5)
<i>Z</i>	4
Calculated density (Mg·m ⁻³)	1.145
Absorption coefficient (mm ⁻¹)	0.417
<i>F</i> (000)	3072
Theta range for collection	1.998 to 32.534°
Reflections collected	221609
Independent reflections	28967
Minimum/maximum transmission	0.5745/0.7464
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	28967 / 1142 / 1692
Goodness-of-fit on <i>F</i> ²	1.015
Final R indices [<i>I</i> >2 σ (<i>I</i>)]	R ₁ = 0.0505, wR ₂ = 0.1142
R indices (all data)	R ₁ = 0.0964, wR ₂ = 0.1347
Maximum/minimum residual electron density (e·Å ⁻³)	0.552 / -0.447

Refinement details: The structure has disordered *tert*-butyl and ferrocenyl groups, thus necessary restraints and constraints were applied to all these disordered atoms. More specifically, the similarity restraint SIMU and the rigid bond restraint RIGU were applied, assuming that the atoms in these moieties move similarly both in direction and magnitude. The same distances restraint SAME was used to enforce similar geometries of all disordered residues within their own class. After applying necessary restraints, some of the ellipsoids were not properly shaped, so equivalent atomic displacement parameters (EADP constraints) were applied to those atoms to make their same anisotropic displacement parameters (ADPs). There were some disagreeable reflections [0 1 11 0 2 -1 1 1 1 1 1 0 0 0 2 -1 0 2 -2 0 2 -6 3 15], and these were omitted.

Crystal data for 8 (CCDC: 2166954)

Empirical formula	C ₉ H ₁₃ Al ₂ Fe ₂ N ₄
Formula weight (g·mol ⁻¹)	1511.74
Temperature (K)	296(2)
Radiation, λ (Å)	MoK α , 0.71073
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>Unit cell dimensions</i>	
<i>a</i> (Å)	15.996(8)
<i>b</i> (Å)	29.021(14)
<i>c</i> (Å)	19.433(10)
α (°)	90
β (°)	91.562(13)
γ (°)	90
Volume (Å ³)	9018(8)
<i>Z</i>	4
Calculated density (Mg·m ⁻³)	1.113
Absorption coefficient (mm ⁻¹)	0.386
<i>F</i> (000)	3272
Theta range for collection	1.261 to 25.382°
Reflections collected	111641
Independent reflections	16515
Minimum/maximum transmission	0.5802/0.6565
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters / restraints	16515 / 1107 / 1140
Goodness-of-fit on <i>F</i> ²	1.052
Final R indices [<i>I</i> > 2 σ (<i>I</i>)]	R ₁ = 0.0594, wR ₂ = 0.1473
R indices (all data)	R ₁ = 0.0836, wR ₂ = 0.1614
Maximum/minimum residual electron density (e·Å ⁻³)	0.748 / -0.554

Computational details

Geometry optimisations and Hessian calculations were performed at the (U)PBE0-D3(BJ)/def2-SVP level of theory.⁷⁻¹¹ All optimised geometries were characterized as minimum energy structures as only real vibrational frequencies were found. Solvation corrections were included using the solvent model based on density (SMD)¹² method at the (U)PBE0-D3(BJ)/def2-TZVP level (solvents: toluene, $\epsilon = 2.3741$; n-hexane, $\epsilon = 1.8819$). A concentration correction of $\Delta G^{0 \rightarrow *}$ = $RT \cdot \ln(24.46)$ = 1.89 kcal mol⁻¹ (T = 298.15 K) was added to the free energies of all calculated species to change the 1.00 atm gas phase values to the condensed phase standard state concentration of 1.00 mol L⁻¹. For toluene, a standard state of 9.41 mol L⁻¹ at 298.15 K was used, whereby its $\Delta G^{0 \rightarrow *}$ correction is 3.22 kcal mol⁻¹.^{13,14} This procedure leads to a proper description of associative/dissociative steps.^{13,14} Mayer bond orders (MBO)^{15,16} were obtained for selected bonds and were calculated using Multiwfn 3.8.¹⁷ All geometry optimizations, vibrational frequencies, canonical Kohn-Sham molecular orbitals, and spin density calculations were performed in Gaussian 16, revision C.01.¹⁸

Cartesian coordinates

Coordinates in angstrom from optimizations at the (U)PBE0-D3(BJ)/def2-SVP level of theory.

2			
I	-2.051439000	0.548449000	2.225204000
I	2.026824000	0.555916000	2.232138000
Fe	-0.020066000	-2.676791000	-0.264769000
Al	-0.007197000	0.610311000	0.667853000
N	0.048786000	2.927669000	-1.375592000
N	0.061851000	3.673901000	0.632548000
C	0.017217000	2.528441000	-0.082449000
C	0.013976000	2.068603000	-2.540557000
H	-0.014553000	1.021488000	-2.218275000
H	0.911201000	2.228727000	-3.154641000
H	-0.879148000	2.283929000	-3.143931000
C	0.117801000	4.305340000	-1.474469000
C	0.130365000	4.781531000	-0.192200000
C	0.088394000	3.756699000	2.079128000
H	-0.372369000	2.858076000	2.506625000
H	-0.489368000	4.631063000	2.403474000
H	1.123070000	3.833641000	2.442347000
C	0.203484000	6.170846000	0.321955000
H	0.301966000	6.877877000	-0.511249000
H	1.069832000	6.312063000	0.986792000
H	-0.700745000	6.446271000	0.888032000
C	0.165154000	5.013407000	-2.776196000
H	0.214455000	6.097934000	-2.617983000
H	-0.728093000	4.803973000	-3.385767000
H	1.048152000	4.720023000	-3.365888000
C	-0.006306000	-0.694107000	-0.802244000
C	-1.165331000	-1.373101000	-1.343607000
C	-0.722517000	-2.459516000	-2.161498000
H	-1.371854000	-3.148121000	-2.700206000
C	0.694976000	-2.467927000	-2.157858000

H	1.338868000	-3.164025000	-2.693509000
C	1.147117000	-1.387658000	-1.336875000
C	2.565274000	-1.032185000	-1.157407000
C	3.538670000	-2.016207000	-0.992204000
H	3.217124000	-3.059163000	-0.956666000
C	4.889721000	-1.689940000	-0.831671000
C	5.242893000	-0.338956000	-0.847417000
H	6.288351000	-0.061807000	-0.711487000
C	4.294967000	0.680285000	-1.016044000
C	2.962916000	0.310305000	-1.180237000
H	2.198336000	1.072912000	-1.313261000
C	4.743476000	2.143367000	-0.982726000
C	5.428960000	2.427463000	0.361946000
H	6.321437000	1.800826000	0.504500000
H	4.739880000	2.225928000	1.196070000
H	5.747871000	3.481114000	0.416323000
C	3.564284000	3.107855000	-1.121417000
H	2.835468000	2.968768000	-0.308396000
H	3.042638000	2.978401000	-2.082703000
H	3.925140000	4.147117000	-1.078658000
C	5.725794000	2.402960000	-2.132784000
H	6.071580000	3.449419000	-2.119145000
H	5.249823000	2.209826000	-3.106820000
H	6.612720000	1.756098000	-2.061629000
C	5.910296000	-2.809838000	-0.615602000
C	-1.179751000	-3.396611000	1.254730000
H	-2.207645000	-3.088368000	1.441567000
C	-0.749549000	-4.454593000	0.401282000
H	-1.393686000	-5.120007000	-0.172312000
C	0.678174000	-4.466948000	0.401674000
H	1.310254000	-5.144050000	-0.171659000
C	1.126542000	-3.416689000	1.255432000
H	2.159393000	-3.126594000	1.444031000
C	-0.021076000	-2.763525000	1.786545000

H	-0.013319000	-1.913680000	2.466547000
C	-2.578770000	-0.997881000	-1.169483000
C	-2.955836000	0.346634000	-1.191321000
H	-2.181353000	1.099380000	-1.323439000
C	-4.285888000	0.737053000	-1.026517000
C	-4.712311000	2.206929000	-0.993477000
C	-5.684681000	2.481287000	-2.148553000
H	-6.581442000	1.847540000	-2.081857000
H	-5.206887000	2.280837000	-3.120193000
H	-6.014748000	3.532821000	-2.136728000
C	-3.517841000	3.153916000	-1.125067000
H	-3.863832000	4.198112000	-1.080634000
H	-2.994673000	3.020033000	-2.084952000
H	-2.794379000	3.002292000	-0.309467000
C	-5.400567000	2.500169000	0.347677000
H	-6.301878000	1.885295000	0.486120000
H	-5.705892000	3.557882000	0.400281000
H	-4.718427000	2.290234000	1.185373000
C	-5.241412000	-0.268444000	-0.860283000
H	-6.286945000	0.017155000	-0.722245000
C	-4.907876000	-1.629169000	-0.845080000
C	-6.003878000	-2.673625000	-0.620849000
C	-7.063161000	-2.546397000	-1.724629000
H	-7.526508000	-1.548710000	-1.732907000
H	-7.865507000	-3.286946000	-1.576451000
H	-6.617717000	-2.716912000	-2.716857000
C	-5.452203000	-4.099771000	-0.644628000
H	-4.980457000	-4.338772000	-1.610024000
H	-6.270710000	-4.818522000	-0.486326000
H	-4.708828000	-4.263909000	0.150401000
C	-6.652769000	-2.429568000	0.749508000
H	-5.904876000	-2.502274000	1.553872000
H	-7.441367000	-3.174771000	0.942043000
H	-7.111197000	-1.431490000	0.811121000

C	-3.566219000	-1.974933000	-1.004945000
H	-3.253097000	-3.017987000	-0.972146000
C	5.533466000	-3.590195000	0.652656000
H	6.263382000	-4.393235000	0.843568000
H	5.513696000	-2.925345000	1.529747000
H	4.540667000	-4.055910000	0.564869000
C	5.889949000	-3.754174000	-1.825880000
H	6.157687000	-3.215651000	-2.748027000
H	6.610211000	-4.576375000	-1.686509000
H	4.895998000	-4.201076000	-1.975756000
C	7.331608000	-2.272609000	-0.446125000
H	7.665770000	-1.713994000	-1.333879000
H	7.415831000	-1.610665000	0.429191000
H	8.030881000	-3.109631000	-0.297653000

3

Al	-1.002396000	-0.754032000	-0.765240000
Al	0.967441000	1.008078000	-0.728348000
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I	-0.105669000	3.129419000	-1.938779000
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C	-2.349197000	0.466115000	-1.767692000
N	-3.129030000	1.344914000	-1.101457000
C	-3.823054000	2.167560000	-1.966184000
C	-3.437830000	1.808187000	-3.226267000
C	-1.794093000	0.232103000	-4.185183000
H	-1.182536000	-0.611715000	-3.846441000
H	-1.138062000	1.019103000	-4.586494000
H	-2.469217000	-0.117701000	-4.978497000
C	-3.054411000	1.590810000	0.320356000
H	-2.616248000	0.724524000	0.825814000
H	-4.055603000	1.756882000	0.732905000
H	-2.417892000	2.467380000	0.509575000
C	-4.793790000	3.185870000	-1.502585000

H	-5.184980000	3.755827000	-2.354679000
H	-4.337415000	3.900213000	-0.800914000
H	-5.646163000	2.706444000	-0.994697000
C	-3.752228000	2.408342000	-4.545531000
H	-4.538981000	3.166001000	-4.438912000
H	-4.102744000	1.663143000	-5.276027000
H	-2.865017000	2.904839000	-4.972005000
N	2.434124000	0.160521000	-3.424630000
C	2.215128000	0.073022000	-2.092076000
N	2.875591000	-1.042468000	-1.711941000
C	3.506652000	-1.650131000	-2.778643000
C	3.218989000	-0.888698000	-3.875560000
C	1.914596000	1.164202000	-4.320736000
H	1.247224000	0.699789000	-5.061226000
H	2.734999000	1.667480000	-4.851995000
H	1.351173000	1.908929000	-3.747699000
C	2.796183000	-1.627537000	-0.392405000
H	2.502298000	-0.867528000	0.340528000
H	3.774558000	-2.017599000	-0.094525000
H	2.049640000	-2.433600000	-0.386075000
C	4.315264000	-2.883639000	-2.651198000
H	4.777266000	-3.135062000	-3.614265000
H	3.698329000	-3.738446000	-2.337693000
H	5.123872000	-2.750820000	-1.914764000
C	3.570058000	-1.067232000	-5.305298000
H	4.209040000	-1.950505000	-5.430597000
H	4.114186000	-0.200224000	-5.712463000
H	2.670284000	-1.218852000	-5.923339000
Fe	-2.806664000	-3.629770000	1.011370000
C	-1.999838000	-1.721028000	0.686526000
C	-3.416061000	-1.701962000	1.017711000
C	-3.608244000	-2.296766000	2.306351000
H	-4.570252000	-2.455785000	2.792159000
C	-2.346982000	-2.731026000	2.779931000

H	-2.147445000	-3.266519000	3.707254000
C	-1.363597000	-2.393111000	1.797632000
C	-3.247942000	-4.622762000	-0.733533000
H	-3.282767000	-4.170844000	-1.722187000
C	-4.317745000	-4.728926000	0.198495000
H	-5.328055000	-4.346040000	0.058852000
C	-3.811587000	-5.359321000	1.373376000
H	-4.373031000	-5.556045000	2.285706000
C	-2.429454000	-5.640571000	1.165024000
H	-1.751637000	-6.089217000	1.889731000
C	-2.086417000	-5.187537000	-0.139724000
H	-1.112296000	-5.237331000	-0.621496000
Fe	3.046615000	3.603578000	0.998408000
C	2.101210000	1.753886000	0.747547000
C	3.518162000	1.629652000	1.041238000
C	3.795187000	2.250297000	2.301039000
H	4.782233000	2.331699000	2.755154000
C	2.585347000	2.786193000	2.802722000
H	2.450816000	3.347554000	3.726322000
C	1.550717000	2.487485000	1.864283000
C	3.380832000	4.544313000	-0.793525000
H	3.260639000	4.088669000	-1.775152000
C	4.555651000	4.553612000	0.012568000
H	5.508195000	4.084674000	-0.231008000
C	4.246914000	5.230025000	1.228647000
H	4.924839000	5.374610000	2.068623000
C	2.883111000	5.640410000	1.171824000
H	2.337095000	6.156075000	1.960722000
C	2.352488000	5.220155000	-0.079388000
H	1.336649000	5.358376000	-0.441626000
C	-4.559966000	-1.222986000	0.213907000
C	-4.667120000	-1.501163000	-1.157028000
H	-3.855563000	-2.055804000	-1.624626000
C	-5.791876000	-1.124341000	-1.885500000

C	-6.805358000	-0.409127000	-1.223776000
H	-7.687748000	-0.110845000	-1.789801000
C	-6.730684000	-0.100952000	0.133552000
C	-5.599564000	-0.534484000	0.838810000
H	-5.516051000	-0.328953000	1.907417000
C	-5.997002000	-1.535458000	-3.345360000
C	-7.147459000	-2.551808000	-3.407295000
H	-7.322772000	-2.875742000	-4.446059000
H	-8.085480000	-2.124255000	-3.022335000
H	-6.912497000	-3.443009000	-2.805323000
C	-4.746191000	-2.187177000	-3.934592000
H	-4.500951000	-3.132936000	-3.430004000
H	-3.868991000	-1.531351000	-3.852950000
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H	-5.569729000	0.455453000	-4.113132000
H	-7.300919000	0.153132000	-3.869780000
H	-6.469465000	-0.589180000	-5.250735000
C	-7.843654000	0.640760000	0.879618000
C	-8.449434000	-0.304935000	1.927471000
H	-9.259026000	0.197010000	2.481531000
H	-8.865978000	-1.203899000	1.447961000
C	-7.266271000	1.874880000	1.587254000
H	-6.473854000	1.605929000	2.300138000
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H	-8.576888000	1.781038000	-0.839708000
H	-9.724204000	1.650773000	0.511733000
C	0.065061000	-2.722213000	2.047741000
C	0.758811000	-2.039554000	3.051664000
H	0.268791000	-1.193220000	3.534003000
C	2.019832000	-2.457751000	3.488366000
C	2.584415000	-3.586347000	2.882127000
H	3.548393000	-3.946224000	3.234916000

C	1.927931000	-4.289509000	1.866002000
C	0.677279000	-3.824797000	1.447849000
H	0.120174000	-4.349748000	0.675966000
C	2.687966000	-1.739200000	4.663329000
C	2.493755000	-5.576879000	1.257209000
C	2.765887000	-0.238322000	4.373205000
H	3.267750000	0.292822000	5.197561000
H	1.772697000	0.214227000	4.248129000
H	3.323599000	-0.037708000	3.448315000
C	4.104538000	-2.251552000	4.927390000
H	4.754428000	-2.125345000	4.048024000
H	4.115551000	-3.315259000	5.209448000
H	4.554981000	-1.686242000	5.757399000
C	1.842733000	-1.975199000	5.924504000
H	1.769613000	-3.049488000	6.154097000
H	0.820167000	-1.588539000	5.800114000
H	2.293667000	-1.466912000	6.792194000
C	2.766884000	-5.360742000	-0.235513000
H	1.871252000	-5.010133000	-0.771592000
H	3.103055000	-6.297354000	-0.708972000
H	3.558098000	-4.609667000	-0.371210000
C	3.797425000	-6.010622000	1.928635000
H	4.587482000	-5.253405000	1.818290000
H	4.162651000	-6.939970000	1.465323000
H	3.657024000	-6.206421000	3.002676000
C	1.469144000	-6.708235000	1.428207000
H	1.222852000	-6.857059000	2.490861000
H	1.873468000	-7.653967000	1.033311000
H	0.533321000	-6.498292000	0.891427000
C	4.603389000	0.955423000	0.291973000
C	4.972074000	1.318290000	-1.010584000
H	4.390529000	2.095759000	-1.501305000
C	6.074660000	0.739337000	-1.637533000
C	6.780962000	-0.261014000	-0.949412000

H	7.647056000	-0.713410000	-1.431713000
C	6.427331000	-0.671871000	0.335465000
C	5.339115000	-0.034327000	0.944885000
H	5.034954000	-0.316047000	1.955414000
C	6.595989000	1.224910000	-2.992467000
C	7.171980000	-1.778629000	1.086617000
C	5.593750000	2.144643000	-3.689279000
H	4.625195000	1.643375000	-3.821481000
H	5.972761000	2.433234000	-4.681664000
H	5.420061000	3.070942000	-3.121920000
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H	7.677892000	-0.615734000	-3.516196000
H	7.219290000	0.387085000	-4.903563000
H	5.983757000	-0.579551000	-4.050570000
C	7.894976000	2.010069000	-2.753933000
H	7.712899000	2.875723000	-2.098695000
H	8.306267000	2.380897000	-3.706898000
H	8.660341000	1.381976000	-2.273703000
C	8.395546000	-2.277661000	0.317869000
H	8.903973000	-3.064388000	0.895835000
H	9.122522000	-1.470379000	0.140678000
H	8.119303000	-2.710591000	-0.655866000
C	7.640212000	-1.250067000	2.449739000
H	6.796802000	-0.927117000	3.077052000
H	8.314278000	-0.388829000	2.325102000
H	8.182803000	-2.034920000	3.000379000
C	6.217420000	-2.962431000	1.298854000
H	5.906876000	-3.396261000	0.335321000
H	5.306460000	-2.662739000	1.837143000
H	6.707807000	-3.758600000	1.881956000
C	0.137481000	2.826232000	2.171593000
C	-0.444036000	4.023264000	1.763795000
H	0.137534000	4.670563000	1.112227000
C	-1.725034000	4.400163000	2.189858000

C	-2.398463000	3.545677000	3.063243000
H	-3.385644000	3.829638000	3.429208000
C	-1.845549000	2.332646000	3.503775000
C	-0.584913000	1.977916000	3.024721000
H	-0.115224000	1.044080000	3.330775000
C	-2.304991000	5.745575000	1.746117000
C	-2.613984000	1.484990000	4.521462000
C	-2.127668000	5.928711000	0.233566000
H	-2.603000000	5.111699000	-0.329204000
H	-1.069680000	5.942814000	-0.062476000
H	-2.576650000	6.880810000	-0.090732000
C	-1.548530000	6.862818000	2.480542000
H	-1.930797000	7.853125000	2.183934000
H	-0.473111000	6.830553000	2.248801000
H	-1.660408000	6.761529000	3.570977000
C	-3.795305000	5.862297000	2.071773000
H	-4.376493000	5.050611000	1.605767000
H	-4.187264000	6.818353000	1.692444000
H	-3.986214000	5.838152000	3.155105000
C	-3.974510000	1.086914000	3.937229000
H	-3.837569000	0.466712000	3.040237000
H	-4.574711000	1.967371000	3.662975000
H	-4.553640000	0.499989000	4.668268000
C	-1.863249000	0.206004000	4.887232000
H	-1.724427000	-0.442090000	4.010465000
H	-2.441056000	-0.367227000	5.628402000
H	-0.878166000	0.421761000	5.328763000
C	-2.821170000	2.311669000	5.798879000
H	-3.365757000	1.721947000	6.553751000
H	-3.400585000	3.226623000	5.605134000
H	-1.854155000	2.612757000	6.230257000
H	-7.694966000	-0.634004000	2.657458000
H	-6.839052000	2.584734000	0.862128000
H	-9.455913000	0.257029000	-0.553717000

4

Al	-2.909439000	-0.951053000	-0.918631000
I	-4.022625000	-2.277365000	-2.883984000
Al	2.793770000	0.983904000	-0.826152000
I	3.803190000	2.233876000	-2.902223000
C	-0.908724000	-1.187161000	-1.072859000
H	-0.669051000	-1.342675000	1.120165000
C	0.231796000	0.843425000	-1.982277000
H	0.462448000	1.479739000	-2.845360000
C	-0.451502000	-0.299127000	-2.180025000
C	0.633419000	0.818368000	1.870062000
H	0.281030000	1.843902000	2.072215000
H	1.718870000	0.854887000	2.056659000
H	0.175226000	0.141569000	2.606760000
N	-3.142605000	1.835676000	-2.318411000
C	-3.045562000	1.100918000	-1.187676000
N	-2.884163000	2.012119000	-0.203628000
C	-2.889381000	3.302403000	-0.700334000
C	-3.047151000	3.191696000	-2.052359000
C	-3.186040000	1.320462000	-3.666259000
H	-4.002660000	1.793792000	-4.228270000
H	-3.358413000	0.239009000	-3.642231000
H	-2.229990000	1.517868000	-4.172841000
C	-2.662086000	1.744147000	1.199266000
H	-3.477863000	2.173075000	1.795392000
H	-1.704002000	2.180379000	1.505967000
H	-2.625526000	0.665444000	1.369157000
C	-2.717807000	4.489259000	0.169047000
H	-2.835380000	5.409918000	-0.416153000
H	-1.717266000	4.509980000	0.630303000
H	-3.465264000	4.507466000	0.977129000
C	-3.082883000	4.228598000	-3.112376000
H	-2.961883000	5.224701000	-2.668260000

H	-4.034402000	4.220762000	-3.667328000
H	-2.267499000	4.090726000	-3.839746000
N	2.847361000	-2.038909000	-0.382804000
C	2.809841000	-1.042793000	-1.293953000
N	2.749519000	-1.678133000	-2.487336000
C	2.775729000	-3.053784000	-2.329640000
C	2.846875000	-3.282020000	-0.984546000
C	2.739871000	-1.876821000	1.048837000
H	3.490170000	-2.496543000	1.551997000
H	1.727451000	-2.154187000	1.372790000
H	2.921690000	-0.831826000	1.314182000
C	2.566078000	-1.076242000	-3.787933000
H	1.624542000	-1.433993000	-4.226533000
H	3.403896000	-1.334534000	-4.451439000
H	2.519311000	0.010904000	-3.688887000
C	2.708892000	-3.993806000	-3.475359000
H	2.772733000	-5.029404000	-3.118251000
H	3.531890000	-3.832006000	-4.189056000
H	1.761442000	-3.891946000	-4.027728000
C	2.935336000	-4.542876000	-0.213908000
H	2.916360000	-5.404598000	-0.892661000
H	2.092384000	-4.646194000	0.486308000
H	3.874070000	-4.587278000	0.361248000
C	-3.791144000	-1.417210000	0.799000000
C	-4.967880000	-1.213291000	2.819669000
H	-5.710010000	-0.903354000	3.554322000
C	-4.021610000	-2.255194000	2.978588000
H	-3.906615000	-2.890965000	3.855507000
C	-6.652744000	-3.124668000	-0.021594000
H	-6.814249000	-2.535027000	-0.921907000
C	-7.307747000	-2.955168000	1.231157000
H	-8.059483000	-2.201737000	1.462367000
C	-5.660635000	0.417062000	0.977635000
C	-6.105777000	0.470490000	-0.348948000

H	-5.864883000	-0.364272000	-1.008420000
C	-6.867747000	1.546584000	-0.811792000
C	-7.158844000	2.582784000	0.083138000
H	-7.752629000	3.429053000	-0.269970000
C	-6.733090000	2.568426000	1.414578000
C	-5.990100000	1.467133000	1.844786000
H	-5.632397000	1.412622000	2.873092000
C	-7.406330000	1.625411000	-2.242479000
C	-7.023527000	0.398955000	-3.067832000
H	-7.420819000	0.494681000	-4.089952000
H	-7.433689000	-0.527407000	-2.638597000
H	-5.935138000	0.268586000	-3.142001000
C	-6.827941000	2.873163000	-2.924093000
H	-7.178608000	2.944718000	-3.966225000
H	-5.729250000	2.830620000	-2.926427000
H	-7.121831000	3.797894000	-2.405353000
C	-8.938106000	1.722943000	-2.205128000
H	-9.344126000	1.778374000	-3.227860000
H	-9.281367000	2.614466000	-1.659617000
H	-9.372461000	0.839762000	-1.712333000
C	-7.106514000	3.726138000	2.344740000
C	-6.632353000	5.053693000	1.737421000
H	-6.906137000	5.896438000	2.391880000
H	-7.079611000	5.238558000	0.749961000
H	-5.538414000	5.060758000	1.614435000
C	-8.633059000	3.756722000	2.510339000
H	-8.934894000	4.581296000	3.176163000
H	-8.997610000	2.813166000	2.944236000
H	-9.141628000	3.898558000	1.545155000
C	-6.471098000	3.581439000	3.728251000
H	-6.750164000	4.439357000	4.358841000
H	-5.371540000	3.553667000	3.671873000
H	-6.809762000	2.669351000	4.242063000
C	-2.256511000	-3.411532000	1.539248000

C	-1.388545000	-3.743661000	2.585323000
H	-1.476318000	-3.192630000	3.524521000
C	-0.432864000	-4.755769000	2.454021000
C	-0.362272000	-5.434542000	1.232047000
H	0.351894000	-6.247679000	1.122062000
C	-1.197263000	-5.115286000	0.152174000
C	-2.133769000	-4.094066000	0.324525000
H	-2.820450000	-3.839381000	-0.485198000
C	0.464610000	-5.107316000	3.645789000
C	1.270373000	-3.871325000	4.070126000
H	1.888519000	-4.098655000	4.953414000
H	0.618344000	-3.023164000	4.325394000
H	1.942687000	-3.545723000	3.262979000
C	-0.418843000	-5.567048000	4.815089000
H	0.200744000	-5.834961000	5.686055000
H	-1.014092000	-6.448605000	4.531929000
H	-1.118058000	-4.778479000	5.129750000
C	1.451169000	-6.229845000	3.320311000
H	2.076045000	-6.442650000	4.201088000
H	2.127301000	-5.955150000	2.496179000
H	0.936211000	-7.162586000	3.045051000
C	-1.126737000	-5.858389000	-1.185441000
C	-0.148873000	-7.033373000	-1.140610000
H	-0.144779000	-7.549431000	-2.112740000
H	-0.429265000	-7.770662000	-0.372690000
H	0.881156000	-6.703943000	-0.937383000
C	-0.669874000	-4.878743000	-2.275016000
H	-0.555787000	-5.401234000	-3.238909000
H	0.294163000	-4.419952000	-2.008942000
H	-1.400068000	-4.069269000	-2.420911000
C	-2.515664000	-6.402610000	-1.548159000
H	-2.469170000	-6.968091000	-2.492332000
H	-3.243825000	-5.591231000	-1.689993000
H	-2.896493000	-7.073873000	-0.763071000

C	3.916023000	1.464119000	0.753744000
C	4.971013000	0.715915000	1.407018000
C	5.266754000	1.320920000	2.670271000
H	6.048340000	1.002312000	3.358929000
C	4.433519000	2.456790000	2.818171000
H	4.459134000	3.170031000	3.641150000
C	3.614724000	2.565202000	1.649833000
Fe	5.583826000	2.632568000	1.149073000
C	6.756964000	2.925829000	-0.505440000
H	6.728621000	2.317450000	-1.407233000
C	7.562785000	2.700283000	0.646039000
H	8.260230000	1.875363000	0.785783000
C	7.250653000	3.708486000	1.604697000
H	7.673138000	3.792788000	2.605025000
C	6.253360000	4.557865000	1.041801000
H	5.773922000	5.401662000	1.536001000
C	5.949788000	4.073110000	-0.261208000
H	5.207712000	4.481492000	-0.943571000
C	2.604267000	3.624687000	1.466800000
C	1.836216000	4.040931000	2.559553000
H	2.001429000	3.552686000	3.522620000
C	0.855875000	5.029171000	2.435392000
C	0.664504000	5.608716000	1.175930000
H	-0.079498000	6.394474000	1.065174000
C	1.405449000	5.213039000	0.054713000
C	2.373296000	4.219887000	0.223178000
H	2.977590000	3.898178000	-0.626491000
C	0.018071000	5.421486000	3.656377000
C	0.946359000	5.873284000	4.792295000
H	0.359367000	6.159489000	5.679700000
H	1.547713000	6.741934000	4.483332000
H	1.640709000	5.075766000	5.094167000
C	-0.954340000	6.561812000	3.350956000
H	-1.523899000	6.818101000	4.257315000

H	-1.681919000	6.284571000	2.572793000
H	-0.427903000	7.469677000	3.019456000
C	-0.797368000	4.202543000	4.113859000
H	-1.399926000	4.449432000	5.002875000
H	-0.149454000	3.351506000	4.370676000
H	-1.484346000	3.870739000	3.319813000
C	1.170576000	5.815588000	-1.333345000
C	2.503903000	6.289240000	-1.928135000
H	2.338737000	6.749178000	-2.915334000
H	3.204139000	5.453776000	-2.071654000
H	2.984624000	7.035535000	-1.276918000
C	0.213689000	7.007960000	-1.289751000
H	0.098037000	7.427206000	-2.300878000
H	0.588091000	7.810171000	-0.635243000
H	-0.788193000	6.719379000	-0.937160000
C	0.567021000	4.733856000	-2.241614000
H	0.356429000	5.146429000	-3.242094000
H	-0.371789000	4.340499000	-1.822646000
H	1.257742000	3.888142000	-2.369182000
C	5.635229000	-0.504241000	0.917533000
C	5.952452000	-0.677426000	-0.437912000
H	5.731577000	0.140805000	-1.124245000
C	6.561230000	-1.845979000	-0.891219000
C	6.824251000	-2.864205000	0.041028000
H	7.295602000	-3.781986000	-0.310137000
C	6.521294000	-2.730185000	1.396291000
C	5.938660000	-1.527846000	1.816290000
H	5.676139000	-1.385747000	2.867246000
C	6.996550000	-2.031861000	-2.346439000
C	8.531250000	-2.065725000	-2.398972000
H	8.879682000	-2.198917000	-3.435925000
H	8.938806000	-2.890965000	-1.795691000
H	8.955183000	-1.126170000	-2.012975000
C	6.503667000	-0.892431000	-3.237336000

H	6.795612000	-1.078283000	-4.282306000
H	6.932900000	0.076822000	-2.944280000
H	5.410152000	-0.787118000	-3.201763000
C	6.437364000	-3.352052000	-2.892141000
H	6.711319000	-3.476930000	-3.951867000
H	5.341449000	-3.367955000	-2.808602000
H	6.826104000	-4.224323000	-2.346274000
C	6.808384000	-3.828121000	2.425093000
H	5.055875000	-3.347597000	3.665765000
C	7.379075000	-5.090297000	1.777964000
H	7.555559000	-5.857565000	2.547127000
H	8.339927000	-4.895498000	1.278273000
C	0.793686000	1.265189000	-0.661445000
H	0.599398000	2.332723000	-0.453360000
C	0.305216000	0.398825000	0.468905000
C	-0.391995000	-0.736041000	0.249789000
H	-0.686563000	-2.249953000	-1.264861000
H	-0.760970000	-0.565591000	-3.198505000
C	-4.847613000	-0.701569000	1.488005000
C	-3.302302000	-2.392608000	1.749470000
Fe	-5.299359000	-2.677156000	1.447106000
C	-5.705940000	-4.179099000	0.114371000
H	-5.030264000	-4.522982000	-0.665240000
C	-6.763111000	-3.907734000	2.142507000
H	-7.031116000	-4.013711000	3.192874000
C	-5.771386000	-4.663875000	1.450801000
H	-5.142827000	-5.444040000	1.877965000
C	7.827539000	-3.298949000	3.444612000
H	8.055406000	-4.067930000	4.200207000
H	7.449057000	-2.410403000	3.971199000
H	8.767489000	-3.016941000	2.946205000
C	5.510791000	-4.208555000	3.154188000
H	5.708023000	-4.980470000	3.914978000
H	4.765122000	-4.614655000	2.453006000

H	6.686958000	-5.516342000	1.034994000
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Al	0.331345000	-1.058531000	-0.860581000
I	0.437620000	-3.065570000	0.795800000
N	-1.829820000	-0.007967000	-2.671181000
C	-1.385991000	-1.083506000	-1.971216000
N	-2.222081000	-2.089369000	-2.333713000
C	-3.187719000	-1.648597000	-3.225699000
C	-2.940314000	-0.322125000	-3.434233000
C	-1.206130000	1.295534000	-2.705292000
H	-1.868036000	2.050337000	-2.259535000
H	-0.976006000	1.570314000	-3.744489000
H	-0.276077000	1.273106000	-2.127268000
C	-2.101916000	-3.475179000	-1.945525000
H	-1.832340000	-4.092416000	-2.815684000
H	-3.049258000	-3.839845000	-1.525259000
H	-1.320254000	-3.576778000	-1.184420000
C	-4.230889000	-2.541274000	-3.787437000
H	-4.871501000	-1.983921000	-4.482507000
H	-4.878381000	-2.962055000	-3.001598000
H	-3.791042000	-3.385731000	-4.341492000
C	-3.646192000	0.679259000	-4.269148000
H	-4.517376000	0.223569000	-4.756342000
H	-2.996864000	1.090171000	-5.058594000
H	-4.003764000	1.524459000	-3.660454000
C	0.441304000	0.682284000	0.084724000
C	-0.624945000	1.545556000	0.553823000
C	-0.063526000	2.802081000	0.948392000
H	-0.613693000	3.631592000	1.391244000
C	1.338954000	2.741976000	0.750036000
H	2.058432000	3.516196000	1.013326000
C	1.658357000	1.452573000	0.221760000
Fe	0.735647000	1.278833000	2.035463000

C	0.153089000	-0.142261000	3.387145000
H	-0.543580000	-0.951957000	3.178529000
C	-0.178715000	1.161790000	3.853828000
H	-1.182614000	1.529649000	4.061575000
C	1.029445000	1.914279000	3.947549000
H	1.111068000	2.958935000	4.244750000
C	2.105233000	1.073820000	3.536846000
H	3.152313000	1.362266000	3.455997000
C	1.562732000	-0.195628000	3.191193000
H	2.117728000	-1.049409000	2.807729000
C	3.016473000	1.013799000	-0.141506000
C	3.928373000	1.929237000	-0.674572000
H	3.603749000	2.962707000	-0.815925000
C	5.221151000	1.545148000	-1.042691000
C	5.582635000	0.204683000	-0.870210000
H	6.584618000	-0.111147000	-1.151530000
C	4.697101000	-0.744339000	-0.344934000
C	3.418149000	-0.316777000	0.019699000
H	2.720872000	-1.022613000	0.475864000
C	6.181859000	2.588118000	-1.621182000
C	6.383656000	3.713820000	-0.596513000
H	7.070211000	4.479267000	-0.993077000
H	6.811511000	3.319700000	0.338093000
H	5.435111000	4.211370000	-0.346106000
C	7.550215000	1.993070000	-1.955583000
H	8.207002000	2.776504000	-2.363978000
H	7.475672000	1.195443000	-2.710312000
H	8.043447000	1.576631000	-1.064126000
C	5.580692000	3.168484000	-2.909591000
H	6.254403000	3.924758000	-3.344117000
H	4.609451000	3.650449000	-2.724102000
H	5.423657000	2.376906000	-3.658349000
C	5.077298000	-2.217964000	-0.181774000
C	4.741451000	-2.690839000	1.239672000

H	5.045463000	-3.741257000	1.372122000
H	3.662553000	-2.638227000	1.445653000
H	5.267195000	-2.083462000	1.992830000
C	6.567647000	-2.459272000	-0.426831000
H	6.800977000	-3.523565000	-0.270492000
H	7.194487000	-1.873130000	0.263207000
H	6.862337000	-2.207734000	-1.457019000
C	4.272091000	-3.041628000	-1.198127000
H	4.506726000	-4.113965000	-1.098815000
H	4.508580000	-2.729691000	-2.227227000
H	3.188935000	-2.916685000	-1.050382000
C	-2.070542000	1.261095000	0.567874000
C	-2.579704000	-0.004338000	0.901481000
H	-1.872625000	-0.782697000	1.190296000
C	-3.950888000	-0.252279000	0.897617000
C	-4.817515000	0.793769000	0.538094000
H	-5.890489000	0.601918000	0.533739000
C	-4.352285000	2.064546000	0.206070000
C	-2.967299000	2.276478000	0.229336000
H	-2.561739000	3.257473000	-0.030192000
C	-4.547858000	-1.607534000	1.283958000
C	-5.508517000	-1.425269000	2.467818000
H	-5.943855000	-2.393949000	2.761091000
H	-6.338227000	-0.744888000	2.225504000
H	-4.977888000	-1.011489000	3.338809000
C	-3.472466000	-2.612716000	1.690454000
H	-3.937073000	-3.575639000	1.952635000
H	-2.903602000	-2.269570000	2.567530000
H	-2.747509000	-2.797810000	0.885879000
C	-5.316916000	-2.171839000	0.081071000
H	-5.737273000	-3.162554000	0.317827000
H	-4.647191000	-2.273842000	-0.785440000
H	-6.148064000	-1.515937000	-0.218382000
C	-5.286953000	3.219363000	-0.164121000

H	-3.914026000	4.035258000	-1.672445000
C	-6.758730000	2.806905000	-0.127305000
H	-7.393586000	3.663707000	-0.400193000
H	-7.063747000	2.473969000	0.876260000
C	-5.081807000	4.370379000	0.831537000
H	-5.746869000	5.214767000	0.589076000
H	-4.047010000	4.742798000	0.816402000
H	-5.303651000	4.041919000	1.858321000
C	-4.960230000	3.706693000	-1.582757000
H	-5.603078000	4.557656000	-1.859042000
H	-5.128923000	2.903518000	-2.317174000
H	-6.973275000	1.994189000	-0.838221000

6'

Al	0.210871000	1.072526000	0.030871000
I	0.418774000	1.825239000	-2.456874000
C	0.040071000	4.001868000	2.800790000
H	0.279309000	2.518267000	4.367583000
C	1.278146000	3.581680000	0.756753000
H	1.666984000	3.930015000	-0.203413000
C	0.512285000	4.415606000	1.531605000
C	1.860107000	0.662546000	3.189170000
H	2.959644000	0.664115000	3.098293000
H	1.527010000	-0.250015000	2.665397000
H	1.601623000	0.566302000	4.254136000
N	-2.130249000	1.230431000	1.957619000
C	-1.566963000	1.749221000	0.844012000
N	-2.326852000	2.827002000	0.548099000
C	-3.351763000	2.988615000	1.463889000
C	-3.228250000	1.965027000	2.359789000
C	-1.621784000	0.123082000	2.734313000
H	-2.410864000	-0.625330000	2.879374000
H	-1.258577000	0.486373000	3.705259000
H	-0.792429000	-0.349949000	2.200469000

C	-2.104478000	3.775397000	-0.518742000
H	-1.912947000	4.770824000	-0.096547000
H	-2.983263000	3.817945000	-1.177949000
H	-1.233692000	3.470318000	-1.107040000
C	-4.312454000	4.116924000	1.405380000
H	-5.041939000	4.035160000	2.221011000
H	-4.872004000	4.135519000	0.457024000
H	-3.800294000	5.086804000	1.509216000
C	-4.035080000	1.614055000	3.552445000
H	-4.843472000	2.342357000	3.693500000
H	-3.424882000	1.606164000	4.469207000
H	-4.493348000	0.617890000	3.447570000
C	0.325597000	-0.911228000	0.112642000
C	-0.751831000	-1.879092000	0.197047000
C	-0.203664000	-3.163961000	0.509958000
H	-0.768130000	-4.092267000	0.589212000
C	1.204389000	-3.032168000	0.596272000
H	1.918221000	-3.839254000	0.755853000
C	1.540817000	-1.665141000	0.344268000
Fe	0.543402000	-2.463298000	-1.245531000
C	-0.058501000	-1.948186000	-3.133939000
H	-0.697518000	-1.101175000	-3.375277000
C	-0.484441000	-3.267782000	-2.812339000
H	-1.517148000	-3.609218000	-2.754285000
C	0.675999000	-4.043565000	-2.520163000
H	0.685705000	-5.086587000	-2.206583000
C	1.817663000	-3.200859000	-2.661684000
H	2.852406000	-3.482211000	-2.471607000
C	1.361949000	-1.907419000	-3.040989000
H	1.981799000	-1.028328000	-3.202323000
C	2.924954000	-1.154605000	0.357277000
C	3.819244000	-1.615859000	1.327445000
H	3.457691000	-2.338000000	2.063131000
C	5.135501000	-1.151072000	1.391212000

C	5.545337000	-0.209823000	0.441131000
H	6.568156000	0.158106000	0.472269000
C	4.682385000	0.272699000	-0.551073000
C	3.372108000	-0.212236000	-0.573861000
H	2.674648000	0.132084000	-1.339509000
C	6.065588000	-1.669385000	2.491633000
C	6.179935000	-3.196596000	2.382839000
H	6.843978000	-3.590855000	3.168858000
H	6.593291000	-3.489388000	1.405454000
H	5.202046000	-3.687937000	2.493395000
C	7.470392000	-1.074047000	2.390320000
H	8.104059000	-1.476527000	3.195439000
H	7.458540000	0.021570000	2.494154000
H	7.951408000	-1.322910000	1.432110000
C	5.479666000	-1.293842000	3.860705000
H	6.127369000	-1.661767000	4.672812000
H	4.478216000	-1.724854000	4.007344000
H	5.390930000	-0.201102000	3.961764000
C	5.129154000	1.307742000	-1.587713000
C	4.777076000	0.813377000	-2.997920000
H	5.126919000	1.535339000	-3.752645000
H	3.691034000	0.703994000	-3.131923000
H	5.249634000	-0.158894000	-3.206844000
C	6.635745000	1.565063000	-1.530612000
H	6.917797000	2.285854000	-2.313101000
H	7.214322000	0.643494000	-1.698933000
H	6.943958000	1.993535000	-0.564802000
C	4.395534000	2.629582000	-1.318995000
H	4.714105000	3.399590000	-2.040192000
H	4.605884000	3.000998000	-0.304155000
H	3.307241000	2.509553000	-1.421170000
C	-2.195054000	-1.630151000	0.035965000
C	-2.686718000	-0.727088000	-0.919751000
H	-1.968864000	-0.231159000	-1.574108000

C	-4.053916000	-0.497758000	-1.057982000
C	-4.933830000	-1.182154000	-0.202658000
H	-6.004063000	-1.003420000	-0.306551000
C	-4.485445000	-2.091850000	0.753783000
C	-3.104163000	-2.304896000	0.852197000
H	-2.711400000	-3.004272000	1.594080000
C	-4.630036000	0.447528000	-2.114607000
C	-5.582363000	-0.333173000	-3.031778000
H	-6.003312000	0.331819000	-3.802777000
H	-6.422329000	-0.773780000	-2.474574000
H	-5.049819000	-1.151451000	-3.540001000
C	-3.537483000	1.072906000	-2.979426000
H	-3.986182000	1.755790000	-3.717039000
H	-2.970867000	0.311224000	-3.535625000
H	-2.812764000	1.647669000	-2.386549000
C	-5.402190000	1.571409000	-1.409859000
H	-5.807681000	2.284877000	-2.145223000
H	-4.740238000	2.115140000	-0.720518000
H	-6.245071000	1.181647000	-0.819672000
C	-5.435669000	-2.865857000	1.671551000
H	-4.047870000	-2.860028000	3.375280000
C	-6.898262000	-2.481999000	1.445702000
H	-7.544219000	-3.053634000	2.129428000
H	-7.224742000	-2.704109000	0.418581000
C	1.542612000	2.184187000	1.156060000
H	2.526528000	1.810882000	0.825590000
C	1.275251000	1.899184000	2.588694000
C	0.500875000	2.767393000	3.323645000
H	-0.563706000	4.670835000	3.416983000
H	0.297338000	5.429772000	1.180398000
C	-5.279906000	-4.368843000	1.397182000
H	-5.954078000	-4.952663000	2.044288000
H	-4.251879000	-4.711644000	1.585731000
H	-5.522708000	-4.601109000	0.349097000

C	-5.083765000	-2.576105000	3.137444000
H	-5.747073000	-3.138090000	3.813962000
H	-5.201754000	-1.504567000	3.362839000
H	-7.073986000	-1.412226000	1.637488000

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Al	1.242865000	0.265010000	-0.313101000
Al	-0.755140000	1.184475000	1.107711000
H	-0.414089000	2.475752000	2.041817000
C	-2.374490000	1.567790000	-0.014592000
C	-2.485734000	2.631837000	-0.990307000
C	-3.788569000	2.599765000	-1.580875000
H	-4.172974000	3.309519000	-2.312613000
C	-4.501838000	1.518363000	-1.007580000
H	-5.528021000	1.224041000	-1.224155000
C	-3.641589000	0.881290000	-0.058308000
Fe	-3.931990000	2.856747000	0.423337000
C	-3.359802000	4.094698000	1.943381000
H	-2.331928000	4.195441000	2.289530000
C	-3.964126000	4.836158000	0.887782000
H	-3.475298000	5.603928000	0.289385000
C	-5.291333000	4.346855000	0.708306000
H	-6.001929000	4.687903000	-0.043081000
C	-5.508354000	3.300719000	1.651682000
H	-6.415801000	2.707084000	1.753358000
C	-4.314863000	3.149515000	2.416369000
H	-4.155686000	2.428015000	3.213752000
C	-1.311884000	-0.128552000	2.631882000
N	-1.280377000	-1.477264000	2.609539000
C	-1.550586000	-2.021362000	3.849834000
C	-1.762321000	-0.964362000	4.691734000
N	-1.612349000	0.176134000	3.918452000
C	-1.758150000	1.511917000	4.446136000
H	-2.780284000	1.670000000	4.819402000

H	-1.534372000	2.221060000	3.639243000
H	-1.048836000	1.675868000	5.269341000
C	-2.053942000	-0.920779000	6.145508000
H	-3.004831000	-0.408645000	6.361589000
H	-1.259075000	-0.398232000	6.701332000
H	-2.127207000	-1.939295000	6.547758000
C	-1.577242000	-3.485173000	4.082546000
H	-2.371137000	-3.965737000	3.487873000
H	-1.768459000	-3.704611000	5.140608000
H	-0.620340000	-3.954487000	3.805330000
C	-1.011159000	-2.285160000	1.443661000
H	-1.833231000	-2.991987000	1.290853000
H	-0.058779000	-2.821460000	1.550919000
H	-0.944326000	-1.633511000	0.567649000
C	3.038294000	1.319647000	-0.438034000
N	4.207557000	1.924275000	-0.147137000
C	4.900325000	1.819879000	1.111726000
H	4.360102000	1.113037000	1.748784000
H	4.942109000	2.797861000	1.614994000
H	5.924912000	1.449864000	0.964266000
C	4.632150000	2.706294000	-1.218625000
C	5.880390000	3.507181000	-1.173452000
H	6.028119000	4.030631000	-2.126956000
H	6.768346000	2.878710000	-0.996511000
H	5.848274000	4.268695000	-0.376947000
C	3.687897000	2.566791000	-2.205294000
C	3.574666000	3.154435000	-3.559832000
H	3.512258000	2.370727000	-4.331240000
H	4.438294000	3.792395000	-3.788364000
H	2.661881000	3.765005000	-3.635684000
N	2.738892000	1.707876000	-1.688976000
C	1.475829000	1.159157000	-2.179207000
H	1.643216000	0.528521000	-3.067953000
H	0.788081000	1.979187000	-2.438449000

C	-4.026260000	-0.386069000	0.609984000
C	-3.910606000	-1.578851000	-0.106460000
H	-3.480304000	-1.538527000	-1.109669000
C	-4.344948000	-2.801981000	0.424397000
C	-4.892501000	-2.792063000	1.709948000
H	-5.258289000	-3.726287000	2.136634000
C	-5.031231000	-1.612209000	2.459185000
C	-4.584601000	-0.419343000	1.892334000
H	-4.684576000	0.527378000	2.416469000
C	-1.424373000	3.559538000	-1.422931000
C	-1.321141000	3.887633000	-2.778805000
H	-2.045617000	3.457197000	-3.471360000
C	-0.302818000	4.710800000	-3.264855000
C	0.621759000	5.222462000	-2.347554000
H	1.416413000	5.874326000	-2.704715000
C	0.544832000	4.930429000	-0.978868000
C	-0.482348000	4.092404000	-0.536750000
H	-0.574122000	3.847784000	0.522887000
C	3.345496000	-1.478566000	1.874008000
C	2.708181000	-0.607297000	2.763440000
H	1.645387000	-0.397454000	2.614762000
C	3.404101000	-0.025813000	3.833064000
C	4.760384000	-0.332905000	3.990842000
H	5.308473000	0.113998000	4.816821000
C	5.432331000	-1.195227000	3.116646000
C	4.704253000	-1.755190000	2.067386000
H	5.187544000	-2.427510000	1.357780000
C	0.395926000	-2.915997000	-2.135615000
C	0.356120000	-4.101926000	-2.878040000
H	0.987912000	-4.934105000	-2.568344000
C	-0.436637000	-4.249688000	-4.017595000
C	-1.200674000	-3.156162000	-4.420444000
H	-1.818610000	-3.234259000	-5.314503000
C	-1.190371000	-1.943558000	-3.717230000

C	-0.400708000	-1.843153000	-2.567642000
H	-0.392996000	-0.911907000	-1.999382000
C	-5.756363000	-1.646431000	3.807734000
C	-5.172968000	-2.738479000	4.711971000
H	-5.712228000	-2.769355000	5.672063000
H	-4.111771000	-2.542780000	4.918952000
H	-5.251323000	-3.737287000	4.258578000
C	-5.648942000	-0.309401000	4.543228000
H	-6.145059000	0.504508000	3.994247000
H	-4.597384000	-0.023095000	4.694856000
H	-6.129536000	-0.382626000	5.530875000
C	-7.241503000	-1.942769000	3.548519000
H	-7.374515000	-2.916183000	3.052977000
H	-7.684913000	-1.173445000	2.898220000
H	-7.805952000	-1.962356000	4.495072000
C	-0.230621000	4.998290000	-4.767534000
C	-0.026250000	3.674751000	-5.521031000
H	-0.849832000	2.969760000	-5.335595000
H	0.904696000	3.179814000	-5.205177000
H	0.029764000	3.851126000	-6.607422000
C	0.916228000	5.945016000	-5.124007000
H	0.922877000	6.130578000	-6.208991000
H	1.897316000	5.524301000	-4.856524000
H	0.813045000	6.917639000	-4.619203000
C	-1.544651000	5.647824000	-5.224675000
H	-2.409150000	4.995181000	-5.034646000
H	-1.515156000	5.858912000	-6.305818000
H	-1.717916000	6.596422000	-4.693598000
C	2.672205000	0.904215000	4.803063000
C	1.571166000	0.100507000	5.508019000
H	1.023461000	0.741990000	6.218391000
H	2.001225000	-0.741147000	6.072684000
H	0.850156000	-0.312721000	4.789331000
C	2.053966000	2.070264000	4.022921000

H	1.346477000	1.740118000	3.249214000
H	2.833874000	2.662477000	3.520236000
H	1.507881000	2.745088000	4.702129000
C	3.601256000	1.480914000	5.872193000
H	3.030119000	2.148842000	6.535070000
H	4.415841000	2.073650000	5.428522000
H	4.049282000	0.695335000	6.499768000
C	-4.283049000	-4.071170000	-0.434190000
C	6.917054000	-1.537073000	3.268166000
H	7.065831000	-1.144699000	5.417936000
C	-0.419924000	-5.577478000	-4.779363000
C	-0.887744000	-6.703392000	-3.846407000
H	-1.917310000	-6.521750000	-3.501459000
H	-0.247553000	-6.787223000	-2.955830000
H	-0.867619000	-7.673220000	-4.369172000
C	-1.339081000	-5.552986000	-6.000893000
H	-1.301191000	-6.524979000	-6.516281000
H	-1.035985000	-4.781056000	-6.724486000
H	-2.386511000	-5.366322000	-5.718730000
C	1.011148000	-5.866031000	-5.256059000
H	1.050701000	-6.818384000	-5.809018000
H	1.715159000	-5.937976000	-4.413703000
H	1.369175000	-5.066789000	-5.923265000
C	-1.468551000	-0.399106000	-5.651838000
H	-1.534386000	-1.233345000	-6.366408000
H	-2.037182000	0.448143000	-6.068415000
H	-3.624415000	-2.067175000	-5.048492000
H	-3.911337000	-1.440161000	-3.408747000
C	1.497698000	5.559834000	0.041673000
C	0.716918000	6.624763000	0.827015000
H	0.326345000	7.403632000	0.153843000
H	1.364664000	7.108826000	1.576302000
H	-0.138752000	6.177031000	1.354644000
C	2.703035000	6.222890000	-0.627766000

H	3.267681000	5.499300000	-1.236663000
H	3.383091000	6.620331000	0.141751000
H	2.411881000	7.066045000	-1.272343000
C	2.018799000	4.494920000	1.012880000
H	1.210332000	3.988365000	1.558871000
H	2.690052000	4.956045000	1.756023000
H	2.579632000	3.719779000	0.473774000
C	2.610223000	-2.195736000	0.809935000
C	1.888460000	-4.020287000	-0.388063000
H	1.761051000	-5.045453000	-0.728326000
C	3.753714000	-2.756832000	-3.027646000
H	3.024322000	-2.964595000	-3.809901000
C	4.048736000	-1.474582000	-2.482429000
H	3.596784000	-0.532620000	-2.782342000
C	4.993857000	-1.647017000	-1.430773000
H	5.383172000	-0.856984000	-0.790280000
C	5.290708000	-3.038560000	-1.330577000
H	5.972063000	-3.503784000	-0.619025000
C	4.521534000	-3.724455000	-2.317291000
H	4.505401000	-4.801016000	-2.480963000
C	-5.271970000	-3.904965000	-1.598702000
H	-5.278380000	-4.807670000	-2.230853000
H	-4.999092000	-3.051505000	-2.235948000
H	-6.293974000	-3.735445000	-1.226380000
C	-2.874693000	-4.287050000	-1.004018000
H	-2.871576000	-5.152729000	-1.683971000
H	-2.142706000	-4.494787000	-0.209036000
H	-2.507760000	-3.424893000	-1.578103000
C	-4.672823000	-5.320344000	0.357504000
H	-5.712810000	-5.277526000	0.715153000
H	-4.015508000	-5.470778000	1.228574000
H	-4.581970000	-6.209563000	-0.284674000
C	7.671607000	-1.093918000	2.006307000
H	7.270195000	-1.572079000	1.100572000

H	8.738974000	-1.356672000	2.080950000
H	7.600740000	-0.003403000	1.870829000
C	7.550184000	-0.845735000	4.475919000
H	7.494491000	0.250707000	4.395140000
H	8.613916000	-1.119518000	4.547547000
C	7.067314000	-3.055125000	3.444140000
H	6.527585000	-3.400455000	4.339232000
H	8.128935000	-3.328170000	3.555720000
H	6.667871000	-3.605448000	2.579501000
C	-2.016181000	-0.779462000	-4.267637000
C	-1.945274000	0.447274000	-3.370705000
H	-2.582312000	1.242562000	-3.782352000
H	-0.925635000	0.846016000	-3.289887000
H	-2.307096000	0.243701000	-2.354561000
H	-0.411937000	-0.097820000	-5.580820000
C	-3.488913000	-1.193215000	-4.394402000
H	-4.082062000	-0.364550000	-4.812319000
C	1.270537000	-2.847180000	-0.945501000
C	1.708180000	-1.685369000	-0.196862000
C	2.716890000	-3.619228000	0.683463000
H	3.327919000	-4.267914000	1.309887000
Fe	3.294730000	-2.709696000	-1.042145000

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C	3.768161000	-1.174839000	-1.488159000
H	5.189595000	1.839712000	-3.461679000
C	3.765743000	0.107600000	-0.928036000
H	3.383714000	0.214533000	0.085413000
C	3.786269000	3.678171000	-1.674068000
H	2.696875000	3.588797000	-1.559407000
H	4.029255000	3.681850000	-2.747978000
H	4.073914000	4.658286000	-1.262890000
C	4.028905000	2.537680000	0.523524000
H	4.199257000	3.515549000	0.991825000

H	4.567885000	1.787080000	1.120833000
H	2.951224000	2.332477000	0.601285000
C	5.349428000	-0.433334000	-4.927156000
C	4.533852000	0.411743000	-5.914162000
H	3.486786000	0.075905000	-5.932462000
H	4.943496000	0.324435000	-6.933399000
H	4.540681000	1.477034000	-5.639150000
H	5.907786000	-2.543110000	-4.742791000
C	0.462607000	3.817644000	1.099817000
C	0.734188000	3.033204000	2.228549000
H	0.118346000	2.152030000	2.416015000
C	1.721738000	3.398058000	3.148510000
C	2.432597000	4.581752000	2.922228000
H	3.185341000	4.891191000	3.650802000
C	2.211902000	5.380192000	1.795973000
C	1.236694000	4.968128000	0.886840000
H	1.049920000	5.561917000	-0.005832000
C	3.004394000	6.679892000	1.620905000
C	2.665323000	7.391976000	0.310749000
H	1.604571000	7.681760000	0.265561000
H	2.885498000	6.761915000	-0.564550000
H	3.264060000	8.311303000	0.220014000
C	2.661912000	7.621444000	2.785319000
H	3.207359000	8.574127000	2.687513000
H	2.928343000	7.178354000	3.756287000
H	1.583517000	7.842003000	2.803922000
C	4.511171000	6.387275000	1.630774000
H	5.085319000	7.324419000	1.553411000
H	4.794899000	5.746391000	0.782243000
H	4.825115000	5.877780000	2.553466000
C	2.007606000	2.580516000	4.411055000
C	3.509354000	2.275579000	4.504340000
H	4.114026000	3.191622000	4.576932000
H	3.855800000	1.715372000	3.623683000

H	3.720830000	1.665679000	5.396723000
C	1.575922000	3.401201000	5.635435000
H	2.121058000	4.355437000	5.697075000
H	1.768213000	2.840140000	6.564306000
H	0.500023000	3.630894000	5.590600000
C	1.242846000	1.257351000	4.420517000
H	0.153783000	1.406806000	4.431381000
H	1.511581000	0.675385000	5.315441000
H	1.472180000	0.642968000	3.537470000
C	0.983467000	-4.255001000	1.505496000
C	0.542913000	-5.564194000	1.315274000
H	1.047046000	-6.175042000	0.562731000
C	-0.546930000	-6.081942000	2.029573000
C	-1.163818000	-5.253050000	2.967042000
H	-2.009211000	-5.634759000	3.538983000
C	-0.723780000	-3.940947000	3.216262000
C	0.339489000	-3.453511000	2.461338000
H	0.694672000	-2.431461000	2.594404000
C	-1.417096000	-3.101504000	4.293146000
C	-0.648854000	-1.814515000	4.593840000
H	-0.608014000	-1.140608000	3.725986000
H	0.379676000	-2.026129000	4.925300000
H	-1.151263000	-1.262503000	5.403182000
C	-2.822094000	-2.726730000	3.801909000
H	-3.359245000	-2.149924000	4.572469000
H	-3.420760000	-3.619535000	3.563938000
H	-2.756609000	-2.108392000	2.896098000
C	-1.523070000	-3.911056000	5.593348000
H	-1.990894000	-3.299982000	6.381357000
H	-0.526639000	-4.218737000	5.946341000
H	-2.133350000	-4.818418000	5.474121000
C	-1.001653000	-7.521822000	1.773887000
C	-2.264543000	-7.876539000	2.559598000
H	-3.105504000	-7.215940000	2.297123000

H	-2.103517000	-7.810469000	3.646105000
H	-2.567929000	-8.909957000	2.332149000
C	0.122668000	-8.477243000	2.199961000
H	1.048332000	-8.287009000	1.636650000
H	-0.171032000	-9.525124000	2.025703000
H	0.352190000	-8.357260000	3.269777000
C	-1.297064000	-7.716616000	0.279670000
H	-2.099227000	-7.041265000	-0.055245000
H	-1.618943000	-8.751959000	0.083666000
H	-0.412329000	-7.519036000	-0.342669000
C	-3.559415000	1.763316000	-1.437445000
C	-4.902091000	2.120193000	-1.321739000
H	-5.139524000	2.997718000	-0.718425000
C	-5.918824000	1.387690000	-1.947174000
C	-5.542522000	0.293318000	-2.724697000
H	-6.311161000	-0.284420000	-3.238225000
C	-4.199515000	-0.079589000	-2.896114000
C	-3.219996000	0.652166000	-2.224582000
H	-2.165082000	0.391977000	-2.318691000
C	-3.871803000	-1.235358000	-3.844858000
C	-4.387750000	-0.893903000	-5.250628000
H	-5.477072000	-0.742374000	-5.262625000
H	-4.154981000	-1.710045000	-5.953799000
H	-3.917264000	0.027879000	-5.626150000
C	-4.552471000	-2.515778000	-3.344523000
H	-5.647750000	-2.413369000	-3.323620000
H	-4.221662000	-2.751099000	-2.323454000
H	-4.308953000	-3.367463000	-4.000196000
C	-2.368900000	-1.484155000	-3.938831000
H	-1.833336000	-0.609267000	-4.336277000
H	-2.171668000	-2.329933000	-4.616585000
H	-1.934782000	-1.727043000	-2.960233000
C	-7.377125000	1.823753000	-1.778531000
C	-8.342792000	0.926003000	-2.552461000

H	-9.376854000	1.271645000	-2.401272000
H	-8.288916000	-0.119946000	-2.212854000
H	-8.140768000	0.946007000	-3.634104000
C	-7.532341000	3.262215000	-2.292819000
H	-8.574745000	3.602009000	-2.183102000
H	-7.259022000	3.328064000	-3.357028000
H	-6.890191000	3.962369000	-1.738426000
C	-7.760446000	1.772351000	-0.292886000
H	-7.114939000	2.421017000	0.317660000
H	-7.680087000	0.746005000	0.098732000
H	-8.800032000	2.107203000	-0.148796000
C	-4.319645000	3.759268000	1.813906000
H	-5.139115000	3.069851000	1.621735000
C	-4.193845000	5.070074000	1.269128000
H	-4.890860000	5.550292000	0.583590000
C	-2.985003000	5.636238000	1.770178000
H	-2.586679000	6.619343000	1.524199000
C	-2.364407000	4.673553000	2.616806000
H	-1.397295000	4.780661000	3.106613000
C	-3.185164000	3.510546000	2.642670000
H	-2.953998000	2.585327000	3.169245000
C	-1.449786000	2.306010000	0.070010000
C	-2.507763000	2.630044000	-0.858302000
C	-2.377133000	3.990203000	-1.290490000
H	-3.043639000	4.498996000	-1.985811000
C	-1.241211000	4.538150000	-0.651055000
H	-0.905862000	5.569465000	-0.740322000
C	-0.669063000	3.525987000	0.193899000
C	3.549305000	-2.297505000	3.242349000
H	2.655835000	-2.463398000	3.841030000
C	3.868466000	-1.110992000	2.519874000
H	3.250538000	-0.216643000	2.465887000
C	5.103563000	-1.327672000	1.841082000
H	5.598268000	-0.627031000	1.169983000

C	5.544421000	-2.648916000	2.142044000
H	6.443010000	-3.125793000	1.753560000
C	4.583152000	-3.248601000	3.008129000
H	4.616036000	-4.264543000	3.398540000
C	2.055080000	-2.402226000	0.040443000
C	3.289636000	-2.330898000	-0.705988000
C	4.003576000	-3.566157000	-0.571078000
H	4.987000000	-3.782165000	-0.987939000
C	3.242580000	-4.417593000	0.273946000
H	3.533988000	-5.408342000	0.621684000
C	2.058766000	-3.708611000	0.660125000
C	0.768628000	-0.852263000	-2.298128000
N	0.794132000	0.326213000	-2.953020000
C	0.945158000	0.152107000	-4.317377000
C	1.023949000	-1.197477000	-4.521814000
N	0.915430000	-1.781369000	-3.270583000
C	0.986610000	-3.206553000	-3.050239000
H	0.116644000	-3.713220000	-3.494343000
H	1.017814000	-3.401329000	-1.973096000
H	1.907413000	-3.610206000	-3.494152000
C	1.154694000	-1.986865000	-5.769943000
H	0.275262000	-2.629913000	-5.937688000
H	2.042772000	-2.638089000	-5.753069000
H	1.250393000	-1.318984000	-6.635610000
C	0.980991000	1.293026000	-5.263405000
H	0.067899000	1.905124000	-5.190746000
H	1.065097000	0.933861000	-6.296965000
H	1.840843000	1.952782000	-5.066153000
C	0.726748000	1.625888000	-2.325497000
H	1.584165000	2.230163000	-2.644066000
H	0.759995000	1.491204000	-1.238377000
H	-0.209795000	2.143188000	-2.578560000
C	-2.600228000	-0.838190000	0.534359000
N	-3.899115000	-0.812073000	0.902041000

C	-4.508831000	-2.034645000	0.692837000
C	-3.537455000	-2.856885000	0.186207000
N	-2.385471000	-2.092820000	0.087215000
C	-1.121611000	-2.586257000	-0.448347000
H	-1.309066000	-2.887658000	-1.493132000
H	-0.872065000	-3.512457000	0.088980000
C	-3.559060000	-4.304477000	-0.132659000
H	-4.578029000	-4.704348000	-0.046559000
H	-2.907751000	-4.859313000	0.563112000
H	-3.195075000	-4.508817000	-1.151098000
C	-5.939890000	-2.278221000	0.995143000
H	-6.593248000	-1.636608000	0.380370000
H	-6.176899000	-2.080267000	2.052844000
H	-6.202480000	-3.322626000	0.783184000
C	-4.522526000	0.322496000	1.531107000
H	-3.855028000	1.183601000	1.419558000
H	-4.689909000	0.130187000	2.602547000
H	-5.477047000	0.555603000	1.043437000
Al	0.441955000	-1.237257000	-0.268694000
H	-1.218115000	0.603670000	2.525491000
Al	-1.075879000	0.504661000	0.910025000
Fe	3.715181000	-2.694163000	1.245940000
Fe	-2.579552000	3.928272000	0.734334000
C	4.302762000	1.200682000	-1.608618000
C	4.768650000	0.992552000	-2.914024000
C	4.770033000	-0.269452000	-3.518452000
C	4.274777000	-1.349215000	-2.779839000
H	4.280731000	-2.356921000	-3.196635000
C	6.811350000	0.036499000	-4.933195000
H	6.901610000	1.095686000	-4.651459000
H	7.250814000	-0.082274000	-5.936711000
H	7.413001000	-0.550413000	-4.222530000
C	5.315902000	-1.887363000	-5.398849000
H	4.288450000	-2.279724000	-5.435970000

H	5.736998000	-1.961430000	-6.413171000
C	4.514554000	2.555299000	-0.924399000
C	6.023033000	2.853262000	-0.918117000
H	6.223215000	3.794630000	-0.381586000
H	6.428891000	2.953209000	-1.936017000
H	6.578069000	2.047662000	-0.413222000

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Al	0.752047000	-1.039525000	0.965271000
Al	-0.832669000	0.860576000	0.516228000
N	1.709478000	0.198866000	3.631813000
C	1.800823000	0.160871000	2.275573000
N	2.654710000	1.165142000	1.967017000
C	3.066749000	1.850125000	3.094258000
C	2.466919000	1.237653000	4.160804000
C	0.946003000	-0.738558000	4.414743000
H	0.543497000	-1.497343000	3.721666000
H	0.097332000	-0.251088000	4.917633000
H	1.579853000	-1.221840000	5.174110000
C	2.888975000	1.615443000	0.617207000
H	2.716057000	0.789431000	-0.078098000
H	3.925062000	1.958079000	0.509395000
H	2.170717000	2.411773000	0.360260000
C	4.000116000	3.001569000	3.028915000
H	4.194298000	3.400624000	4.033053000
H	3.595326000	3.818871000	2.411346000
H	4.965980000	2.699289000	2.591379000
C	2.566991000	1.495890000	5.618383000
H	3.170203000	2.393762000	5.805696000
H	3.045667000	0.658161000	6.152622000
H	1.578271000	1.656334000	6.078903000
N	-2.081659000	0.907081000	3.371236000
C	-2.076889000	0.428624000	2.104254000
N	-2.897696000	-0.641286000	2.138393000

C	-3.389616000	-0.866151000	3.409280000
C	-2.876464000	0.125518000	4.202169000
C	-1.360553000	2.082885000	3.789164000
H	-0.674828000	1.854500000	4.618055000
H	-2.050339000	2.878865000	4.110441000
H	-0.762916000	2.433336000	2.933167000
C	-3.059218000	-1.542177000	1.022259000
H	-2.954255000	-0.985214000	0.085533000
H	-4.059246000	-1.990303000	1.046599000
H	-2.262435000	-2.303256000	1.044100000
C	-4.287577000	-2.003889000	3.725345000
H	-4.547953000	-2.007084000	4.791754000
H	-3.811404000	-2.968833000	3.489898000
H	-5.224637000	-1.941706000	3.148402000
C	-3.066828000	0.421023000	5.643735000
H	-3.717167000	-0.334461000	6.103296000
H	-3.537613000	1.404910000	5.803907000
H	-2.112836000	0.417897000	6.196383000
Fe	2.869633000	-3.719415000	-0.423675000
C	2.025938000	-1.803295000	-0.384978000
C	3.452553000	-1.785329000	-0.636089000
C	3.731115000	-2.536291000	-1.824345000
H	4.722684000	-2.724259000	-2.236069000
C	2.504324000	-3.053748000	-2.315644000
H	2.373221000	-3.703084000	-3.180803000
C	1.462357000	-2.619998000	-1.438136000
C	3.263478000	-4.463745000	1.452525000
H	3.316857000	-3.884457000	2.371659000
C	4.337328000	-4.739222000	0.559032000
H	5.360895000	-4.380318000	0.658954000
C	3.818031000	-5.516131000	-0.517986000
H	4.379607000	-5.865074000	-1.383363000
C	2.424571000	-5.715332000	-0.290429000
H	1.737574000	-6.240061000	-0.952771000

C	2.086126000	-5.066004000	0.931283000
H	1.103115000	-5.013328000	1.395699000
Fe	-2.623776000	3.586248000	-0.981171000
C	-1.994361000	1.594671000	-0.932520000
C	-3.423530000	1.720087000	-1.132713000
C	-3.664911000	2.471816000	-2.325579000
H	-4.647688000	2.739590000	-2.713142000
C	-2.410464000	2.849741000	-2.869843000
H	-2.243513000	3.457293000	-3.758603000
C	-1.386091000	2.323206000	-2.023963000
C	-2.773766000	4.408174000	0.895818000
H	-2.798722000	3.853028000	1.831376000
C	-3.894533000	4.773481000	0.095278000
H	-4.936804000	4.528776000	0.294323000
C	-3.406308000	5.469592000	-1.046822000
H	-4.010134000	5.856199000	-1.866276000
C	-1.986983000	5.536465000	-0.951222000
H	-1.323769000	5.984980000	-1.688974000
C	-1.595798000	4.877747000	0.249934000
H	-0.579467000	4.727057000	0.610770000
C	4.518322000	-1.116747000	0.142035000
C	4.646797000	-1.283066000	1.528477000
H	3.913943000	-1.912934000	2.026278000
C	5.691876000	-0.696695000	2.239776000
C	6.589284000	0.127531000	1.540339000
H	7.408272000	0.594051000	2.088099000
C	6.474637000	0.347998000	0.167195000
C	5.443524000	-0.307089000	-0.517539000
H	5.326733000	-0.161820000	-1.592032000
C	5.942047000	-0.997500000	3.721138000
C	7.202284000	-1.870427000	3.824053000
H	7.413990000	-2.126686000	4.875063000
H	8.083225000	-1.352532000	3.415845000
H	7.073904000	-2.807232000	3.260462000

C	4.773570000	-1.753673000	4.354381000
H	4.640777000	-2.750137000	3.908180000
H	3.831958000	-1.198834000	4.236508000
H	4.959080000	-1.898532000	5.430031000
C	6.156868000	0.297396000	4.514518000
H	5.259660000	0.930811000	4.470062000
H	7.006869000	0.882330000	4.134225000
H	6.363963000	0.066482000	5.571717000
C	7.399855000	1.294359000	-0.601826000
C	8.020051000	0.559296000	-1.798022000
H	8.691774000	1.231330000	-2.355702000
H	8.605331000	-0.310599000	-1.462648000
C	6.566970000	2.481811000	-1.108910000
H	5.734137000	2.148160000	-1.745635000
H	7.190435000	3.174812000	-1.697000000
C	8.532011000	1.835003000	0.271558000
H	8.149509000	2.418436000	1.123095000
H	9.176271000	2.501692000	-0.321874000
C	0.030324000	-2.959234000	-1.666317000
C	-0.674641000	-2.349245000	-2.707061000
H	-0.169848000	-1.582151000	-3.293766000
C	-1.987970000	-2.716828000	-3.023041000
C	-2.591700000	-3.723992000	-2.261571000
H	-3.601914000	-4.041074000	-2.511785000
C	-1.920300000	-4.359296000	-1.209563000
C	-0.617891000	-3.946355000	-0.919742000
H	-0.056417000	-4.417551000	-0.117999000
C	-2.686976000	-2.062073000	-4.218278000
C	-2.525658000	-5.531543000	-0.427645000
C	-2.692999000	-0.539350000	-4.045416000
H	-3.227661000	-0.054823000	-4.877776000
H	-1.677100000	-0.123753000	-4.022834000
H	-3.176649000	-0.240051000	-3.105139000
C	-4.133196000	-2.533421000	-4.373633000

H	-4.734915000	-2.302894000	-3.481897000
H	-4.198337000	-3.616737000	-4.556861000
H	-4.600361000	-2.024013000	-5.230314000
C	-1.920950000	-2.427991000	-5.498655000
H	-1.906925000	-3.518414000	-5.650247000
H	-0.877405000	-2.082743000	-5.455573000
H	-2.394967000	-1.963359000	-6.378553000
C	-2.616643000	-5.186598000	1.065102000
H	-1.650257000	-4.845541000	1.466730000
H	-2.935851000	-6.068007000	1.644472000
H	-3.349958000	-4.385236000	1.236115000
C	-3.925721000	-5.896437000	-0.921953000
H	-4.627643000	-5.056340000	-0.816300000
H	-4.322011000	-6.737797000	-0.332676000
H	-3.917588000	-6.205054000	-1.978407000
C	-1.619773000	-6.760300000	-0.603807000
H	-1.501612000	-7.009393000	-1.669520000
H	-2.051707000	-7.634880000	-0.090861000
H	-0.617248000	-6.589546000	-0.185505000
C	-4.535940000	1.150468000	-0.330321000
C	-4.863761000	1.639787000	0.940648000
H	-4.235952000	2.423057000	1.350981000
C	-5.975320000	1.176606000	1.641279000
C	-6.735663000	0.148158000	1.063152000
H	-7.610898000	-0.220807000	1.598362000
C	-6.423908000	-0.394087000	-0.184954000
C	-5.325833000	0.137849000	-0.875923000
H	-5.061193000	-0.245949000	-1.863355000
C	-6.441556000	1.828384000	2.947129000
C	-7.218681000	-1.549330000	-0.799763000
C	-5.406341000	2.812711000	3.494195000
H	-4.437540000	2.316960000	3.653340000
H	-5.747954000	3.218685000	4.458840000
H	-5.247227000	3.664534000	2.816872000

C	-6.709176000	0.771873000	4.025378000
H	-7.455461000	0.030428000	3.704854000
H	-7.091979000	1.249782000	4.941183000
H	-5.783885000	0.236519000	4.279712000
C	-7.740104000	2.597262000	2.657576000
H	-7.576342000	3.361453000	1.882398000
H	-8.105202000	3.101409000	3.567185000
H	-8.533672000	1.924054000	2.300087000
C	-8.491363000	-1.861876000	-0.011625000
H	-9.040006000	-2.681372000	-0.500434000
H	-9.162966000	-0.991020000	0.038279000
H	-8.269939000	-2.184410000	1.017180000
C	-7.621315000	-1.202237000	-2.239578000
H	-6.748026000	-1.030650000	-2.884592000
H	-8.241167000	-0.292888000	-2.264607000
H	-8.201970000	-2.026474000	-2.683140000
C	-6.329193000	-2.801329000	-0.802434000
H	-6.082416000	-3.108046000	0.226335000
H	-5.381457000	-2.624905000	-1.331511000
H	-6.841426000	-3.645389000	-1.292088000
C	0.060739000	2.490300000	-2.342081000
C	0.773410000	3.622816000	-1.953112000
H	0.267008000	4.348061000	-1.322818000
C	2.089974000	3.854465000	-2.373973000
C	2.681769000	2.904379000	-3.204092000
H	3.696300000	3.070946000	-3.566568000
C	2.002601000	1.748876000	-3.622755000
C	0.699327000	1.551104000	-3.166779000
H	0.136308000	0.669284000	-3.467146000
C	2.798963000	5.148075000	-1.957908000
C	2.686609000	0.809850000	-4.620685000
C	2.959156000	5.186472000	-0.431912000
H	3.615978000	4.373575000	-0.089670000
H	1.991459000	5.077258000	0.081098000

H	3.404515000	6.143145000	-0.114419000
C	1.956099000	6.350425000	-2.407881000
H	2.463519000	7.294228000	-2.151322000
H	0.970005000	6.361141000	-1.921551000
H	1.795077000	6.330527000	-3.496532000
C	4.186215000	5.275488000	-2.588345000
H	4.850420000	4.453246000	-2.284546000
H	4.656464000	6.217728000	-2.267438000
H	4.133773000	5.286773000	-3.687653000
C	4.034450000	0.341663000	-4.059788000
H	3.880175000	-0.222310000	-3.129162000
H	4.711805000	1.183263000	-3.851281000
H	4.540418000	-0.322098000	-4.779073000
C	1.847104000	-0.431576000	-4.915032000
H	1.694922000	-1.030697000	-4.006301000
H	2.367481000	-1.069011000	-5.646255000
H	0.865329000	-0.174155000	-5.340712000
C	2.908701000	1.573798000	-5.934756000
H	3.397241000	0.924607000	-6.679324000
H	3.546129000	2.458700000	-5.788347000
H	1.950362000	1.917026000	-6.354089000
H	7.253869000	0.198221000	-2.499432000
H	6.136218000	3.046999000	-0.267050000
H	9.163112000	1.024420000	0.667096000

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Al	-0.716003000	1.260128000	1.035099000
N	1.967971000	1.887366000	2.447667000
C	1.347824000	1.730365000	1.251855000
N	2.183374000	2.315172000	0.363833000
C	3.322284000	2.808490000	0.977315000
C	3.185980000	2.538776000	2.311887000
C	1.391210000	1.451936000	3.696054000
H	1.614841000	2.174987000	4.491746000

H	1.766489000	0.462292000	3.997926000
H	0.295702000	1.397678000	3.561212000
C	1.888850000	2.456117000	-1.041489000
H	1.022640000	1.824787000	-1.276665000
H	2.737561000	2.115957000	-1.647519000
H	1.656067000	3.504469000	-1.285841000
C	4.429609000	3.436471000	0.216466000
H	5.219846000	3.778171000	0.897245000
H	4.088353000	4.306845000	-0.366015000
H	4.879739000	2.716600000	-0.487675000
C	4.074952000	2.838442000	3.461627000
H	5.003661000	3.307519000	3.112029000
H	4.349921000	1.926167000	4.015012000
H	3.602426000	3.531862000	4.176402000
Fe	-0.796124000	-2.007839000	0.238984000
C	-0.551360000	-0.089567000	-0.495890000
C	0.497228000	-0.987457000	-0.953172000
C	-0.091702000	-2.074885000	-1.672185000
H	0.456403000	-2.909439000	-2.109116000
C	-1.498025000	-1.898053000	-1.672540000
H	-2.235179000	-2.561919000	-2.122676000
C	-1.783780000	-0.685375000	-0.976012000
C	-0.377108000	-2.022332000	2.244226000
H	0.119339000	-1.232550000	2.807417000
C	0.257258000	-3.120650000	1.591989000
H	1.327787000	-3.313298000	1.543819000
C	-0.756499000	-3.909737000	0.977601000
H	-0.594683000	-4.807695000	0.383332000
C	-2.015434000	-3.299562000	1.250443000
H	-2.983678000	-3.655516000	0.902233000
C	-1.784156000	-2.129621000	2.026988000
H	-2.537592000	-1.416055000	2.358746000
C	1.970425000	-0.839661000	-0.880453000
C	2.707093000	-0.934608000	0.308281000

H	2.157369000	-1.099688000	1.232050000
C	4.099876000	-0.854065000	0.304608000
C	4.748696000	-0.629035000	-0.920312000
H	5.836790000	-0.567938000	-0.929600000
C	4.051994000	-0.514772000	-2.123033000
C	2.657263000	-0.640167000	-2.079289000
H	2.069095000	-0.572527000	-2.997977000
C	4.946389000	-1.088004000	1.559110000
C	4.749465000	-0.268070000	-3.463476000
C	4.089531000	-1.152734000	2.822486000
H	3.515844000	-0.225642000	2.955962000
H	4.731019000	-1.289958000	3.706440000
H	3.379080000	-1.992413000	2.797757000
C	5.971286000	0.041253000	1.729084000
H	6.678871000	0.086882000	0.888601000
H	6.561501000	-0.110435000	2.646839000
H	5.465922000	1.015265000	1.797818000
C	5.685005000	-2.426107000	1.403045000
H	4.970477000	-3.254719000	1.282952000
H	6.306226000	-2.632675000	2.289681000
H	6.342729000	-2.421818000	0.521015000
C	6.269857000	-0.194822000	-3.319578000
H	6.729541000	-0.016144000	-4.303565000
H	6.688022000	-1.132380000	-2.922813000
H	6.579352000	0.626944000	-2.655390000
C	4.409595000	-1.411168000	-4.430420000
H	3.327383000	-1.485207000	-4.611182000
H	4.748538000	-2.377487000	-4.026772000
H	4.902293000	-1.253072000	-5.403141000
C	4.256478000	1.062757000	-4.050206000
H	4.511995000	1.903205000	-3.385109000
H	3.166017000	1.065321000	-4.195583000
H	4.725904000	1.253224000	-5.028609000
C	-3.137735000	-0.131419000	-0.789612000

C	-4.223335000	-0.948931000	-0.479452000
H	-4.046652000	-2.019604000	-0.363888000
C	-5.504100000	-0.421567000	-0.277595000
C	-5.667155000	0.960169000	-0.394971000
H	-6.651411000	1.395804000	-0.221953000
C	-4.603663000	1.815169000	-0.719045000
C	-3.348207000	1.247517000	-0.926477000
H	-2.498412000	1.868226000	-1.207603000
C	-6.652991000	-1.362932000	0.093385000
C	-4.835364000	3.326365000	-0.778487000
C	-6.325075000	-2.051172000	1.426800000
H	-6.196937000	-1.307943000	2.228641000
H	-5.395459000	-2.636202000	1.364844000
H	-7.136117000	-2.737790000	1.718988000
C	-6.816927000	-2.423041000	-1.004910000
H	-7.635560000	-3.116715000	-0.753729000
H	-5.901438000	-3.018731000	-1.135718000
H	-7.050132000	-1.951867000	-1.972122000
C	-7.981457000	-0.622069000	0.248377000
H	-7.939108000	0.128429000	1.052284000
H	-8.779395000	-1.336355000	0.503399000
H	-8.274518000	-0.112386000	-0.682228000
C	-5.206322000	3.811511000	0.631264000
H	-4.400999000	3.573743000	1.343307000
H	-6.128933000	3.333166000	0.993104000
H	-5.366275000	4.902157000	0.635992000
C	-3.582408000	4.079405000	-1.228270000
H	-2.745707000	3.922540000	-0.529812000
H	-3.790802000	5.159992000	-1.263441000
H	-3.259508000	3.767608000	-2.233788000
C	-5.972846000	3.646616000	-1.757047000
H	-6.148881000	4.733599000	-1.798963000
H	-6.918095000	3.168767000	-1.459938000
H	-5.726420000	3.299707000	-2.772550000

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Al	-0.124837000	1.683466000	0.177650000
C	1.002142000	1.579322000	-1.552644000
N	1.987033000	1.329161000	-2.432959000
C	3.340050000	0.979155000	-2.072278000
H	3.395394000	0.874485000	-0.982986000
H	4.048316000	1.756198000	-2.396582000
H	3.626771000	0.023563000	-2.534157000
C	1.505594000	1.416331000	-3.736484000
C	2.368156000	1.175613000	-4.919872000
H	1.792034000	1.314672000	-5.843645000
H	2.770639000	0.149501000	-4.929901000
H	3.224883000	1.867901000	-4.952211000
C	0.170946000	1.730230000	-3.644695000
C	-0.872355000	1.931198000	-4.678706000
H	-1.692237000	1.205030000	-4.560277000
H	-0.455185000	1.811148000	-5.686875000
H	-1.315102000	2.937172000	-4.608512000
N	-0.094145000	1.821708000	-2.292473000
C	-1.306484000	1.986586000	-1.481975000
H	-2.039700000	1.200281000	-1.723955000
H	-1.765106000	2.971892000	-1.661357000
C	2.333527000	-0.489679000	1.366425000
C	2.731620000	0.822447000	1.640058000
H	1.972750000	1.540422000	1.961396000
C	4.068092000	1.222281000	1.529429000
C	5.011712000	0.264202000	1.140753000
H	6.054843000	0.558455000	1.049707000
C	4.651985000	-1.062178000	0.863464000
C	3.307632000	-1.418524000	0.984511000
H	2.984874000	-2.436158000	0.755633000
C	-2.768611000	-0.403059000	1.175252000
C	-3.766702000	-1.315182000	0.831022000

H	-3.497112000	-2.370315000	0.747647000
C	-5.075223000	-0.901875000	0.556633000
C	-5.359273000	0.463293000	0.633246000
H	-6.367491000	0.810480000	0.407173000
C	-4.389642000	1.410628000	0.995899000
C	-3.103784000	0.954262000	1.278350000
H	-2.334894000	1.655402000	1.608741000
C	4.442560000	2.676604000	1.826953000
C	4.025352000	3.021152000	3.264032000
H	4.293015000	4.063268000	3.500891000
H	4.530208000	2.363228000	3.988070000
H	2.940744000	2.914107000	3.409451000
C	3.701103000	3.597892000	0.846523000
H	2.609449000	3.480893000	0.916385000
H	3.997081000	3.384666000	-0.192566000
H	3.941189000	4.652621000	1.056157000
C	5.944391000	2.926501000	1.687044000
H	6.167940000	3.980128000	1.913464000
H	6.299995000	2.725996000	0.664469000
H	6.529939000	2.305479000	2.382268000
C	5.669776000	-2.115326000	0.415814000
H	7.432379000	-1.190423000	1.329122000
C	-6.127388000	-1.945248000	0.170930000
C	-6.294256000	-2.940930000	1.327804000
H	-6.628622000	-2.426311000	2.241589000
H	-5.349684000	-3.454408000	1.560577000
H	-7.041715000	-3.709328000	1.072343000
C	-7.488595000	-1.313606000	-0.122153000
H	-8.212806000	-2.097353000	-0.392340000
H	-7.437472000	-0.604200000	-0.962289000
H	-7.888007000	-0.780227000	0.753801000
C	-5.662603000	-2.694264000	-1.086639000
H	-6.411632000	-3.443560000	-1.389267000
H	-4.712697000	-3.223401000	-0.919366000

H	-5.516461000	-1.997335000	-1.926471000
C	-5.169397000	3.349660000	-0.360221000
H	-6.031355000	2.780706000	-0.739838000
H	-5.444229000	4.416845000	-0.357038000
H	-6.830602000	2.529536000	1.701575000
H	-5.673445000	2.765929000	3.030375000
C	0.915971000	-0.873676000	1.488841000
C	-0.980310000	-2.090577000	1.976985000
H	-1.647211000	-2.882455000	2.315440000
C	-1.341315000	-2.422519000	-1.497160000
H	-2.406996000	-2.219848000	-1.593754000
C	-0.290441000	-1.553864000	-1.906167000
H	-0.413075000	-0.589647000	-2.390552000
C	0.949276000	-2.159462000	-1.551454000
H	1.938338000	-1.725969000	-1.690309000
C	0.664753000	-3.410970000	-0.930882000
H	1.396460000	-4.111827000	-0.530857000
C	-0.752443000	-3.572629000	-0.895739000
H	-1.288346000	-4.415354000	-0.461372000
C	5.284760000	-2.624902000	-0.981042000
H	4.278265000	-3.068978000	-0.991021000
H	5.995103000	-3.394704000	-1.322809000
H	5.297207000	-1.802712000	-1.713882000
C	7.091390000	-1.556596000	0.348906000
H	7.172968000	-0.729540000	-0.372993000
H	7.787708000	-2.346435000	0.028173000
C	5.656280000	-3.286323000	1.408745000
H	5.922280000	-2.944038000	2.420463000
H	6.381059000	-4.058692000	1.105138000
H	4.665268000	-3.759980000	1.466066000
C	-4.763737000	2.893884000	1.049485000
C	-3.598680000	3.764762000	1.521372000
H	-3.910285000	4.820257000	1.546312000
H	-2.728333000	3.690731000	0.852232000

H	-3.269139000	3.491243000	2.535168000
H	-4.337556000	3.211030000	-1.067988000
C	-5.940450000	3.095133000	2.014490000
H	-6.220557000	4.159685000	2.061679000
C	-1.381657000	-0.835727000	1.414455000
C	-0.208554000	-0.061684000	1.105783000
C	0.438469000	-2.114569000	2.023403000
H	1.057489000	-2.926196000	2.403804000
Fe	-0.200047000	-1.892641000	0.114221000
H	0.134530000	2.977390000	1.097716000

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