SUPPORTING INFORMATION

Snapshots of Sequential Polyphosphide Rearrangement upon Metallatetrylene Addition

Xiaofei Sun,[a] Alexander Hinz,[a] Stephan Schulz,[b] Lisa Zimmermann,[c] Manfred Scheer[c] and Peter W. Roesky*[a]

[a] Dr. X. Sun, Dr. A. Hinz, Prof. Dr. P. W. Roesky, Institute of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), Engesserstraße 15, 76131, Karlsruhe, Germany.

[b] Prof. Dr. S. Schulz, Institute for Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (Cenide), University of Duisburg-Essen, Universitätsstraße 5–7, 45117, Essen, Germany.

[c] Lisa Zimmermann, Prof. Dr. M. Scheer, Institute of Inorganic Chemistry, University of Regensburg, Universitätsstr.31, 93040 Regensburg, Germany.

Table of Contents

I. Synthesis and characterization

I.1 General procedures

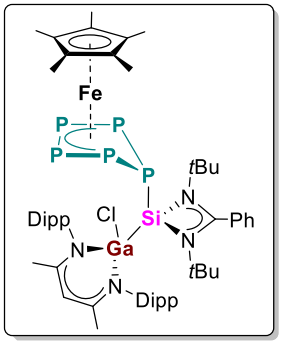
All air- and moisture-sensitive manipulations were performed under dry N_2 or Ar atmosphere using standard Schlenk techniques or in an argon-filled MBraun glovebox, unless otherwise stated. Et_2O, *n*-pentane, and toluene were dried using an MBraun solvent purification system (SPS-800) and degassed. THF, benzene and *n*-hexane were distilled under nitrogen from potassium benzophenone ketyl. C_6D_6, toluene-d_8 and THF-d_8 were dried over Na-K alloy and degassed by freeze-pump-thaw cycles. $[L^{BDI}Ga(Cl)\text{-}SiL^{Ph}]$[S1] ($L^{BDI}$ = {N(Dipp)C(Me)}$_2$CH, Dipp = 2,6-*i*Pr-C_6H_3, L^{Ph} = PhC(N*t*Bu)$_2$), $[L^{BDI}Ga]$,[S2] $[L^{Ph}GeCl]$,[S3] $[Cp^*Fe(\eta^5\text{-}P_5)]$,[S4] and $[Cp^*Fe(\eta^5\text{-}As_5)]$[S5] were prepared according to the literature procedures. All other chemicals were obtained from commercial sources and used without further purification.

Elemental analyses were carried out with an Elementar vario MICRO cube.

NMR spectra were recorded on Bruker spectrometers (Avance Neo 300 MHz, Avance Neo 400 MHz or Avance III 400 MHz). Chemical shifts are referenced internally using signals of the residual protio solvent (^1H) or the solvent ($^{13}C\{^1H\}$) and are reported relative to tetramethylsilane (^1H, $^{13}C\{^1H\}$), or externally relative to tetramethylsilane (^{29}Si), H_3PO_4 (^{31}P). All NMR spectra were measured at 298 K, unless otherwise specified. The multiplicity of the signals is indicated as s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet and br = broad. Assignments were determined based on unambiguous chemical shifts, coupling patterns and ^{13}C-DEPT experiments or 2D correlations (^1H-^1H COSY, ^1H-^{13}C HMQC and ^1H-^{13}C HMBC).

Infrared (IR) spectra were recorded in the region 4000–400 cm^{-1} on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLaTGS detector, a diamond attenuated total reflection (ATR) unit and a nitrogen-flushed chamber. In terms of their intensity, the signals were classified into different categories (vs = very strong, s = strong, m = medium, w = weak, and sh = shoulder).

I.2 Synthesis of 1

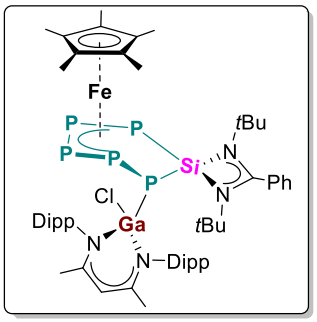


To a J. Young NMR tube containing a mixture of [Cp*Fe(η^5-P_5)] (10.0 mg, 0.029 mmol) and [L^{NacNac}Ga(Cl)-SiL^{Ph}] (22.6 mg, 0.029 mmol) was condensed toluene-d_8 (*ca.* 0.4 mL) at –196 °C, and the resulting mixture was carefully warmed up to -80 °C. The NMR tube was then shacked until everything dissolved and low-temperature variable temperature $^{31}P\{^1H\}$ NMR measurements were performed (from –80 °C to 25 °C). The low temperature $^{31}P\{^1H\}$ NMR spectra indicates the clean formation of the title compound **1**. However, at already –10 °C, traces of compound **2** are formed and at room temperature after 2 h, all signals belonging to **1** disappeared and only **2** and small amounts of [Cp*Fe(η^5-P_5)] are visible (see Figure S1).

Crystals suitable for X-ray diffraction analysis were obtained from benzene.

$^{31}P\{^1H\}$ NMR (162 MHz, toluene-d_8): AA'MM'X spin system δ (ppm) = 37.4 (1P, P_X), 31.3 (2P, P_M, $P_{M'}$), –50.6 (2P, P_A, $P_{A'}$), for details, see Figure S21 and Table S1.

I.3 Synthesis of 2



To a mixture of [Cp*Fe(η^5-P_5)] (50.0 mg, 0.145 mmol) and [L^{NacNac}Ga(Cl)-SiL^{Ph}] (113.1 mg, 0.145 mmol) was condensed toluene (*ca.* 5 mL) at –78 °C, and the resulting mixture was warmed up to room temperature and turned dark brown. After stirring for 1 h at room temperature, all solvents were removed under reduced pressure and *n*-hexane was added to the residue. Single-crystals of **2**, suitable for X-ray diffraction analysis could be obtained from *n*-hexane at room temperature.

Yield (based on crystals): 41% (69.5 mg, 0.059 mmol).

Anal. Calcd. For $C_{54}H_{79}ClFeGaN_4P_5Si$ (0.5 C_6H_{14}) (1171.31 g/mol): C 58.45; H 7.40; N 4.78. Found: C 58.76; H 7.06; N 4.77.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.38-7.36 (m, 1H, CH_{Ar}), 7.32-7.23 (m, 3H, CH_{Ar}), 7.20-7.18 (m, 1H, CH_{Ar}), 6.98-6.91 (m, 5H, CH_{Ar}), 6.87-6.83 (m, 1H, CH_{Ar}), 4.98 (s, 1H, C*H*), 3.96, 3.74, 3.58, 3.40 (four sets of sept, ^3J = 6.9 Hz, 4H, C*H* $_{Dipp}$), 2.09 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.70 (s, 15H, $C_5(CH_3)_5$), 1.64 (s, 3H, L^{NacNac}-NCCH_3), 1.49-1.43 (overlapped signals of 9H, 3H of L^{NacNac}-NCCH_3+ 6H CH_3 $_{Dipp}$), 1.39-1.33 (overlapped signals of 15H, 9H of $C(CH_3)_3$ + 6H of CH_3 $_{Dipp}$), 1.28-1.19 (m, overlapped signals of ca. 4H CH_3 $_{n\text{-hex}}$ + 6H CH_3 $_{Dipp}$), 1.06 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 0.89 (t, ^3J = 5.6 Hz, *ca.* 3H, CH_3 $_{n\text{-hex}}$), 0.74 (s, 9H, $C(CH_3)_3$).

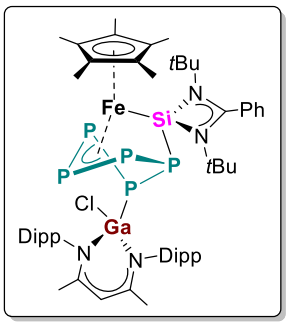
^{31}P{^{1}H} NMR (162 MHz, C_6D_6): AMXYZ spin system δ (ppm) = 85.9 (1P, P_A), 44.8 (1P, P_M), 28.8 (1P, P_X), –3.6 (1P, P_Y), –219.2 (P_Z), for details, see Figure S22 and Table S2.

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 172.4 (N*C*N), 170.3 (L^{NacNac}-N*C*CH$_3$), 169.2 (L^{NacNac}-NC*C*H$_3$), 145.3 (Dipp-*o*-*C*), 145.1 (Dipp-*o*-*C*), 144.6 (Dipp-*m*-*C*), 144.2 (Dipp-*m*-*C*), 142.9 (Dipp-*m*-*C*), 141.3 (Dipp-*m*-*C*), 130.6 (Ph-C_q), 130.7, 129.3, 128.3, 128.04, 128.01, 127.8, 127.5, 125.0, 124.72, 124.67, 124.5, 98.8 (L^{NacNac}-*γ*-*C*H), 89.3 ($C_5(CH_3)_5$), 55.9 ($C(CH_3)_3$), 55.4 ($C(CH_3)_3$), 31.8 (*n*-hex-*C*H$_2$), 31.8 ($C(CH_3)_3$), 31.2 ($C(CH_3)_3$), 23.1 (*n*-hex-*C*H$_2$), 14.4 (*n*-hex-*C*H$_3$), 11.1 ($C_5(CH_3)_5$).

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): δ (ppm) = 57.1 (t, $^1J_{SiP}$ = 159 Hz).

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 2961 (w), 1614 (w), 1524 (m), 1385 (s), 1313 (s), 1236 (vs), 1180 (s), 1128 (s), 1022 (s), 983 (s), 936 (m), 867 (m), 796 (m), 759 (s), 707 (m), 644 (m), 553 (w), 532 (w), 491 (w), 411 (w).

I.4 Synthesis of 3



A J. Young NMR tube containing a C_6D_6 solution (*ca.* 0.4 mL) of compound **2** (30.0 mg, 0.026 mmol) was heated for 24 h at 80 °C and a $^{31}P\{^1H\}$ NMR spectrum was recorded, showing the thermolysis was complete. All solvents were removed under reduced pressure and *n*-hexane was condensed to the NMR tube. Keeping the *n*-hexane solution undisturbed at room temperature afford complex **3** as green crystalline materials.

Single crystals of **3** which were suitable for X-ray diffraction analysis could be obtained from a concentrated C_6D_6 solution.

Yield (based on crystals): 72% (21.5 mg, 0.018 mmol).

Anal. Calcd. For $C_{54}H_{79}ClFeGaN_4P_5Si$ (0.5 C_6H_{14}) (1171.31 g/mol): C 58.45; H 7.40; N 4.78. Found: C 59.09; H 7.21; N 4.76.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.45 (dd, ^3J = 5.8 Hz, ^4J = 3.5 Hz, 1H, CH_{Ar}), 7.34-7.44 (m, 1H, CH_{Ar}), 7.23-7.18 (m, 3H, CH_{Ar}), 7.15-7.11 (m, 1H, CH_{Ar}), 7.02-6.87 (m, 5H, CH_{Ar}), 4.95 (s, 1H, CH), 3.95, 3.75, 3.56, (three sets of sept in 1:2:1 ratio, ^3J = 6.6 Hz, 4H, CH $_{Dipp}$), 2.10 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.82 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.75-1.72 (overlapped signals of 18H, 15H of $C_5(CH_3)_5$ and 3H of CH_3 $_{Dipp}$), 1.70 (s, 3H, L^{NacNac}-NCCH_3), 1.62 (s, 3H, L^{NacNac}-NCCH_3), 1.58 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.31 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.24-1.21 (overlapped signals of ca 16H, 9H of C(CH_3)$_3$ + 3H of CH_3 $_{Dipp}$ + ca. 4H of CH_2 $_{n\text{-}hex}$), 1.18 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 1.15 (d, ^3J = 6.9 Hz, 3H, CH_3 $_{Dipp}$), 0.97 (s, 9H, C(CH_3)$_3$), 0.89 (t, ^3J = 7.0 Hz, ca. 3H, CH_3 $_{n\text{-}hex}$)

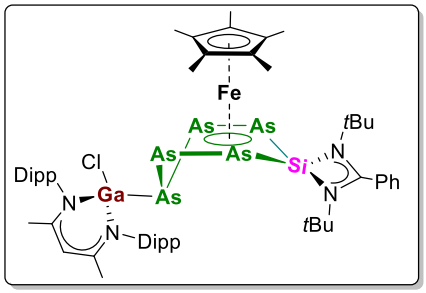
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 172.0 (N*C*N), 169.2 (L^{NacNac}-N*C*CH$_3$), 168.8 (L^{NacNac}-N*C*CH$_3$), 146.41 (Dipp-*o*-*C*), 146.44 (Dipp-*o*-*C*), 143.3 (Dipp-*m*-*C*), 143.1 (Dipp-*m*-*C*), 142.4 (Dipp-*m*-*C*), 141.8 (Dipp-*m*-*C*), 132.4 (Ph-C_q), 130.3, 129.8, 129.4, 128.6, 127.6, 127.5, 127.1, 125.9, 125.4, 123.9, 123.5, 97.6 (L^{NacNac}-*γ*-*C*H), 88.3 ($C_5(CH_3)_5$), 54.9 (*C*(CH_3)$_3$), 33.3 (C(*C*H$_3$)$_3$), 32.3 (C(*C*H$_3$)$_3$), 31.9 (*n*-hex-*C*H$_2$), 30.3, 29.6, 28.4, 28.1, 27.9, 27.4, 25.3, 25.2, 25.1, 24.9, 24.7, 24.5 (L^{NacNac}-iPr-*C*H, iPr-*C*H$_3$), 23.9, 23.8 (L^{NacNac}-NC*C*H$_3$), 23.1 (*n*-hex-*C*H$_2$), 14.4 (*n*-hex-*C*H$_3$), 11.7 ($C_5(CH_3)_5$).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6): AMNXZ spin system δ (ppm) = 224.0 (1P, P_A), 88.5 (1P, P_M), 12.1 (1P, P_N), –57.6 (1P, P_X), –67.7 (P_Z), for details, see Figure S23 and Table S3.

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): δ (ppm) = 63.4 (m).

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 2969 (w), 2894 (w), 2866 (w), 1549 (sh), 1523 (m), 1440 (m), 1389 (vs), 1317 (s), 1254 (m), 1194 (m), 1177 (m), 1102 (w), 1077 (w), 1058 (w), 1021 (s), 939 (w), 863 (w), 793 (s), 755 (s), 726 (s), 708 (s), 619 (vs), 498 (s), 464 (s), 435 (s).

I.5 Synthesis of 4



To a J. Young NMR tube containing a mixture of [Cp*Fe(η^5-As_5)] (15.0 mg, 0.027 mmol) and [L^{NacNac}Ga(Cl)-SiL^{Ph}] (20.8 mg, 0.027 mmol) was condensed C_6D_6 (*ca.* 0.4 mL) at –78 °C, and the resulting mixture was warmed up to room temperature and turned red-brown. The NMR tube was sonicated for 10 min at room temperature and a ^{1}H NMR spectrum was recorded, showing the reaction was complete. All solvents were removed under reduced pressure and *n*-hexane was condensed to the NMR tube. Keeping the *n*-hexane solution undisturbed at room temperature for *ca.* 30 min led to the formation of single-crystals, which were suitable for X-ray diffraction analysis.

Yield (based on crystals): 49% (18.3 mg, 0.013 mmol).

Anal. Calcd. For $C_{54}H_{79}ClFeGaN_4As_5Si$ (0.5 C_6H_{14}) (1389.10 g/mol): C 49.22; H 6.23; N 4.03. Found: C 48.82; H 5.94; N 3.73.

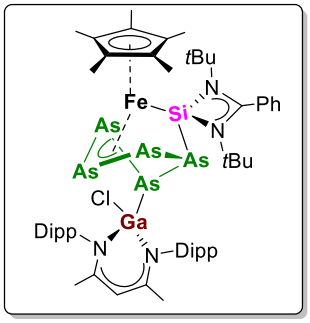
^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.30 (dd, ^3J = 7.5 Hz, ^4J = 1.8 Hz, 2H, CH_{Ar}), 7.19 (t, ^3J = 7.6 Hz, 3H, CH_{Ar}), 6.89-6.84 (m, 2H, CH_{Ar}), 6.74 (t, ^3J = 7.6 Hz, 2H, CH_{Ar}), 6.54 (d, ^3J = 7.1 Hz, 2H, CH_{Ar}), 5.00 (s, 1H, *γ*-C*H*), 4.04, 3.41, (two sets of sept in 1:1 ratio, ^3J = 6.8 Hz, 4H, CH_{Dipp}), 1.96 (d, ^3J = 6.8 Hz, 6H, C$H_{3\ Dipp}$), 1.79 (s, 15H, $C_5(CH_3)_5$), 1.70 (s, 6H, L^{NacNac}-NCCH_3), 1.50 (d, ^3J = 6.8 Hz, 6H, C$H_{3\ Dipp}$), 1.30 (d, ^3J = 6.8 Hz, 6H, C$H_{3\ Dipp}$), 1.27 (s, 9H, C(CH_3)$_3$). 1.25-1.20 (m, *ca*. 4H, CH_2 *n*-hex), 1.11 (d, ^3J = 6.8 Hz, 6H, C$H_{3\ Dipp}$), 0.90-0.87 (m, *ca*. 6H, CH_3 *n*-hex), 0.82 (s, 9H, C(CH_3)$_3$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): *δ* (ppm) = 168.5 (N*C*N), 146.2 (Dipp-*o*-*C*), 143.9 (Dipp-*o*-*C*), 143.1 (Dipp-*m*-*C*), 141.8 (Dipp-*m*-*C*), 131.6, 130.1, 128.3, 127.8, 127.4, 125.5, 123.76, 123.73, 97.6 (L^{NacNac}-*γ*-*C*H), 84.8 ($C_5(CH_3)_5$), 56.8 (*C*(CH_3)$_3$), 55.3 (*C*(CH_3)$_3$), 33.1 (C(*C*H_3)$_3$), 31.7 (C(*C*H_3)$_3$), 31.9 (*n*-hex-*C*H_2), 31.5, 29.7, 28.4, 27.6, 25.0, 24.82, 23.9 (L^{NacNac}-iPr-*C*H, iPr-*C*H_3), 25.0 (L^{NacNac}-NC*C*H_3), 23.1 (*n*-hex-*C*H_2), 14.4 (*n*-hex-*C*H_3), 11.7 ($C_5(CH_3)_5$). Two ^{13}C signals could not be detected.

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): *δ* (ppm) = –4.7 (s).

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 2996 (s), 2890 (s), 2831 (s), 1552 (m), 1524 (s), 1441 (sh), 1400 (vs), 1317 (s), 1256 (m), 1176 (s), 1107 (w), 1080 (w), 1020 (s), 940 (w), 859 (w), 792 (s), 756 (vs), 726 (m), 708 (m), 613 (s), 482 (w), 437 (m).

I.6 Synthesis of 5



A J. Young NMR tube containing a C_6D_6 solution (*ca.* 0.4 mL) of compound **4** (25.0 mg, 0.018 mmol) was heated for 6 h at 80 °C and a ^{1}H NMR spectrum was recorded, showing the thermolysis was complete. All solvents were removed under reduced pressure and *n*-hexane was condensed to the NMR tube. Keeping the *n*-hexane solution undisturbed at room temperature for *ca.* 15 min led to the formation of green prisms, which were suitable for X-ray diffraction analysis.

Yield (based on crystals): 47% (11.7 mg, 0.008 mmol).

Anal. Calcd. For $C_{54}H_{79}ClFeGaN_4As_5Si$ (0.5 C_6H_{14}) (1389.10 g/mol): C 49.22; H 6.23; N 4.03. Found: C 49.97; H 5.46; N 3.97.

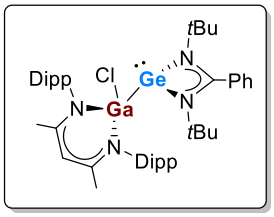
^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.43 (dd, ^3J = 7.4 Hz, ^4J = 1.9 Hz, 1H, C*H*$_{Ar}$), 7.32-7.18 (m, 5H, C*H*$_{Ar}$), 7.15-7.14 (m, 1H, C*H*$_{Ar}$), 6.97-6.79 (m, 4H, C*H*$_{Ar}$), 4.96 (s, 1H, *γ*-C*H*), 3.99, 3.79, 3.63, (three sets of sept in 1:2:1 ratio, ^3J = 6.6 Hz, 4H, C*H* $_{Dipp}$), 2.18 (d, ^3J = 6.9 Hz, 3H, C*H*$_{3\ Dipp}$), 1.78-1.76 (overlapped signals of 21H, 15H of $C_5(CH_3)_5$ and 6H of C*H*$_{3\ Dipp}$), 1.71 (s, 3H, L^{NacNac}-NCC*H*$_3$), 1.62 (s, 3H, L^{NacNac}-NCC*H*$_3$), 1.58 (d, ^3J = 6.9 Hz, 3H, C*H*$_{3\ Dipp}$), 1.32 (d, ^3J = 6.9 Hz, 3H, C*H*$_{3\ Dipp}$), 1.21-1.14 (overlapped signals of ca 19H, 9H of C(C*H*$_3$)$_3$ + 9H of C*H*$_{3\ Dipp}$ + C*H*$_{2\ n\text{-}hex}$), 1.03 (s, 9H, C(C*H*$_3$)$_3$), 0.89 (C*H*$_{3\ n\text{-}hex}$)

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 170.3 (N*C*N), 168.8 (L^{NacNac}-N*C*CH$_3$), 168.5 (L^{NacNac}-N*C*CH$_3$), 146.51 (Dipp-*o*-*C*), 146.49 (Dipp-*o*-*C*), 143.3 (Dipp-*m*-*C*), 143.0 (Dipp-*m*-*C*), 142.2 (Dipp-*m*-*C*), 141.9 (Dipp-*m*-*C*), 132.6 (Ph-C_q), 130.1, 130.0, 129.6, 127.6, 127.5, 127.4, 127.2, 126.0, 125.6, 123.8, 123.7, 97.5 (L^{NacNac}-*γ*-*C*H), 87.0 ($C_5(CH_3)_5$), 54.7 (*C*(CH$_3$)$_3$), 54.6 (*C*(CH$_3$)$_3$), 33.4 (C(*C*H$_3$)$_3$), 32.5 (C(*C*H$_3$)$_3$), 31.9 (*n*-hex-*C*H$_2$), 30.3, 29.8, 28.39, 28.35, 28.0, 27.6, 25.3, 25.13, 25.10, 24.82, 24.6, 24.5 (L^{NacNac}-iPr-*C*H, iPr-*C*H$_3$), 23.8 (L^{NacNac}-NC*C*H$_3$), 23.1 (*n*-hex-*C*H$_2$), 14.4 (*n*-hex-*C*H$_3$), 12.2 ($C_5(CH_3)_5$).

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): δ (ppm) = 37.1.

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 2964 (w), 2901 (w), 2865 (w), 1551 (m), 1524 (m), 1461 (sh), 1438 (s), 1393 (vs), 1318 (s), 1250 (m), 1195 (m), 1178 (m), 1099 (w), 1074 (w), 1022 (s), 933 (w), 864 (m), 793 (s), 753 (s), 724 (sh), 708 (m), 613 (s), 484 (m), 436 (s), 383 (m).

I.7 Synthesis of 6



To a mixture of [L^{BDI}Ga] (72.0 mg, 0.148 mmol) and [L^{Ph}GeCl] (50.2 mg, 0.148 mmol) was condensed toluene (*ca.* 5 mL) at –78 °C, the reaction mixture turned bright yellow and it was allowed to warm up to room temperature. After stirring the reaction mixture at room temperature for 1 h, the resulting solution was concentrated to about one third of its volume and stored in a 5 °C fridge. After 2 days, the solution was carefully decanted and the crystals were isolated, dried for 2 h under vacuum to afford the title compound **7**. The mother liquid was stored in the fridge again for further crystallization.

Single-crystals of **6**, suitable for X-ray diffraction analysis could be obtained from toluene at room temperature.

Yield (based on crystals): 85% (103.8 mg, 0.126 mmol).

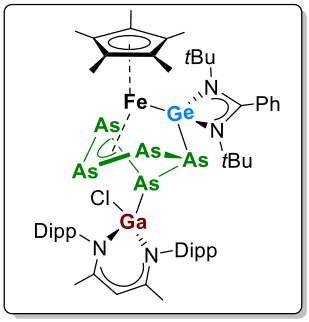
Anal. Calcd. For $C_{44}H_{64}ClGaGeN_4$ (826.83 g/mol): C 63.92; H 7.80; N 6.78. Found: C 63.79; H 7.73; N 6.73.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.59-7.58 (m, 1H, C*H*$_{Ar}$), 7.17-7.14 (m, 3H, C*H*$_{Ar}$), 7.12-7.09 (m, 3H, C*H*$_{Ar}$), 7.06-7.05 (m, 1H, C*H*$_{Ar}$), 6.98-6.92 (m, 2H, C*H*$_{Ar}$), 6.89-6.85 (m, 1H, C*H*$_{Ar}$), 5.07 (s, 1H,*γ* C*H*), 3.88, 3.83, (two sets of sept, ^3J = 6.8 Hz, 4H, C*H* $_{Dipp}$), 1.66 (s, 6H, L^{NacNac}-NCC*H*$_3$), 1.63 (d, ^3J = 6.8 Hz, 12H, C*H*$_3$ $_{Dipp}$), 1.25 (d, ^3J = 6.8 Hz, 6H, C*H*$_3$ $_{Dipp}$), 1.17 (d, ^3J = 6.8 Hz, 6H, C*H*$_3$ $_{Dipp}$), 0.73 (s, 18H, C(C*H*$_3$)$_3$)

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 167.3 (L^{NacNac}-NC*C*H$_3$), 162.5 (N*C*N), 146.2 (Dipp-*m*-*C*), 144.2 (Dipp-*o*-*C*), 143.0 (Dipp-*m*-*C*), 137.2 (Ph-*C*$_q$), 132.2, 129.1, 128.7, 128.0, 127.2, 126.9, 125.5, 124.1 (*C*H^{Ar}), 97.8 (L^{NacNac}-*γ*-*C*H), 52.9 (*C*(CH$_3$)$_3$), 30.7 (C(*C*H$_3$)$_3$), 30.3, 28.0, 27.6, 25.1, 24.7, 24.3, 24.2, (L^{NacNac}-iPr-*C*H, iPr-*C*H$_3$, NC*C*H$_3$).

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 3054 (w), 2961 (m), 2926 (w), 2867 (w), 1612 (w), 1557 (m), 1524 (m), 1463 (m), 1388 (s), 1360 (vs), 1320 (s), 1288 (m), 1251 (m), 1202 (m), 1177 (m), 1102 (w), 1060 (w), 1020 (m), 938 (m), 899 (w), 856 (m), 793 (s), 763 (m), 743 (sh), 704 (s), 640 (w), 581 (w), 522 (w), 475 (m), 446 (m), 400 (w).

I.8 Synthesis of 7



To a J. Young NMR tube containing a mixture of [Cp*Fe(η^5-As_5)] (15.0 mg, 0.027 mmol) and [L^{NacNac}Ga(Cl)-GeL^{Ph}] (21.8 mg, 0.027 mmol) was condensed C_6D_6 (*ca.* 0.4 mL) at –78 °C, and the resulting mixture was warmed up to room temperature and turned brown. The NMR tube was sonicated for 10 min at room temperature and kept at room temperature for 48 h. An ^{1}H NMR spectrum was recorded, showing the reaction was complete. The solvent was removed to *ca.* one third of the volume and kept undisturbed at room temperature overnight to afford green crystals suitable for X-ray diffraction analysis.

Yield (based on crystals): 53% (19.7 mg, 0.014 mmol).

Anal. Calcd. For $C_{54}H_{79}ClFeGaN_4As_5Ge$ (1392.51 g/mol): C 46.58; H 5.72; N 4.02. Found: C 45.95; H 5.38; N 3.58.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 7.43 (dd, ^3J = 7.4 Hz, ^4J = 1.9 Hz, 1H, CH_{Ar}), 7.34-7.27 (m, 2H, CH_{Ar}), 7.23-7.18 (m, 2H, CH_{Ar}), 7.12-7.19 (m, 1H, CH_{Ar}), 6.99-6.83 (m, 5H, CH_{Ar}), 4.95 (s, 1H, C*H*), 4.02, 3.81, 3.72, 3.62 (four sets of sept in 1:1:1:1 ratio, ^3J = 6.6 Hz, 4H, CH_{Dipp}), 2.22 (d, ^3J = 6.6 Hz, 3H, C$H_{3\ Dipp}$), 1.78-1.73 (overlapped signals of 21H, 15H of $C_5(CH_3)_5$ and 6H of C$H_{3\ Dipp}$), 1.72 (s, 3H, L^{NacNac}-NCCH_3), 1.61 (s, 3H, L^{NacNac}-NCCH_3), 1.45 (d, ^3J = 6.6 Hz, 3H, C$H_{3\ Dipp}$), 1.34 (d, ^3J = 6.9 Hz, 3H, C$H_{3\ Dipp}$), 1.21-1.20 (overlapped signals of 12H, 9H of C(CH_3)$_3$ + 3H of C$H_{3\ Dipp}$), 1.14 (d, ^3J = 6.6 Hz, 3H, C$H_{3\ Dipp}$), 1.12 (d, ^3J = 6.9 Hz, 3H, C$H_{3\ Dipp}$), 0.96 (s, 9H, C(CH_3)$_3$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 169.9 (N*C*N), 168.9 (L^{NacNac}-N*C*CH_3), 168.7 (L^{NacNac}-N*C*CH_3), 146.5 (Dipp-*o*-*C*), 146.4 (Dipp-*o*-*C*), 143.2 (Dipp-*m*-*C*), 143.1 (Dipp-*m*-*C*), 142.1 (Dipp-*m*-*C*), 141.7 (Dipp-*m*-*C*), 133.9 (Ph-C_q), 130.0, 129.6, 129.5, 127.61, 127.56, 127.4, 127.3, 125.9, 125.7, 123.9, 123.8, 97.5 (L^{NacNac}-*γ*-*C*H), 86.8 ($C_5(CH_3)_5$), 54.5 (*C*(CH_3)$_3$), 54.1 (*C*(CH_3)$_3$), 33.1 (C(*C*H_3)$_3$), 32.6 (C(*C*H_3)$_3$), 30.3, 29.8, 28.39, 28.3, 27.9, 27.5, 25.24, 25.15, 25.11, 24.8, 24.6, 23.8 (L^{NacNac}-iPr-*C*H, iPr-*C*H_3), 12.1 ($C_5(CH_3)_5$).

IR (ATR): $\tilde{\nu}$ (cm^{-1}) = 2964 (w), 1550 (w), 1525 (m), 1389 (m), 1360 (m), 1312 (s), 1237 (vs), 1177 (s), 1127 (s), 1061 (m), 1018 (m), 983 (s), 864 (m), 794 (m), 763 (m), 739 (m), 708 (s), 576 (m), 528 (m), 497 (m), 474 (m), 448 (m), 426 (m), 400 (m).

II. NMR spectra

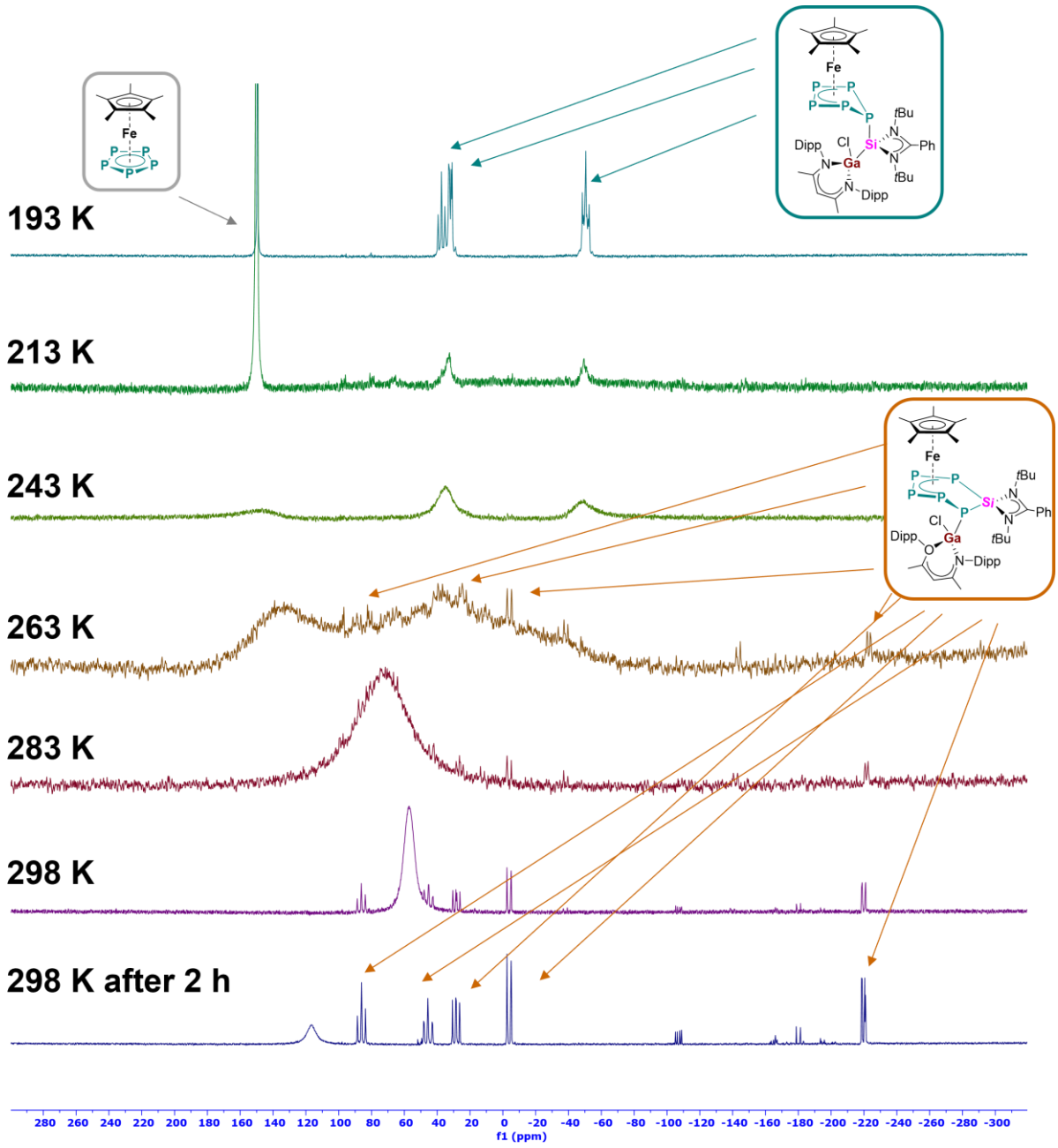


Figure S1. Variable temperature (from 193 K to 298 K) $^{31}P\{^{1}H\}$ NMR (162 MHz, toluene-d_8) spectra of the reaction between [Cp*Fe(η^5-P_5)] and [L^{NacNac}Ga(Cl)-SiL^{Ph}] (1:1 molar ratio).

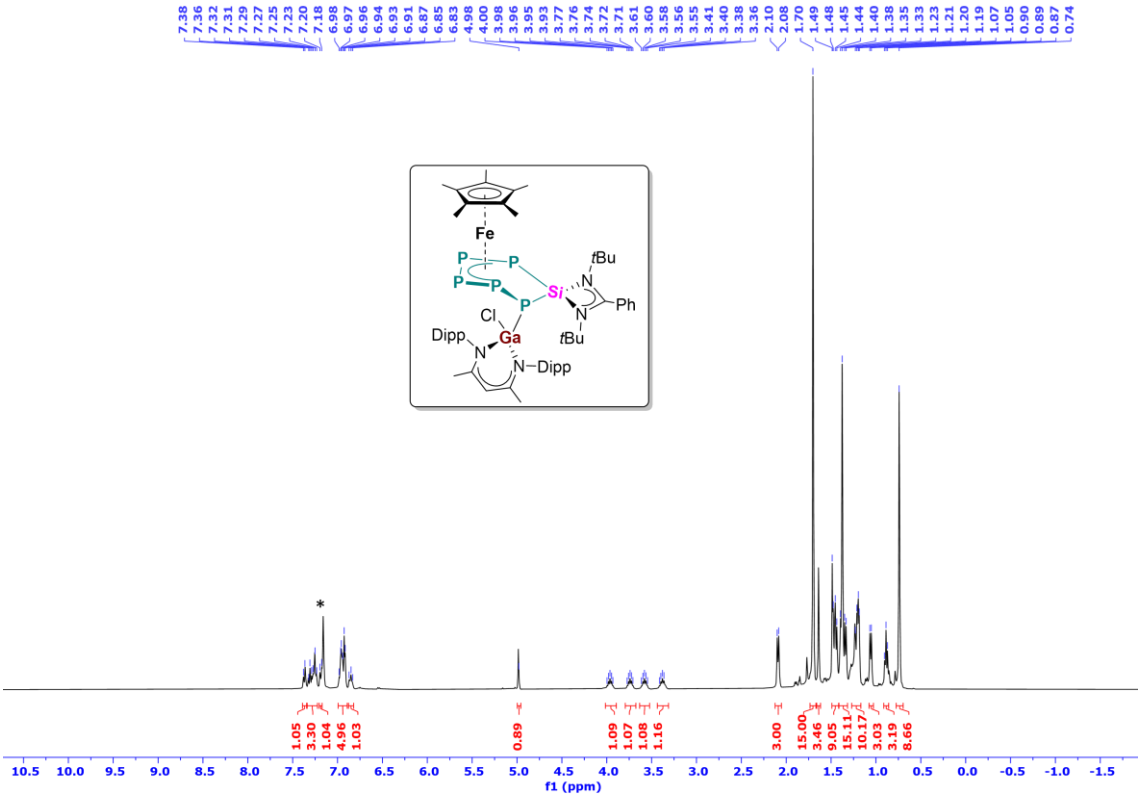


Figure S2. ^{1}H NMR spectrum of compound **2** in C_6D_6, *, residual protio solvent signal.

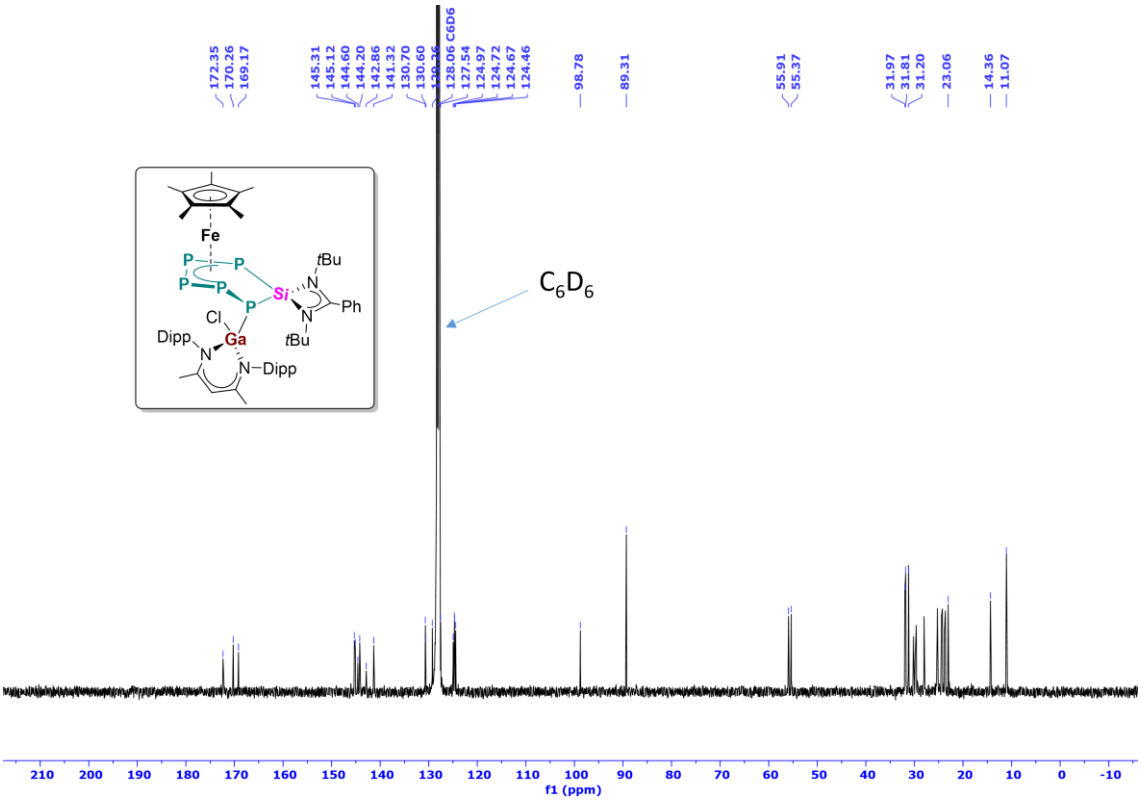


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2** in C_6D_6.

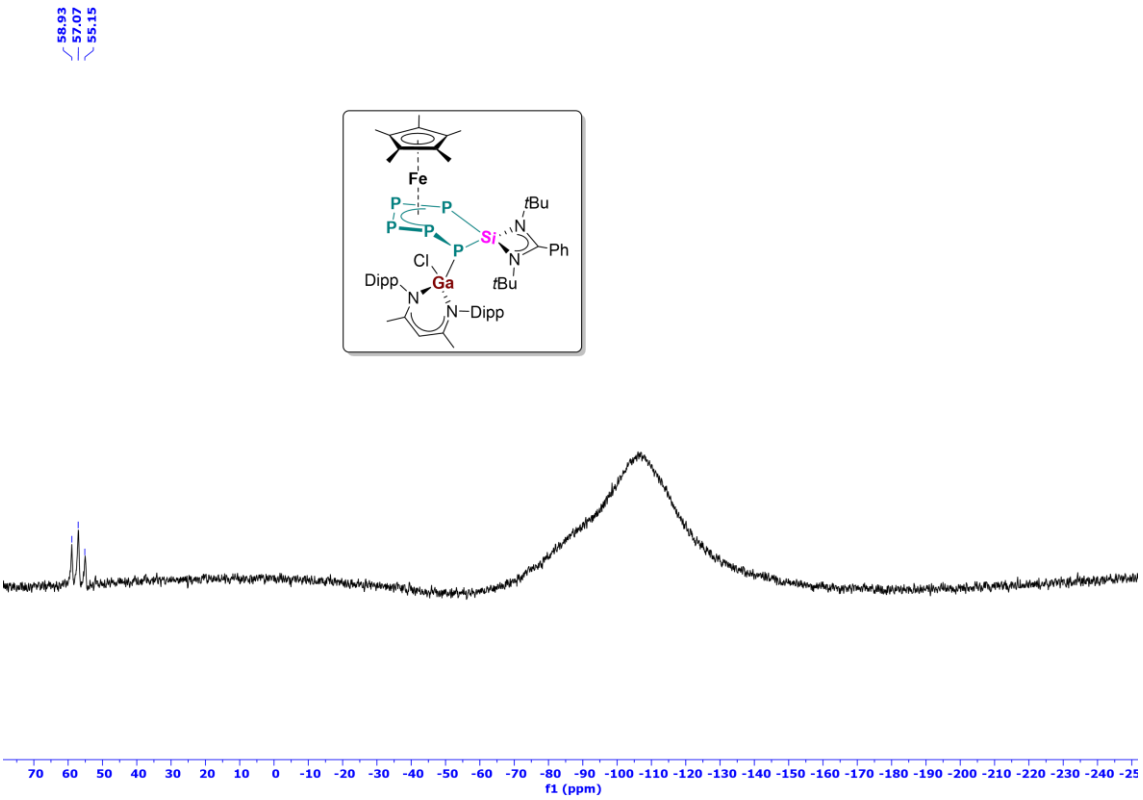


Figure S4. $^{29}Si\{^{1}H\}$ NMR spectrum of compound **2** in C_6D_6.

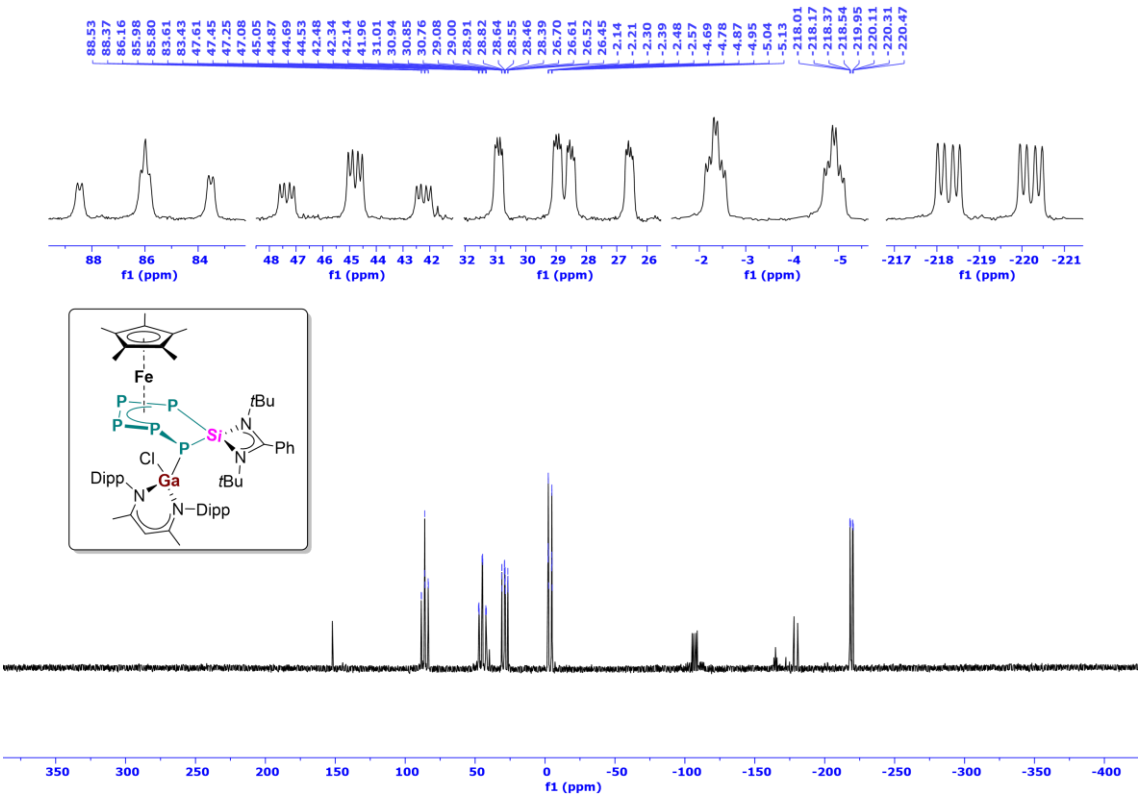


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of compound **2** in C_6D_6.

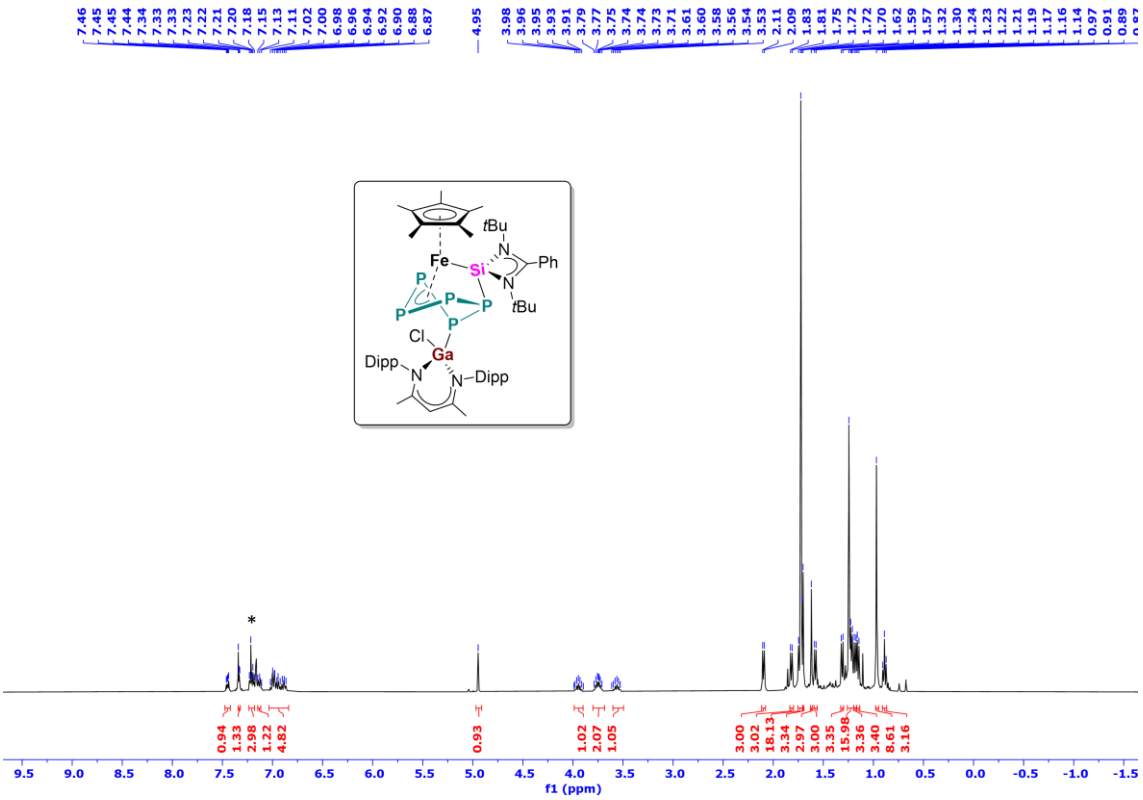


Figure S6. ^{1}H NMR spectrum of compound **3** in C_6D_6, *, residual protio solvent signal.

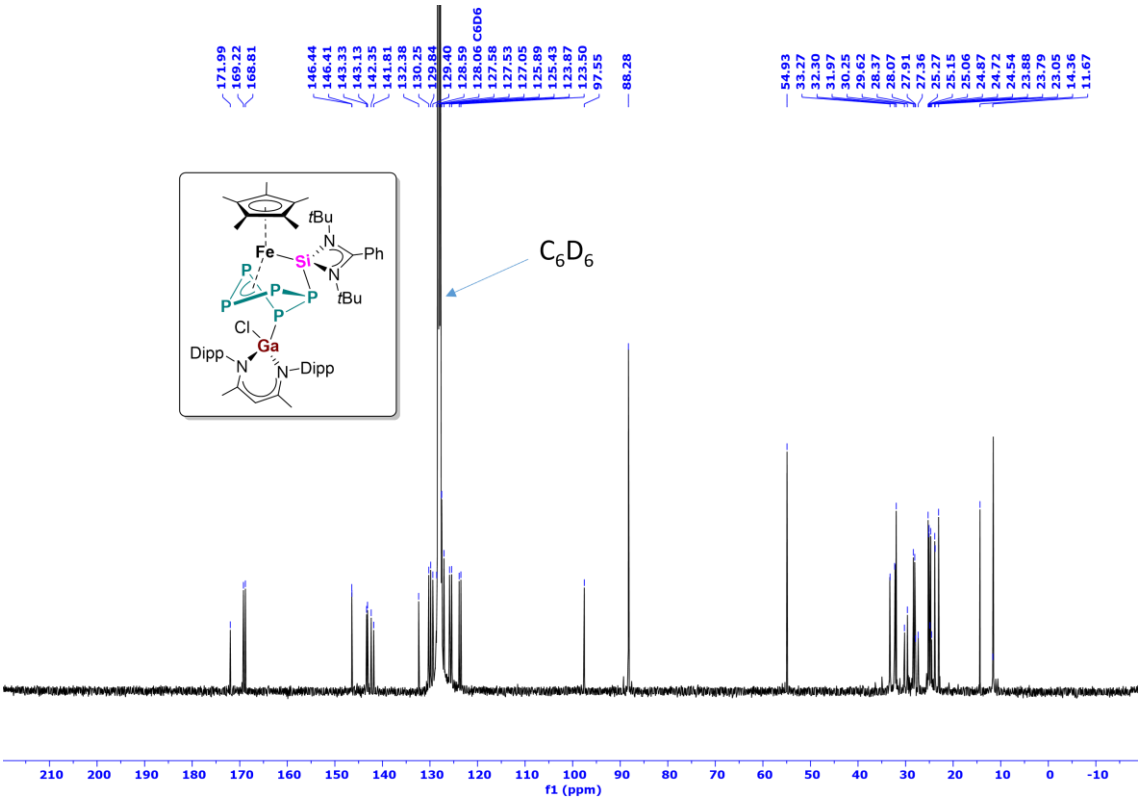


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** in C_6D_6.

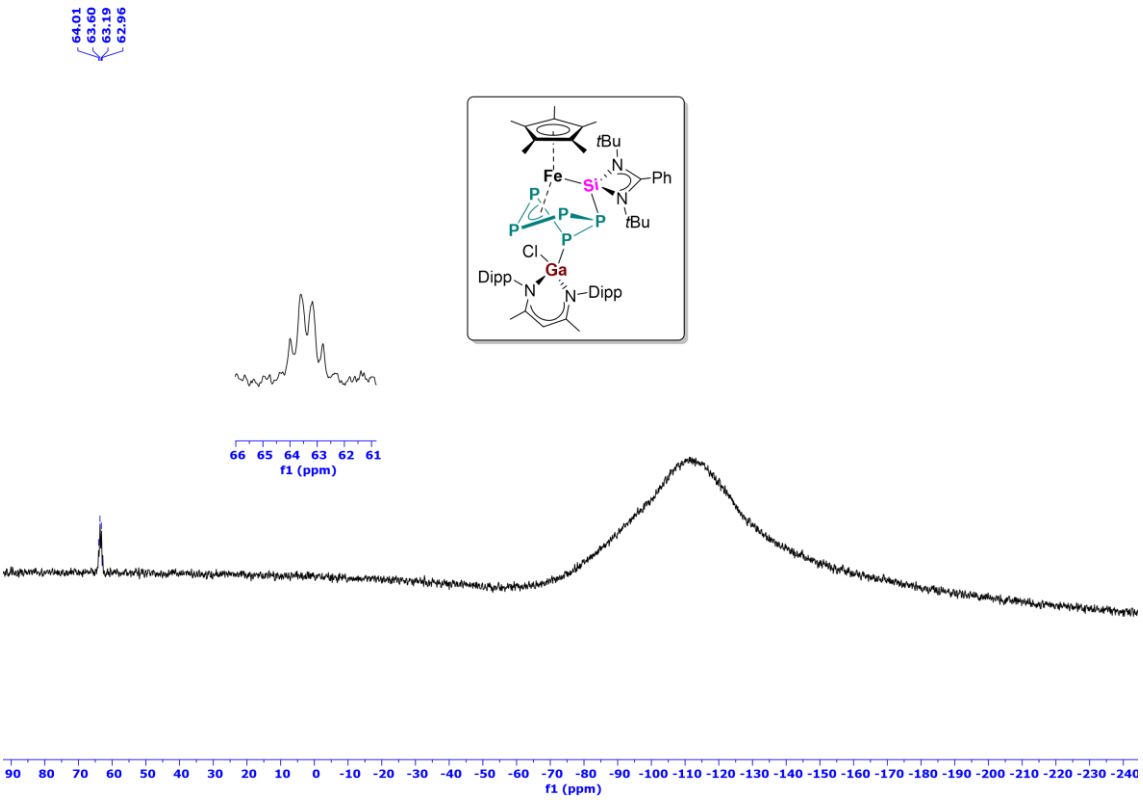


Figure S8. $^{29}Si\{^{1}H\}$ NMR spectrum of compound **3** in C_6D_6.

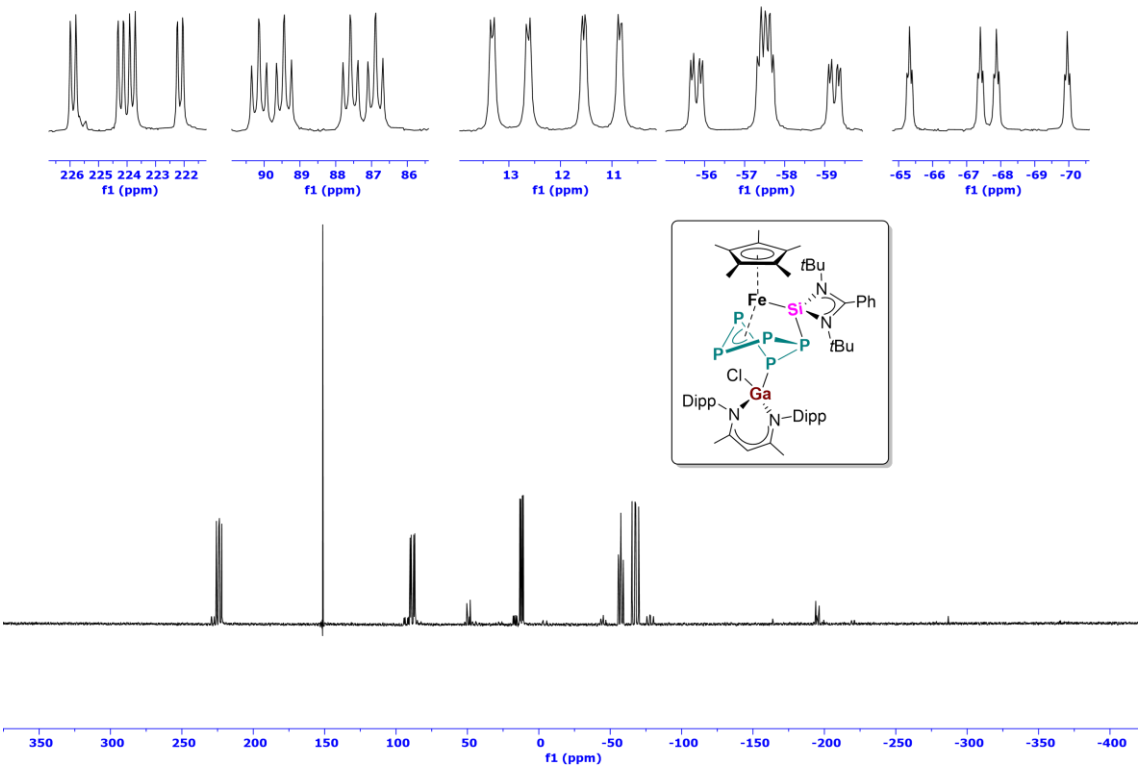


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of compound **3** in C_6D_6.

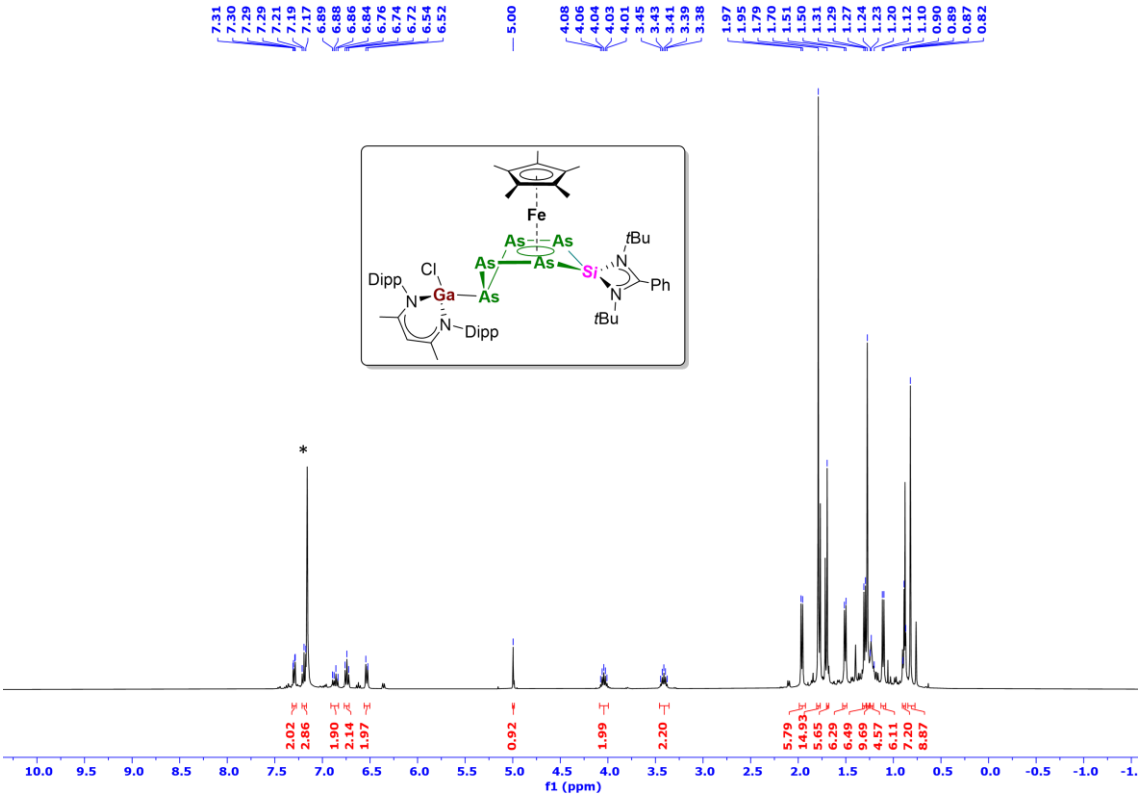


Figure S10. ^{1}H NMR spectrum of compound **4** in C_6D_6, *, residual protio solvent signal.

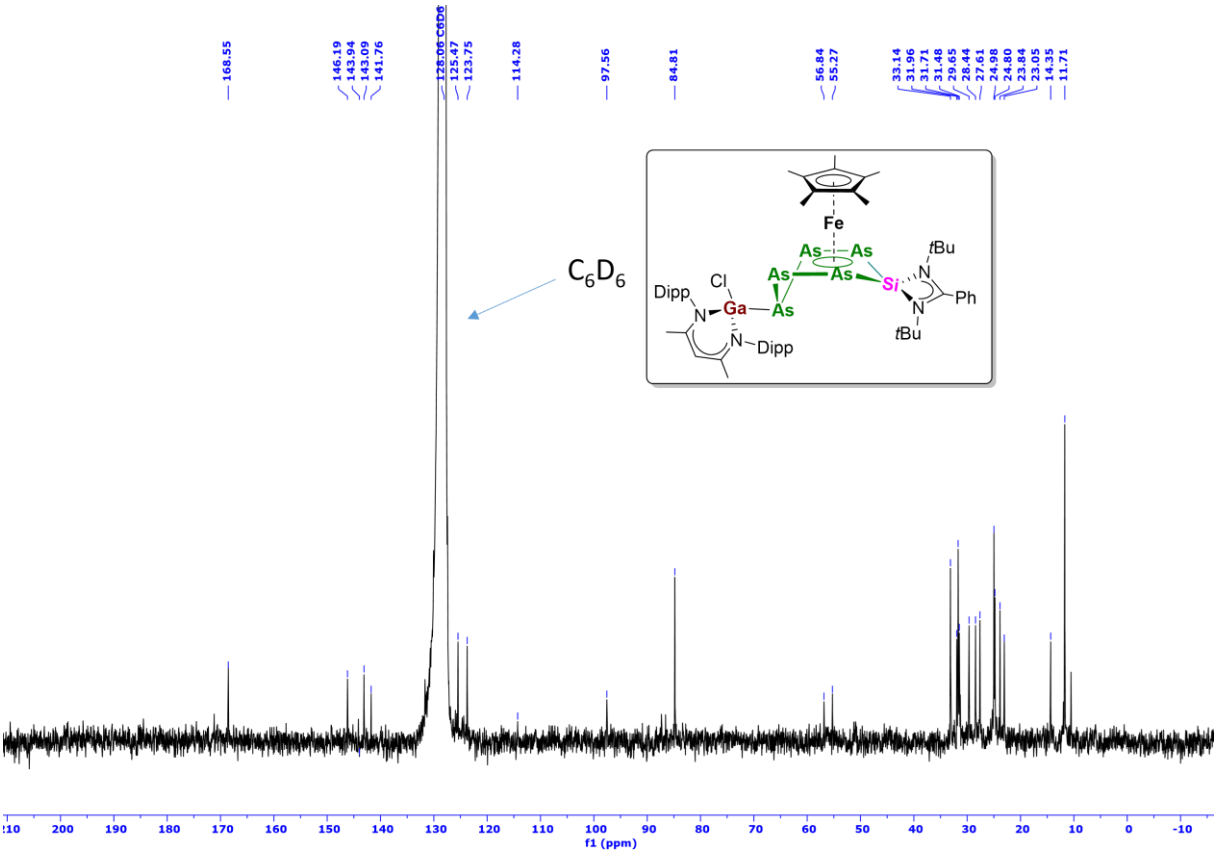


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** in C_6D_6.

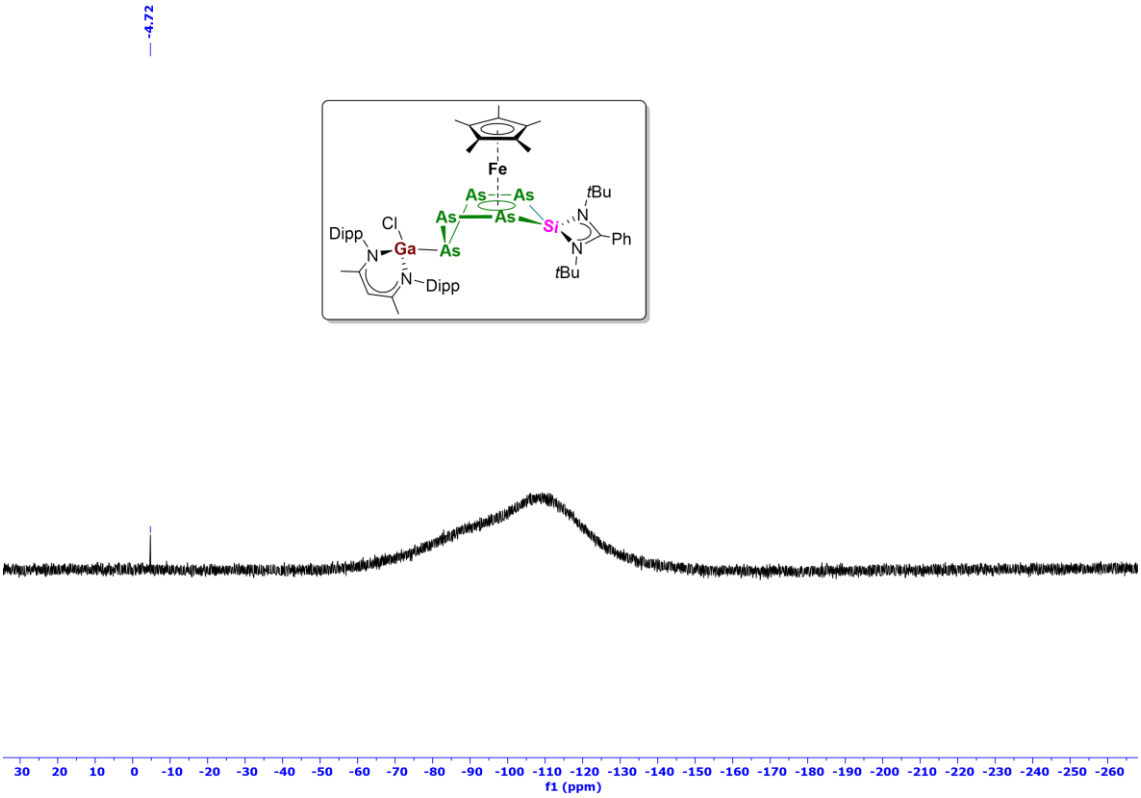


Figure S12. $^{29}Si\{^{1}H\}$ NMR spectrum of compound **3** in C_6D_6.

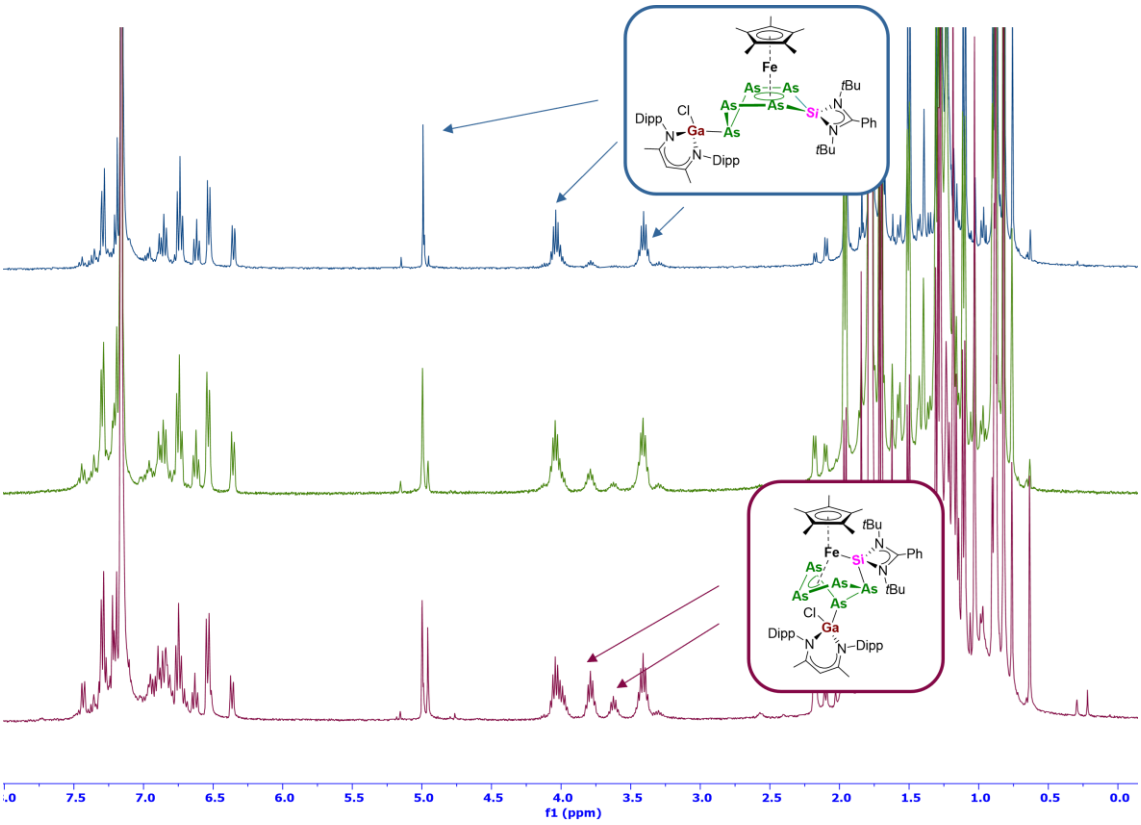


Figure S13. ^{1}H NMR spectrum of compound **4** recorded after dissolving in C_6D_6 (top), overnight (middle), after three days (bottom), showing complex **4** is unstable and already slowly isomerizes to **5** at room temperature.

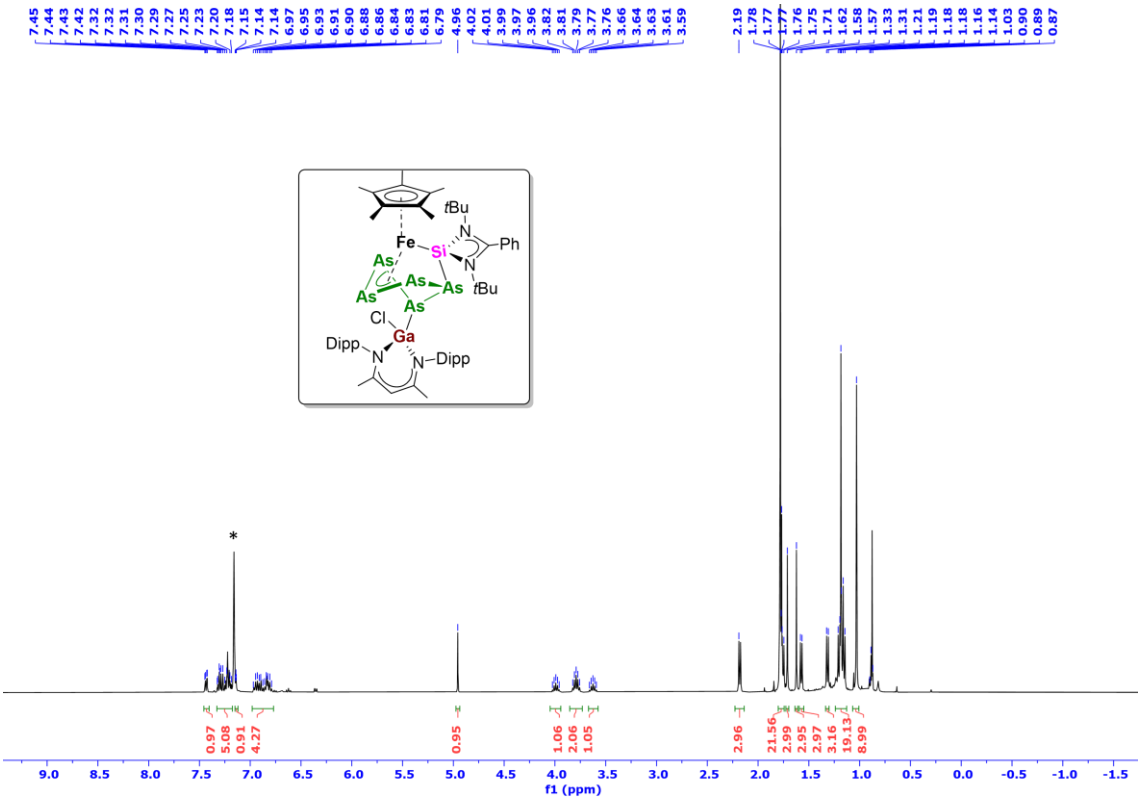


Figure S14. ^{1}H NMR spectrum of compound **5** in C_6D_6, *, residual protio solvent signal.

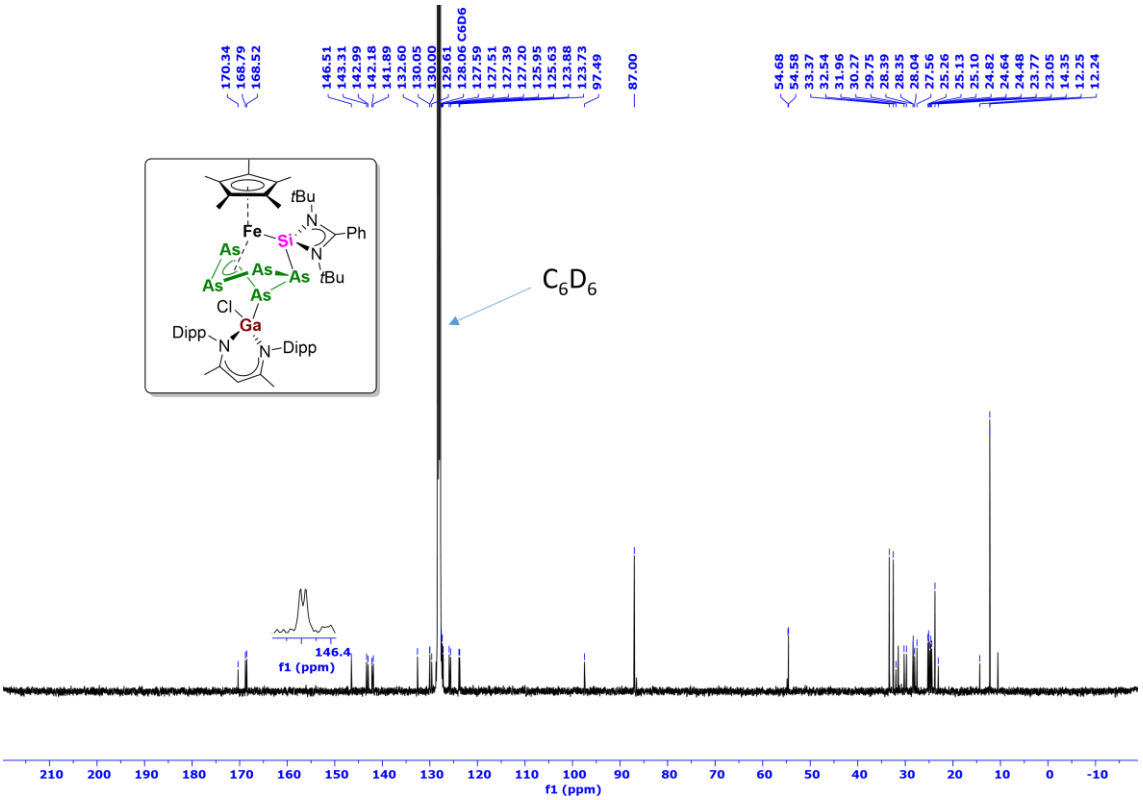


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5** in C_6D_6.

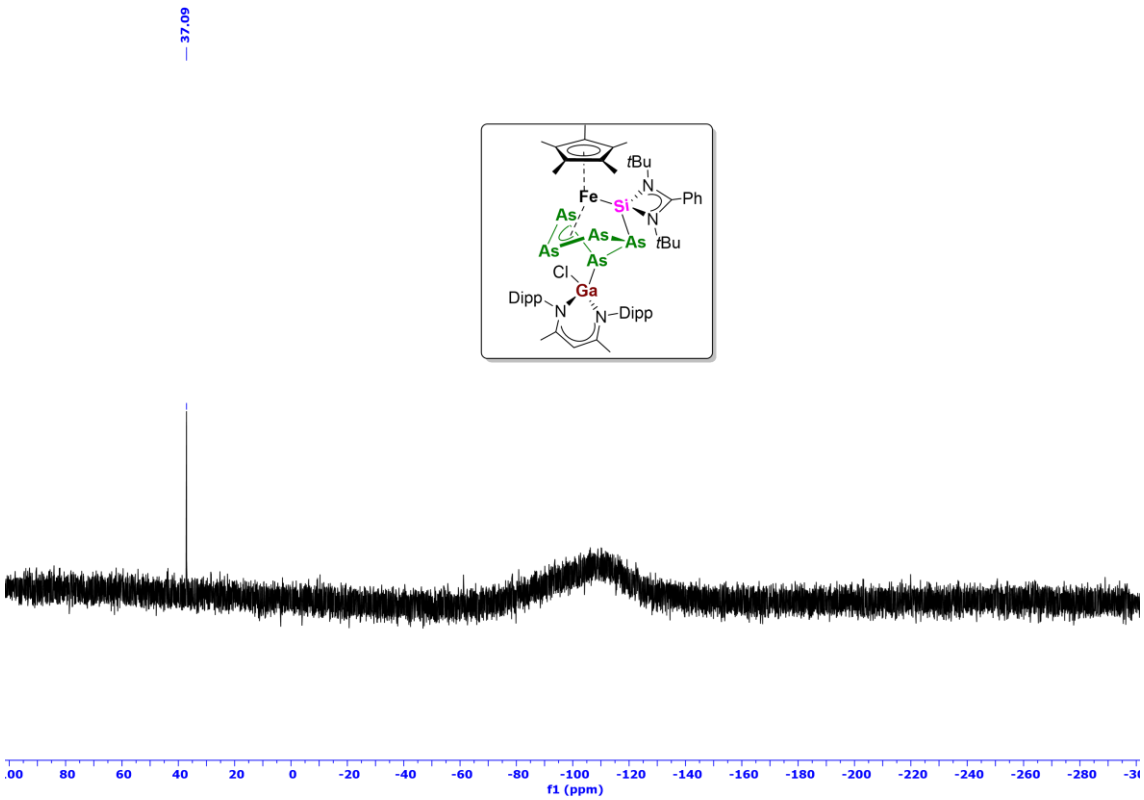


Figure S16. $^{29}Si\{^{1}H\}$ NMR spectrum of compound **5** in C_6D_6.

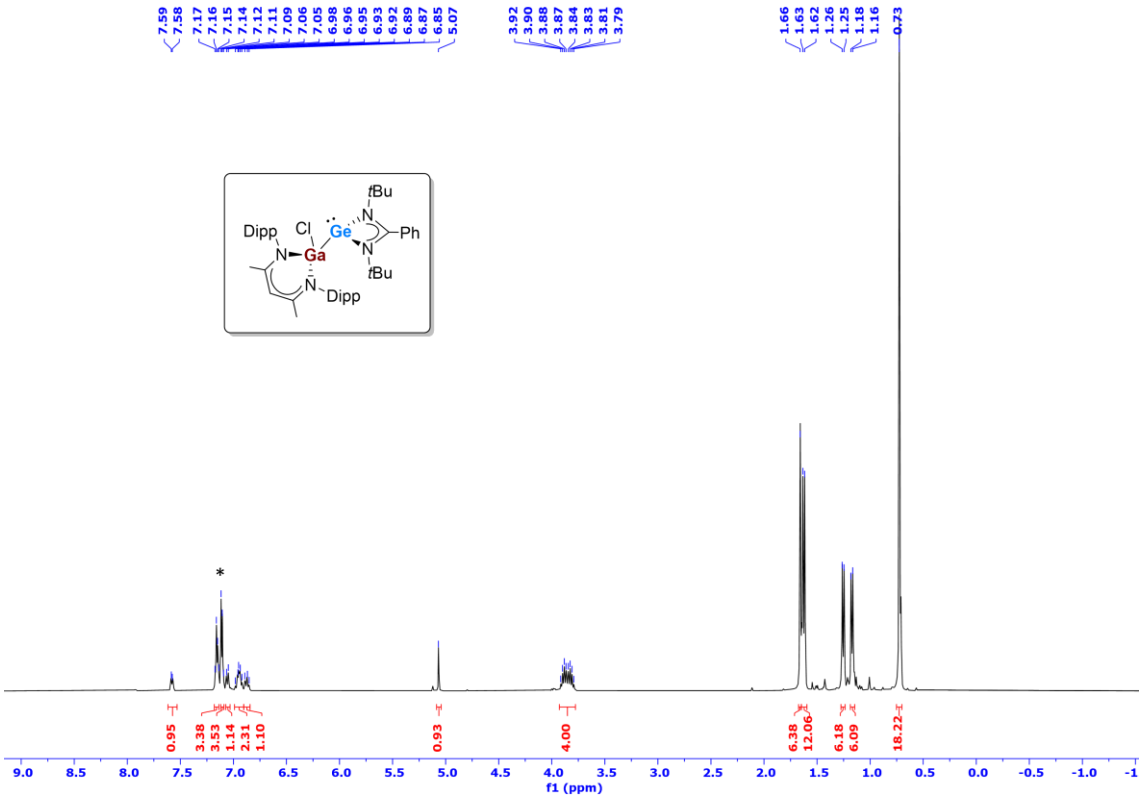


Figure S17. ^{1}H NMR spectrum of compound **6** in C_6D_6, *, residual protio solvent signal.

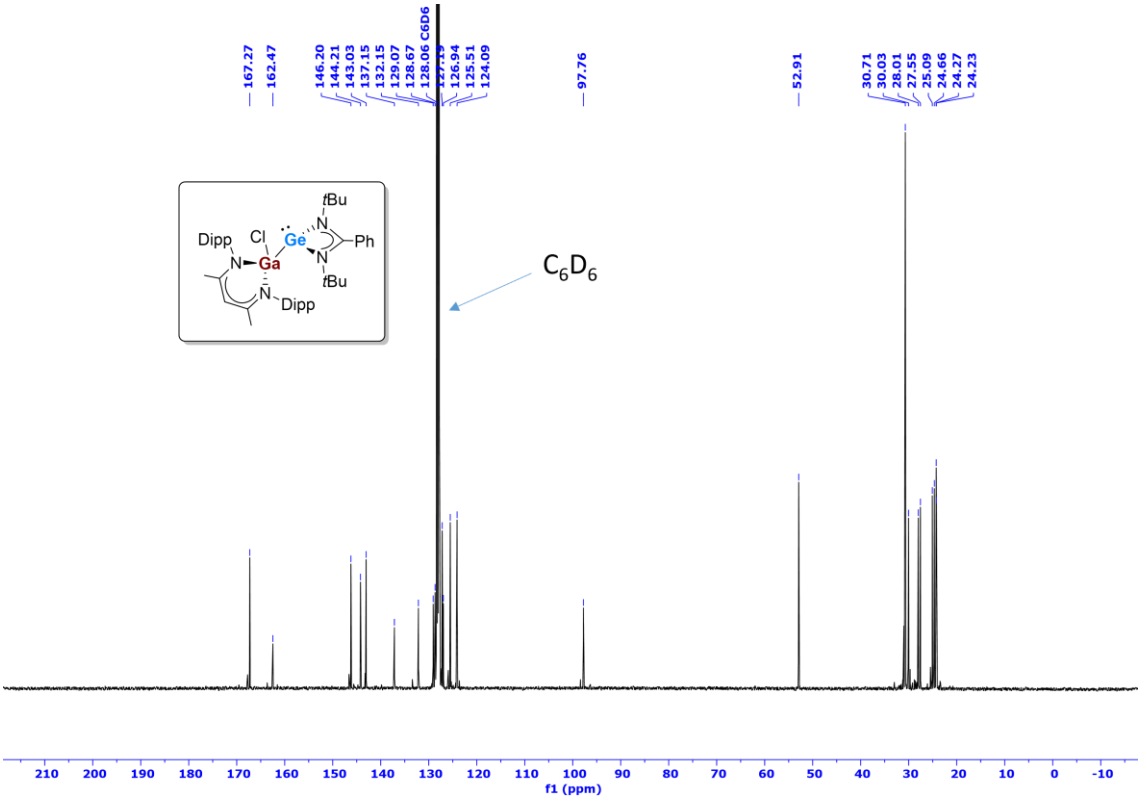


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** in C_6D_6.

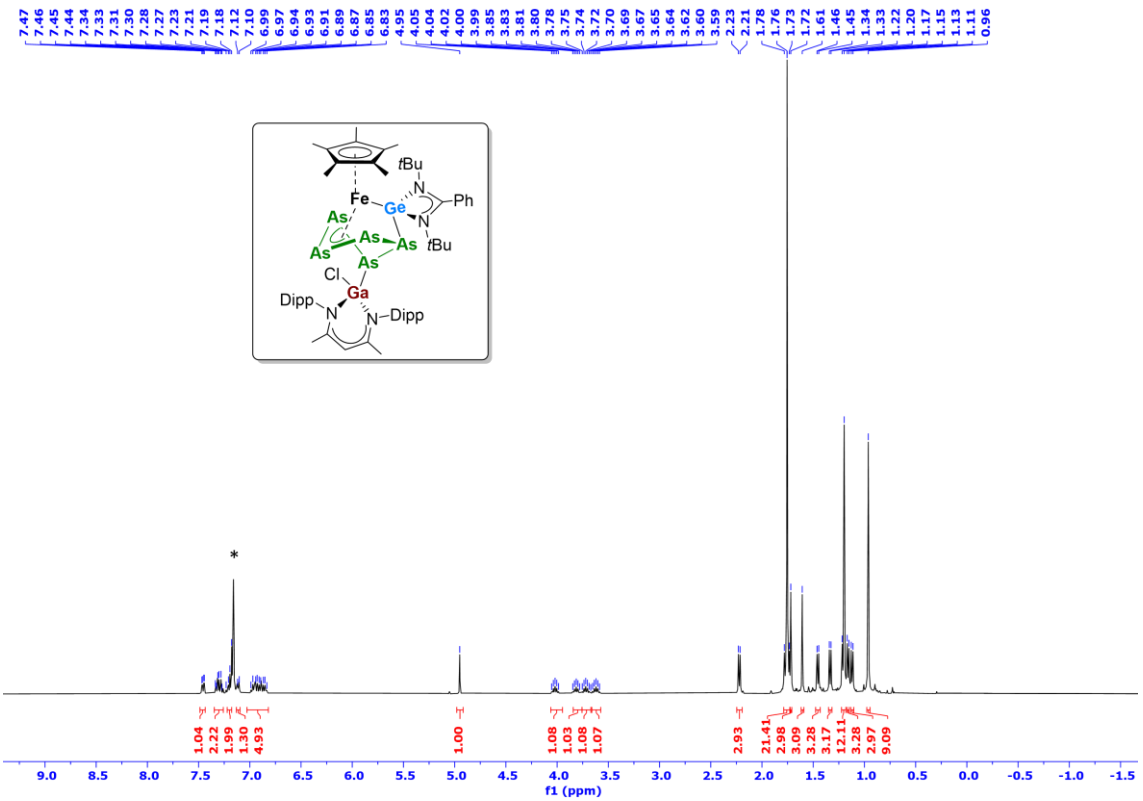


Figure S19. ^{1}H NMR spectrum of compound **7** in C_6D_6, *, residual protio solvent signal.

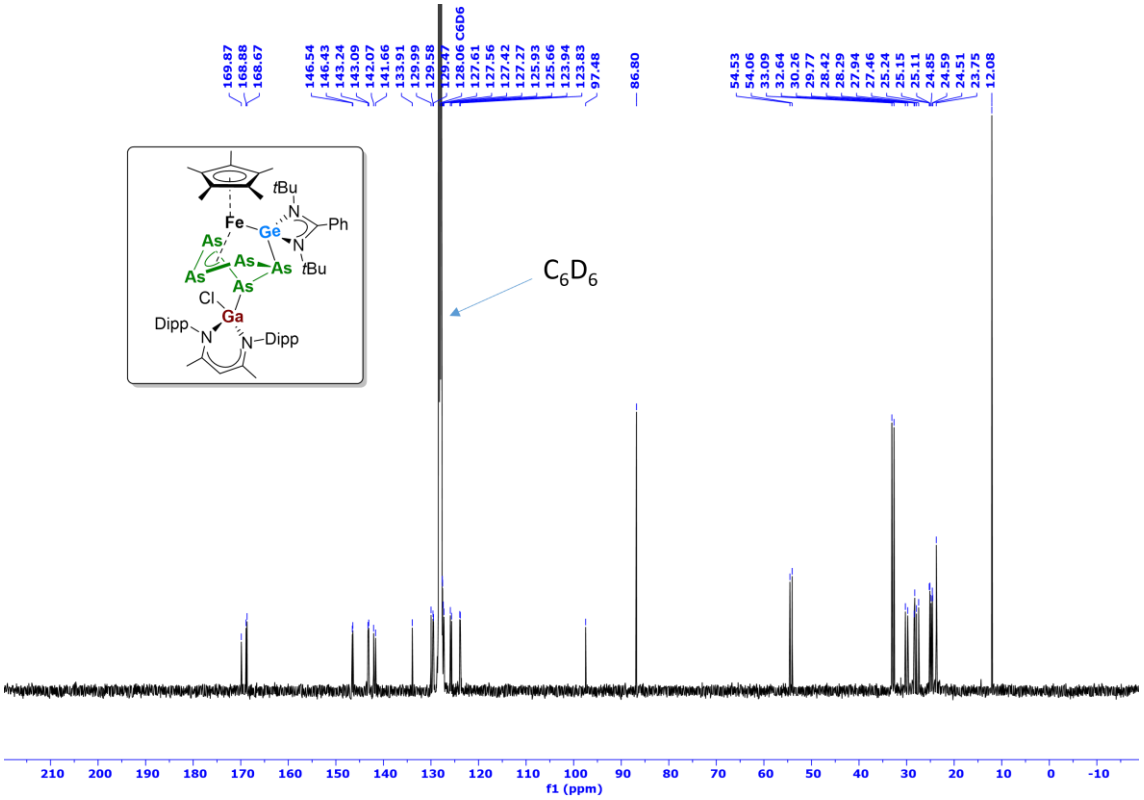


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of compound **7** in C_6D_6.

III. Details of the simulation of the NMR spectra

Simulations of the $^{31}P\{^{1}H\}$ NMR spectra were performed using *gNMR* NMR simulation software, version 5.0.6.0.[S6] The parameters chemical shifts (δ) and coupling constant (J) for the simulation of the phosphorus NMR spectra are compiled in Table S1, S2 and S3.

III.1 Experimental and simulated spectra of 1 (at 193 K)

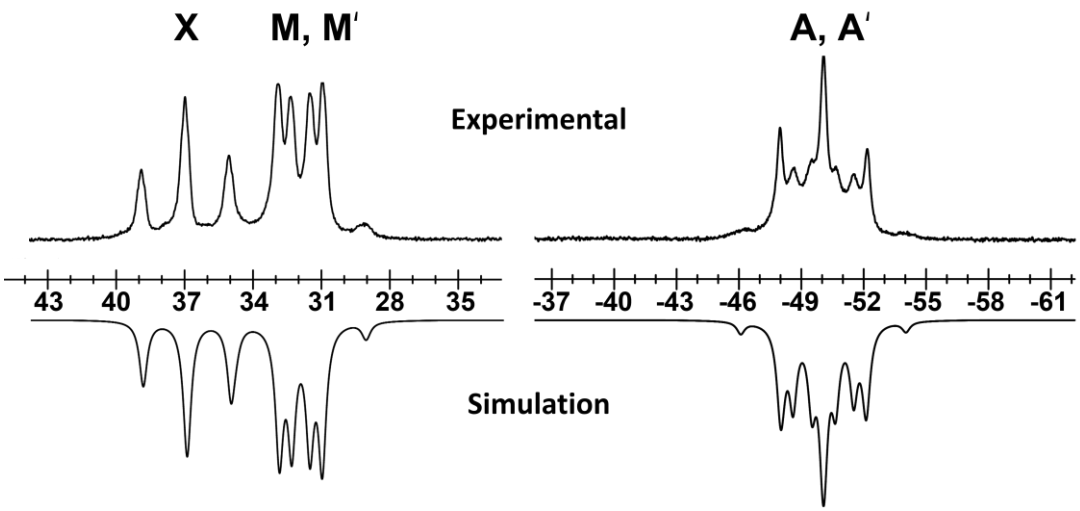


Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz, 193 K, toluene-d_8) of complex **1** with nuclei assigned to an AA'MM'X spin system; experimental (upwards) and simulation (downwards).

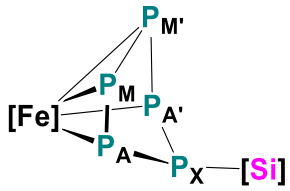


Table S1. Chemical shifts and couplings constants from the iterative fit of the AA'MM'X spin system of **1** and schematic representation of **1**. [Fe] = Cp*Fe; [Si] =L^{Ph}Si-Ga(Cl)L^{BDI}.

Parameters	Iteration values
$\delta(P_A) = \delta(P_{A'})$	-50.6 ppm
$\delta(P_M) = \delta(P_{M'})$	31.3 ppm
$\delta(P_X)$	37.4 ppm
$^{1}J(MM')$	422.9 Hz
$^{1}J(AM) = {}^{1}J(A'M')$	351.7 Hz
$^{1}J(AX) = {}^{1}J(A'X)$	335.5 Hz
$^{2}J(A'M) = {}^{2}J(AM')$	22.8 Hz
$^{2}J(AA')$	0.6 Hz
$^{2}J(MX) = {}^{2}J(M'X)$	0.7 Hz

III.2 Experimental and simulated spectra of 2

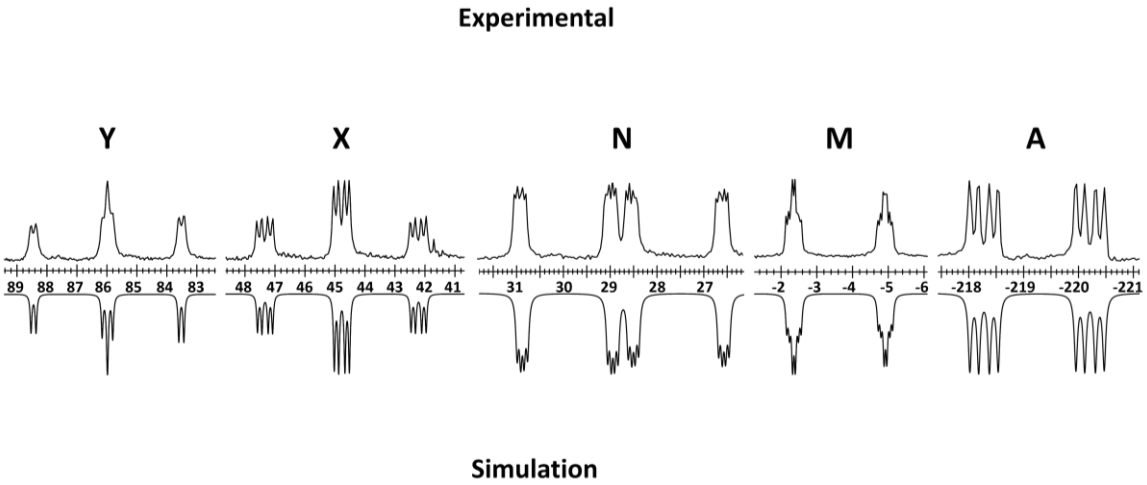


Figure S22. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, 298 K, C_6D_6) of complex **2** with nuclei assigned to an AMNXY spin system; experimental (upwards) and simulation (downwards).

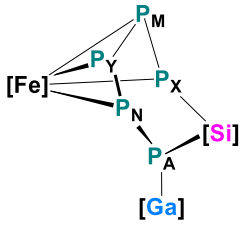


Table S2. Chemical shifts and couplings constants from the iterative fit of the AMNXY spin system of **2** and schematic representation of **2**. [Fe] = Cp*Fe; [Si] =$L^{Ph}Si$; [Ga] = Ga(Cl)L^{BDI}.

Parameters	Iteration values
$\delta(P_A)$	85.9 ppm
$\delta(P_M)$	44.8 ppm
$\delta(P_N)$	28.8 ppm
$\delta(P_X)$	–3.6 ppm
$\delta(P_Y)$	–219.2 ppm
^{1}J(AN)	314.2 Hz
^{1}J(NY)	386.1 Hz
^{1}J(YM)	413.8 Hz
^{1}J(MX)	413.8 Hz
^{2}J(AX)	27.1 Hz
^{2}J(XY)	25.8 Hz
^{2}J(AY)	0.2 Hz
^{3}J(AM)	58.8 Hz
^{3}J(MN)	24.8 Hz
^{3}J(NX)	11.7 Hz

III.3 Experimental and simulated spectra of 3

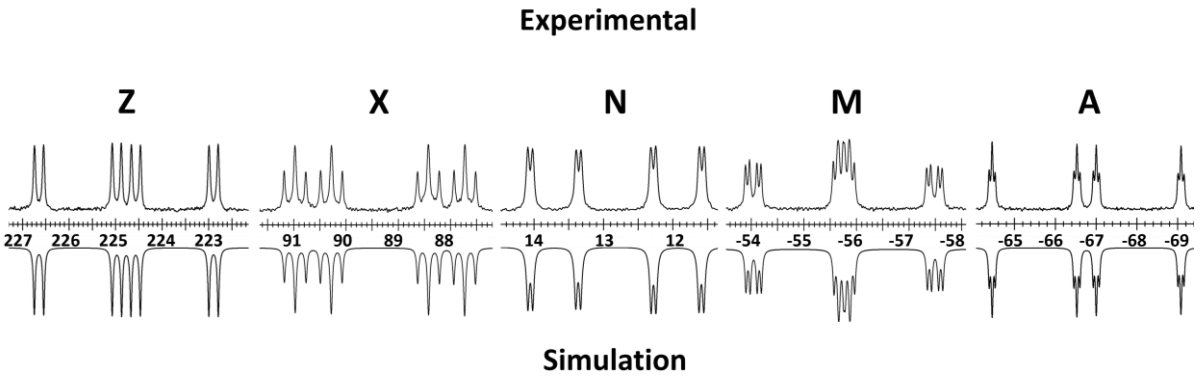


Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, 298 K, C_6D_6) of complex **3** with nuclei assigned to an AMNXY spin system; experimental (upwards) and simulation (downwards).

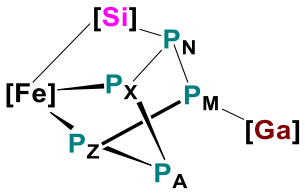


Table S3. Chemical shifts and couplings constants from the iterative fit of the AMNXZ spin system of **3** and schematic representation of **3**. [Fe] = Cp*Fe; [Si] =$L^{Ph}Si$; [Ga] = $Ga(Cl)L^{BDI}$.

Parameters	Iteration values
$\delta(P_A)$	–66.8 ppm
$\delta(P_M)$	–56.8 ppm
$\delta(P_N)$	12.8 ppm
$\delta(P_X)$	89.3 ppm
$\delta(P_Z)$	224.8 ppm
$^{1}J(AX)$	413.4 Hz
$^{1}J(AZ)$	336.4 Hz
$^{1}J(MN)$	287.5 Hz
$^{1}J(MZ)$	271.2 Hz
$^{1}J(NX)$	111.8 Hz
$^{2}J(AN)$	11.3 Hz
$^{2}J(AM)$	13.0 Hz
$^{2}(MX)$	34.5 Hz
$^{2}J(NZ)$	0.1 Hz
$^{2}J(XZ)$	32.8 Hz

IV. IR spectra

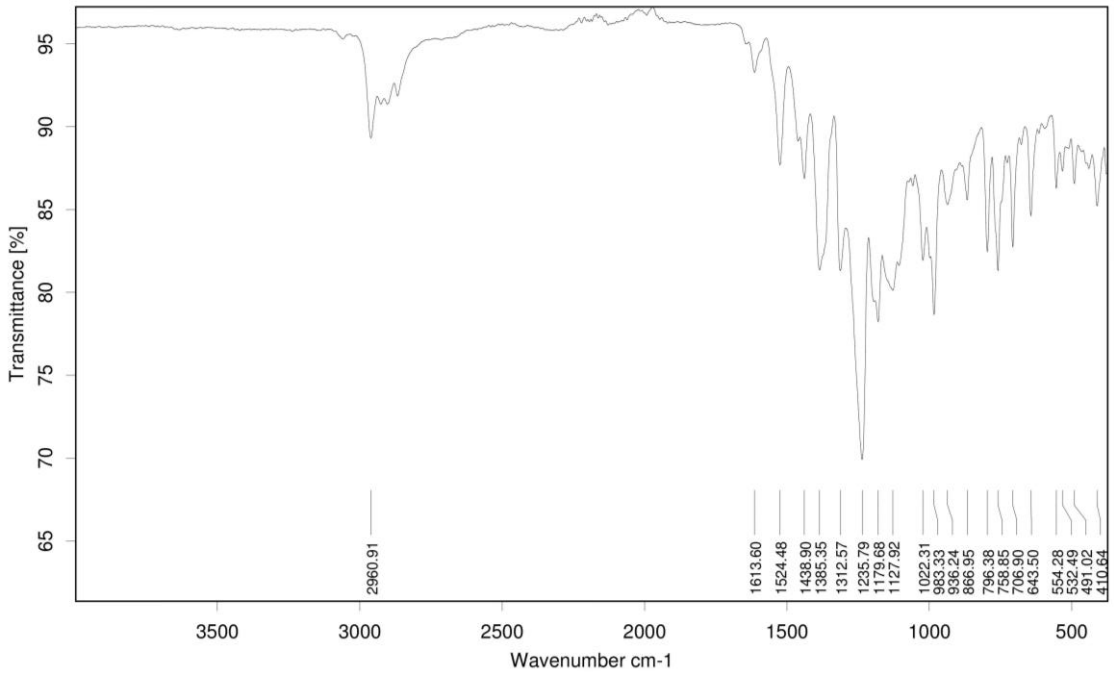


Figure S24. IR spectrum of complex **2**.

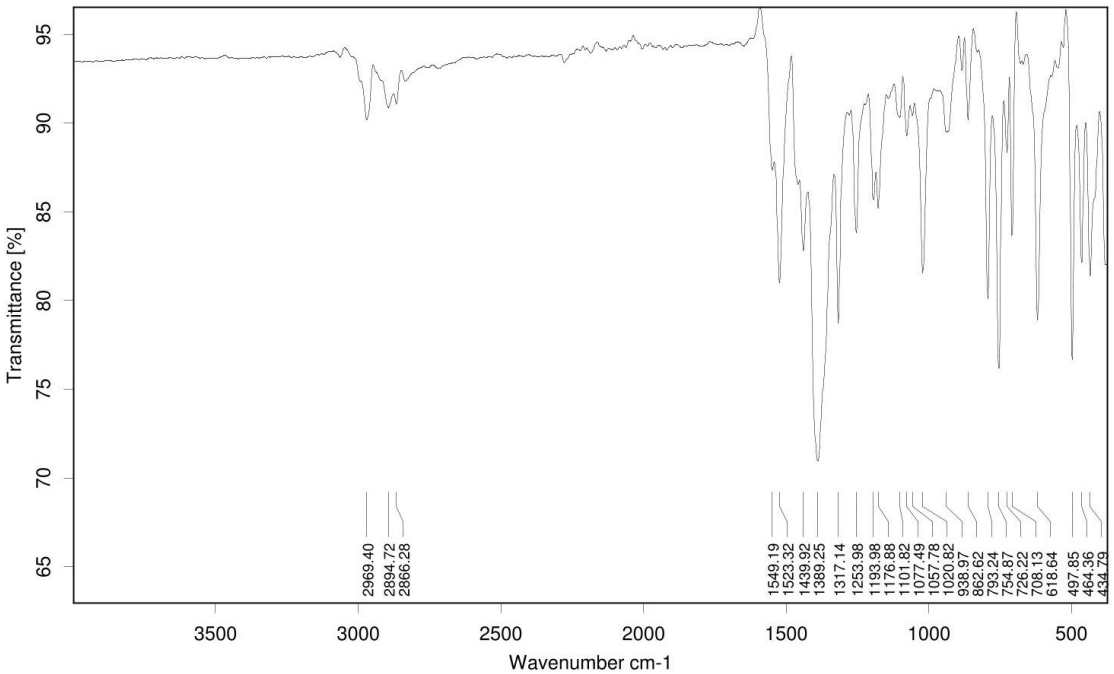


Figure S25. IR spectrum of complex **3**.

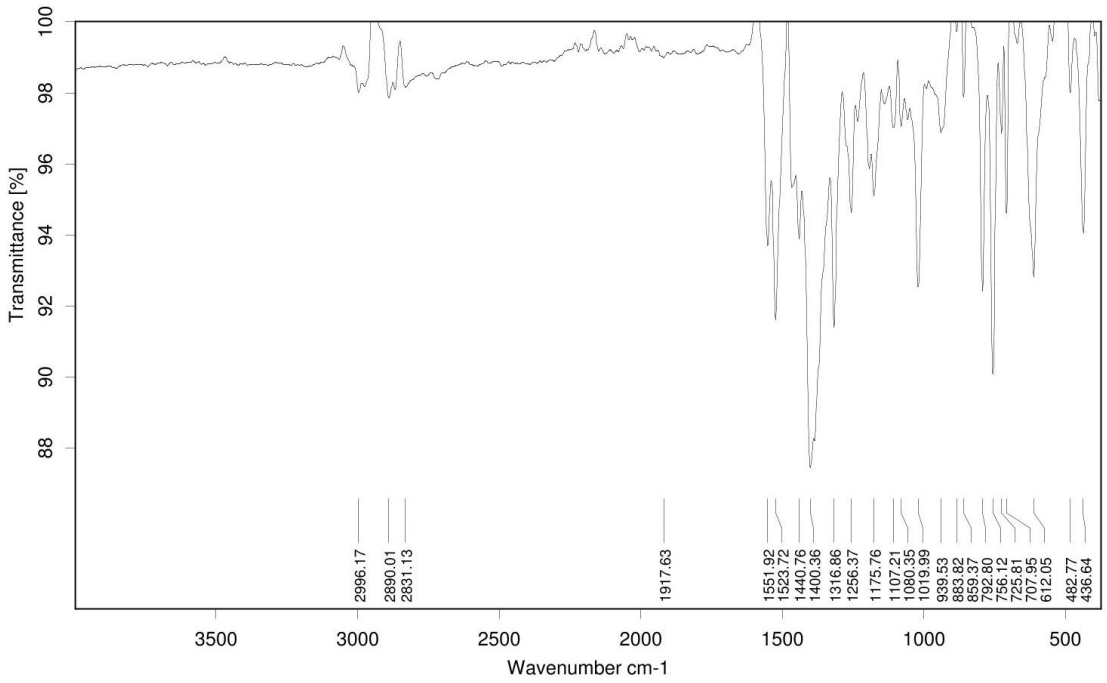


Figure S26. IR spectrum of complex **4**.

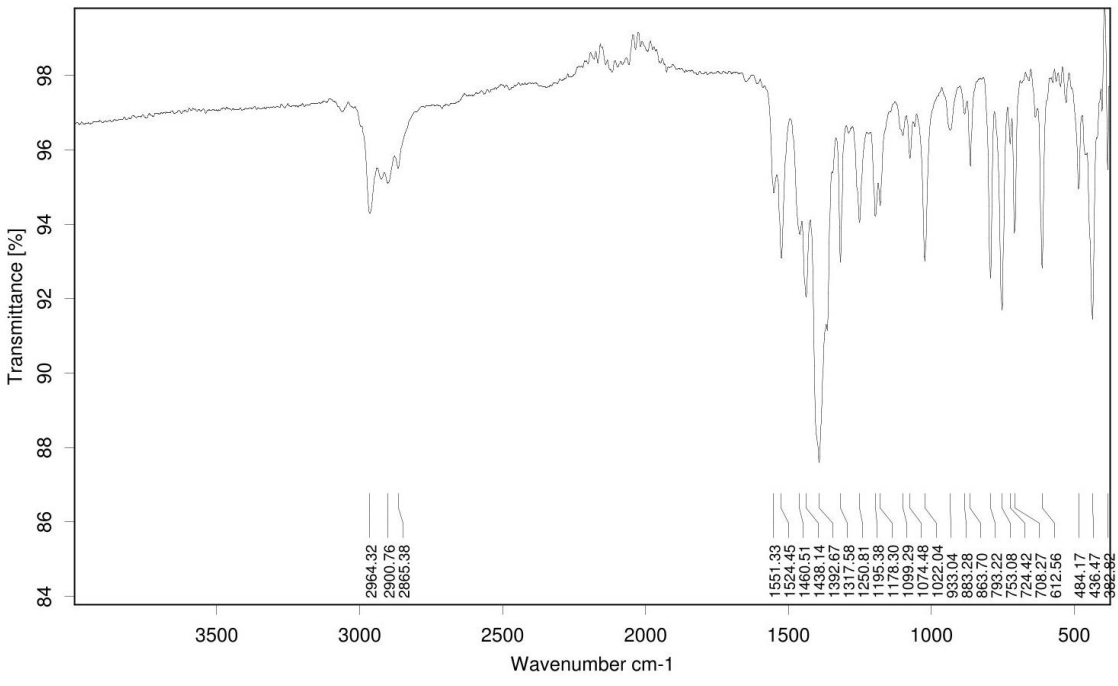


Figure S27. IR spectrum of complex **5**.

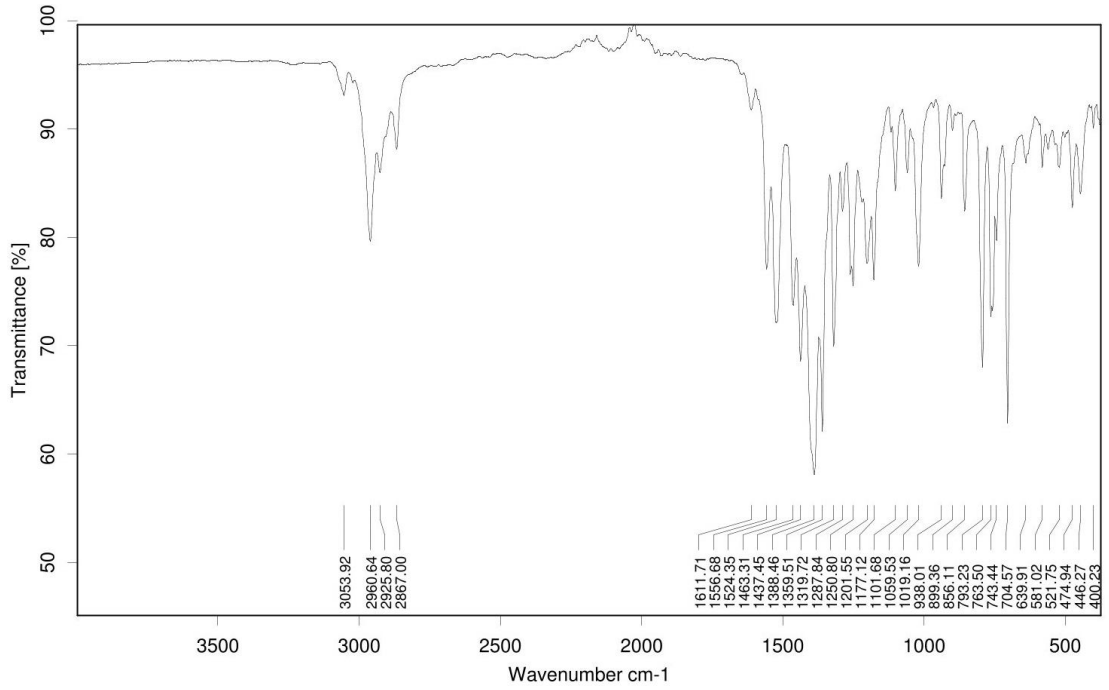


Figure S28. IR spectrum of complex **6**.

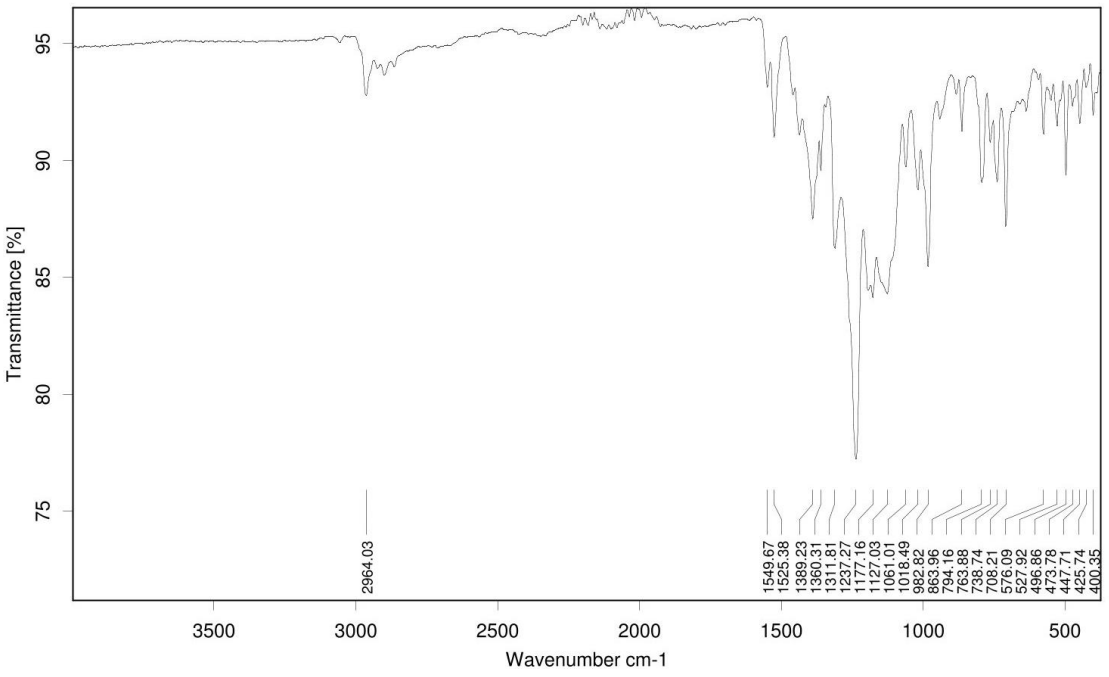


Figure S29. IR spectrum of complex **7**.

V. X-ray crystallography

V.1 General methods

Suitable crystals for the X-ray analysis of all compounds were obtained as described above. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fibre. The crystal was transferred directly to the cold stream of a STOE StadiVari (100 K) diffractometer. All structures were solved by using the program SHELXS/T[S7,S8] and Olex2.[S9] The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F_o^2 by using the program SHELXL.[S7,S8] The H-atoms were introduced into the geometrically calculated positions (SHELXL procedures) unless otherwise stated and refined riding on the corresponding parent atoms. In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance. Specific comments for each data set are given below. Summary of the crystal data, data collection and refinement for compounds are given in Table S4.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2225385-2225391. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

The following special comments were applied to the models of the structures:

- For the refinement of compound **1**, solvent mask was used to treat the solvent region, and the removed electron density (126 electrons per asymmetric unit) is consistent with three benzene molecules.
- In the crystal structure of compound **3**, in one of the two molecules, the two Dipp groups are disordered over two positions occupancy ratios of 0.38/0.62 and 0.41/0.59, respectively. The $L^{Ph}Si$ moiety is disordered over two positions with an occupancy ratio of 0.19/0.81, the FeP_5 moiety is disordered over three positions with an occupancy ratio of 0.73/0.11/0.16 and the Cp* fragment is disordered over three positions with an occupancy ratio of 0.45/0.35/0.11.
- In the crystal structure of compound **4**, one *i*Pr group is disordered over two positions with an occupancy ratio of 0.55/0.45.
- In the crystal structure of compound **7**, in one of the two molecules, one Cp* group is disordered over two positions with an occupancy ratio of 0.55/0.45. The co-crystallized C6D6 molecule is disordered over two positions with an occupancy ratio of 0.39/0.61.

V.2 Summary of crystal data

Table S4.

Compounds	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Chemical formula	$C_{54}H_{79}ClFeGaN_4P_5Si$	$C_{54}H_{79}ClFeGaN_4P_5Si$ (C_6H_{14})	$C_{54}H_{79}ClFeGaN_4P_5Si$ (0.5 C_6D_6)	$C_{54}H_{79}ClFeGaN_4As_5Si$ (0.5 C_6H_{14})	$C_{54}H_{79}ClFeGaN_4As_5Si$ (0.5 C_6H_{14})	$C_{44}H_{64}ClGaGeN_4$	$C_{54}H_{79}ClFeGaN_4As_5Ge$
CCDC Number	2225385	2225386	2225387	2225388	2225389	2225390	2225391
Formula Mass	1128.17	1214.34	1167.22	1391.00	1391.00		
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
Wavelength/Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	orthorhombic	monoclinic	triclinic	monoclinic	triclinic	monoclinic
a/Å	20.5768(7)	26.1402(8)	37.7246(8)	13.5496(7)	15.3662(10)	10.233(2)	37.8546(6)
b/Å	16.8498(4)	17.8110(4)	16.1228(2)	15.4580(8)	17.8212(14)	12.188(2)	16.4222(2)
c/Å	22.4111(8)	27.9689(6)	19.9295(4)	16.9929(9)	23.9686(14)	18.128(6)	19.9888(4)
α/°				91.392(4)		83.16(2)	
β/°	102.858(3)		96.801(2)	107.271(4)	106.448(5)	75.84(2)	96.7960(10)
γ/°				110.499(4)		74.80(2)	
Unit cell volume/Å^3	7575.4(4)	13021.8(6)	12036.4(4)	3150.6(3)	6295.1(8)	2112.0(10)	12338.8(3)
Temperature/K	100	100	100	100	100	100	100
Space group	$P2_1/n$	*Pbca*	$P2_1/c$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P2_1$/c
Z	4	8	8	2	4	2	8
Absorption coefficient μ/mm^{-1}	0.733	0.857	0.925	3.362	3.366	1.447	3.890
No. of reflections measured	55507	42559	78223	47817	61060	22665	84634
No. of independent reflections	14803	13952	23569	13020	12319	8285	22519
R_{int}	0.0401	0.0268	0.0423	0.0359	0.0274	0.0319	0.0353
Final R_1 values ($I > 2\sigma(I)$)	0.0633	0.0399	0.0612	0.0343	0.0309	0.0437	0.0568
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1505	0.0934	0.1182	0.0761	0.0602	0.1167	0.1377
Final R_1 values (all data)	0.0776	0.0638	0.1118	0.0567	0.0463	0.0513	0.0824
Final $wR(F^2)$ values (all data)	0.1587	0.1035	0.1395	0.0825	0.0658	0.1228	0.1574
Goodness of fit on F^2	1.045	1.022	1.055	1.028	1.052	1.049	1.046

V.3 Crystal structures

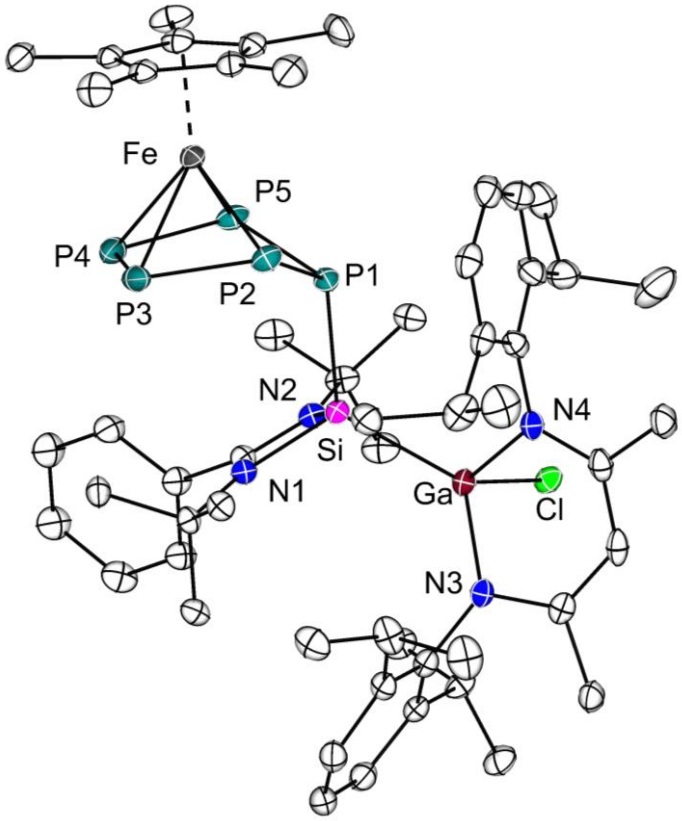


Figure S30. Molecular structure of the complex **1** in the solid state with thermal ellipsoids at 30% level. Selected bond distances [Å] and angles [°]: Ga–Si 2.4293(11), P1–P2 2.1583(15), P2–P3 2.148(2), P3–P4 2.133(2), P4–P5 2.145(2), P1–P5 2.1682(14), P1–Si 2.2516(14), Fe–P2 2.3096(12), Fe–P3 2.3305(13), Fe–P4 2.3245(13), Fe–P5 2.3063(12); P1–P2–P3 109.04(6), P2–P3–P4 103.87(6), P3–P4–P5 104.41(7), P4–P5–P1 108.56(6), P2–P1–P5 94.68(6).

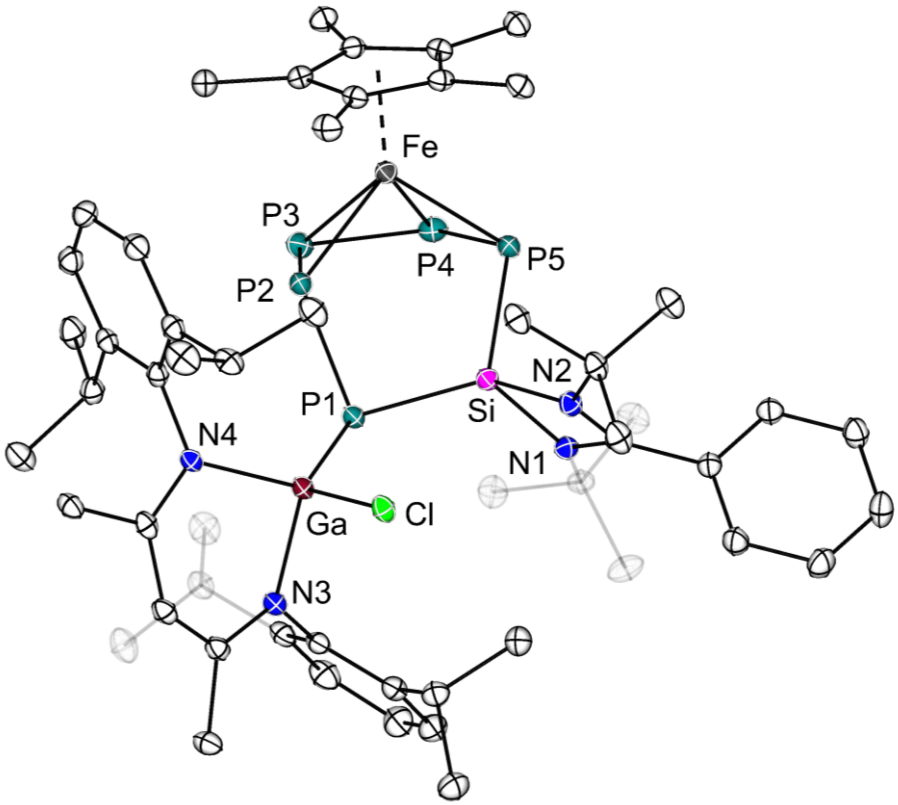


Figure S31. Molecular structure of the complex **2** in the solid state with thermal ellipsoids at 30% level. Selected bond distances [Å] and angles [°]: P1–P2 2.2403(9), P2–P3 2.1467(10), P3–P4 2.1619(10), P4–P5 2.1565(10), Si–P1 2.1771(9), Si–P5 2.1985(9), Ga–P1 2.3062(7), Fe–P2 2.2653(7), Fe–P3 2.3266(8), Fe–P4 2.3471(7), Fe–P5 2.2595(7); P1–P2–P3 100.56(4), P2–P3–P4 105.26(4), P3–P4–P5 108.18(4), P4–P5–Si 106.33(4), P1–Si–P5 113.40(4), Si–P1–P2 95.90(3).

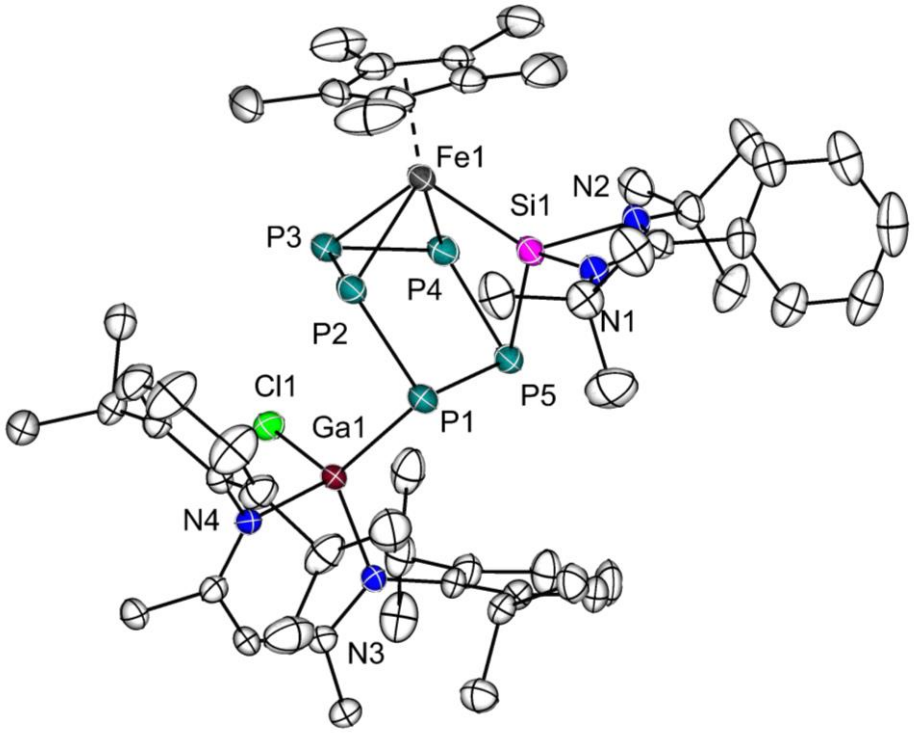


Figure S32. Molecular structure of the complex **3** in the solid state with thermal ellipsoids at 30% level. Two molecules are found in the asymmetric unit, only one of them is depicted here. Selected bond distances [Å] and angles [°]: Ga1–Cl1 2.2108(11), Ga1–P1 2.3117(12), Fe1–Si1 2.2081(14), Si1–P5 2.255(2), P1–P2 2.218(2), P2–P3 2.149(2), P3–P4 2.111(2), P4–P5 2.318(2), P1–P5 2.187(2); P2–P1–P5 101.74(5), P1–P2–P3 103.72(7), P2–P3–P4 99.07(7), P3–P4–P5 107.78(6), P4–P5–P1 102.12(6).

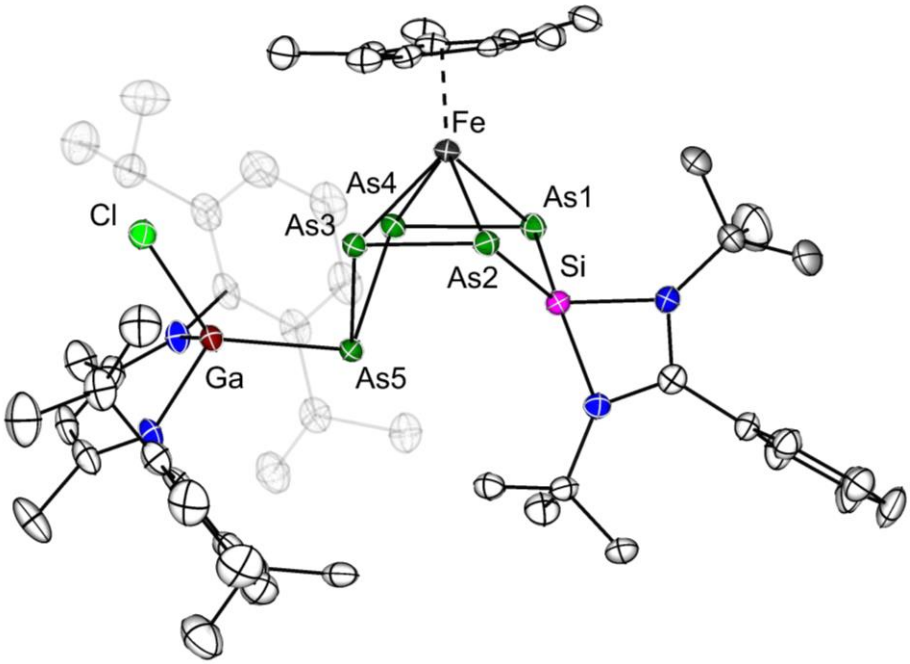


Figure S33. Molecular structure of the complex **4** in the solid state with thermal ellipsoids at 30% level. Selected bond distances [Å] and angles [°]: Si–As1 2.2787(10), Si–As2 2.2985(9), As1–As4 2.3764(5), As2–As3 2.3623(5), As3–As5 2.4563(4), As4-As5 2.4641(5), Ga–As5 2.4046(5); As1–Si–As2 105.00(4), Si–As1–As4 102.03(3), Si–As2–As3 105.34(3), As2–As3–As5 103.27(2), As1–As4–As5 107.12(2), As3–As5–As4 74.030(14).

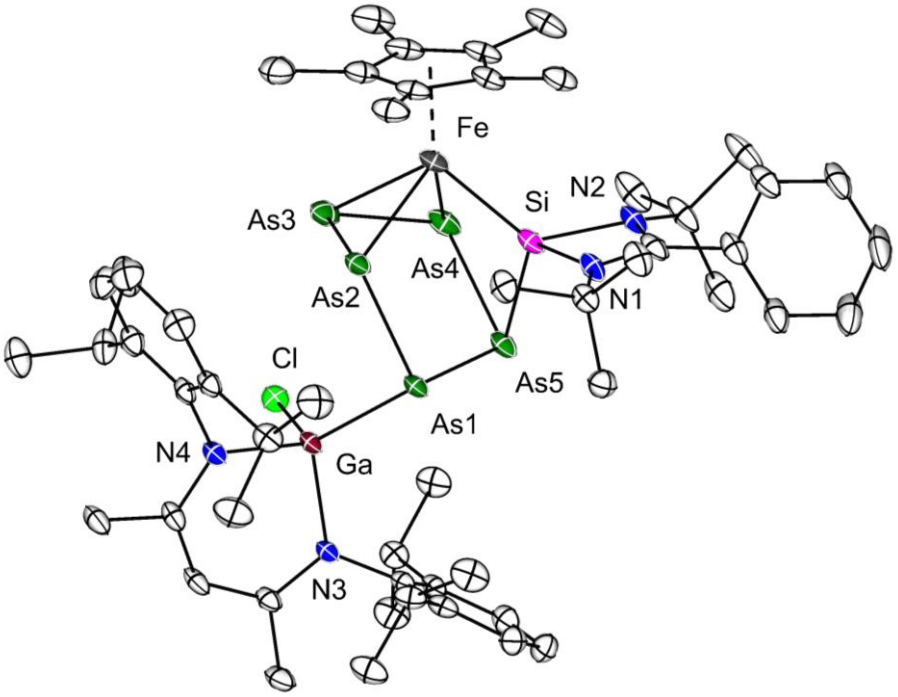


Figure S34. Molecular structure of the complex **5** in the solid state with thermal ellipsoids at 30% level. Selected bond distances [Å] and angles [°]: As1–As2 2.4467(4), As2–As3 2.3669(5), As3–As4 2.3222(5), As4–As5 2.5375(5), As1–As5 2.3986(4), Ga1–As1 2.4080(4), Si–As5 2.3711(8); As1–As2–As3 103.59(2), As2–As3–As4 97.33(2), As3–As4–As5 107.00(2), As1–As5–As4 103.31(2), As2–As1–As5 99.135(15).

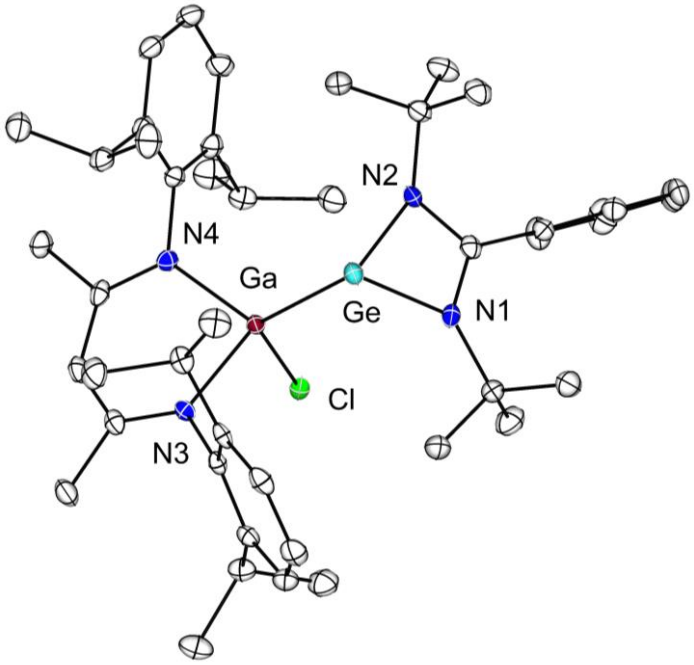


Figure S35. Molecular structure of the complex **6** in the solid state with thermal ellipsoids at 30% level. Selected bond distances [Å] and angles [°]: Ga–Ge 2.5512(10), Ga–Cl 2.3485(10); Ge–Ga–Cl 120.67(3), N1–Ge–N2 65.31(11), N3–Ga–N4 92.73(11).

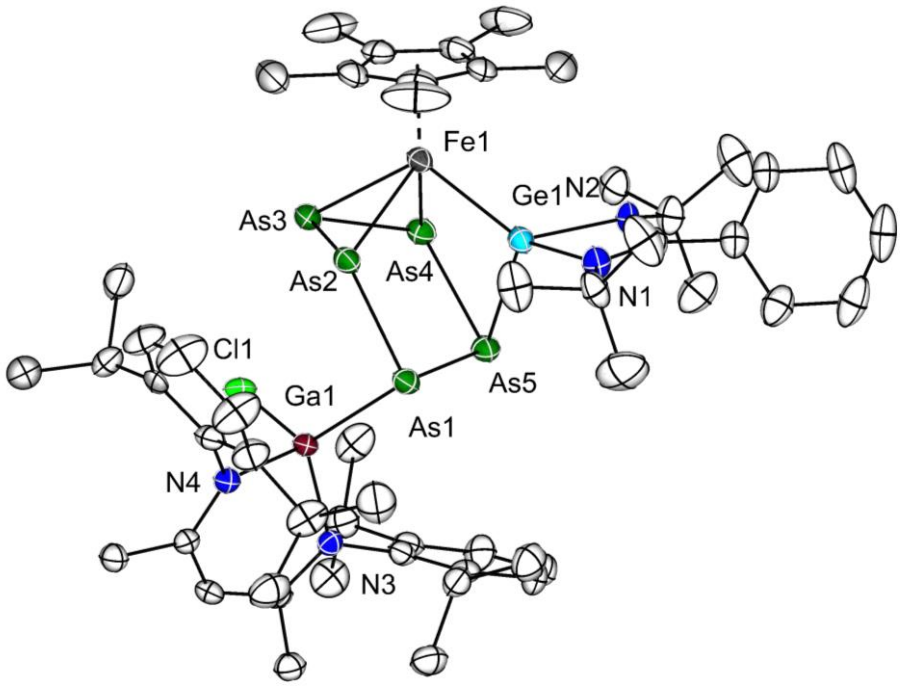


Figure S36. Molecular structure of the complex **7** in the solid state with thermal ellipsoids at 30% level. Two molecules are found in the asymmetric unit, only one of them is depicted here. Selected bond distances [Å] and angles [°]: As1–As2 2.4345(10), As2–As3 2.3638(12), As3–As4 2.3210(11), As4–As5 2.5510(10), As1–As5 2.4027(10), Ga1–As1 2.4014(9), Ge1–As5 2.4325(9); As1–As2–As3 103.04(4), As2–As3–As4 98.62(4), As3–As4–As5 107.50(4), As1–As5–As4 101.91(3), As2–As1–As5 101.23(3).

VI. Quantum chemical calculations

All computations wer performed using Gaussian16[S10] utilizing the PBE0 level of theory, Def2SVP basis sets and empirical dispersion correction (GD3). The temperature is the default temperature of 298.15 K. No solvent corrections were applied. All optimized molecular structures where checked to be minima on the energy hypersurface and possess no imaginary vibrational frequencies. Transition states were checked to possess exactly one imaginary vibrational frequency. Calculated NMR data were obtained on the aforementioned level of theory and are referenced to Me_4Si at 0 ppm (data given are relative to 407 ppm absolute chemical shift) for ^{29}Si and to PH_3 at –248 ppm (data given are relative to 380 ppm absolute chemical shift) for ^{31}P.

VI.1 Computed Energetics and NMR data

Table S5. Relative energies of the intermediates of the rearrangement, complete molecule.

P_5+GaSi	G [a.u.]	ΔG [kJ/mol]
1 / Int1	-7961.788048	0.0
4-P / Int4	-7961.803983	-41.8
2 / Int7	-7961.811135	-60.6
3 / Int9	-7961.816024	-73.5

Table S6. Relative energies of the intermediates of the rearrangement, complete molecule.

As_5+GaSi	G [a.u.]	ΔG [kJ/mol]
1-As / Int1	-17432.91379	0.0
4 / Int4	-17432.93855	-65.0
2-As / Int7	-17432.93857	-65.1
5 / Int9	-17432.94467	-81.1

Table S7. Calculated ^{29}Si and ^{31}P NMR data for 1, 2, 3 and Int4 in (δ in ppm).

P_5+GaSi	^{29}Si	^{31}P				
1 / Int1	13	42	-83	-119	92	85
4-P / Int4	54	138	108	-9	-19	-230
2 / Int7	104	209	77	-16	-48	-77
3 / Int9	18	-109	-115	-251	-253	-230

Table S8. Imaginary frequencies in calculated species.

Compound	# of imaginary frequencies	Energy of imaginary frequency [cm^{-1}]
$TS1^M$ – P/Si	1	–47.68
$TS2^M$ – P/Si	1	–75.98
$TS3^M$ – P/Si	1	–62.67
$TS4^M$ – P/Si	1	–173.51
$TS5^M$ – P/Si	1	–34.92
$TS6^M$ – P/Si	1	–47.10
$TS7^M$ – P/Si	1	–24.94
$TS8^M$ – P/Si	1	–253.28
$TS9^M$ – P/Si	1	–89.34
$TS10^M$ – P/Si	1	–71.09

VI.2 Reaction pathway with model compounds

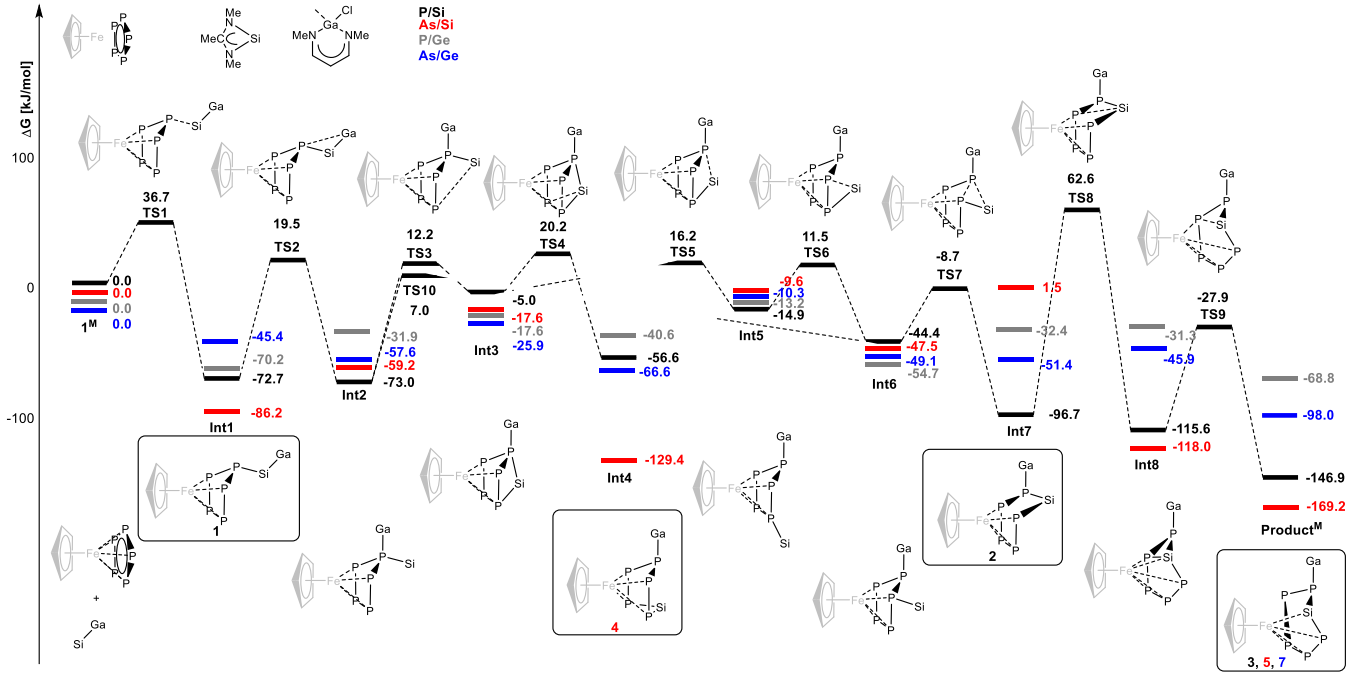


Figure S37. Computed reaction pathway for model compounds with methyl substituents on N (black: $CpFeP_5$+gallasilylene, red: $CpFeAs_5$+gallasilylene, grey: $CpFeP_5$+gallagermylene, blue: $CpFeAs_5$+gallagermylene). Transition states are given for P_5/Si. The highlighted intermediates were isolated. **TS10^M** conntects **Int2** and **Int6**.

Table S9. Energies of the intermediates in the reaction relative to the respective starting materials in kJ/mol. Bold numbers are correlated with isolated compounds.

Intermediate	P_5+Si	As_5+Si	P_5+Ge	As_5+Ge
start	0.0	0.0	**0.0**	0.0
Int1^M	**-72.7**	-86.2	18.3	-18.1
Int2^M	-73.0	-59.2	-31.9	-57.6
Int3^M	-5.0	-17.6	-17.6	-25.9
Int4^M	-56.6	**-129.4**	-40.6	-66.6
Int5^M	-14.9	-9.6	-13.2	-10.3
Int6^M	-44.4	-47.5	-54.7	-49.1
Int7^M	**-96.7**	1.5	-32.4	-51.4
Int8^M	-115.6	-118.0	-31.3	-45.9
Int9^M	**-146.9**	**-169.2**	-68.8	**-98.0**

VI.3 Optimized structures Complete molecules

VI.3.1 compound 1, P

```
0 1
 Ga                -2.25505300   -0.70705100    0.81639700
 Fe                 4.46473400   -0.12398900   -0.55587800
 Cl                -2.99764400   -0.24857900    2.89063300
 P                  1.75563700   -0.30690900    0.73340500
 Si                -0.27611700    0.64519600    0.46779400
 P                  2.51150200   -1.31474300   -1.03466900
 P                  3.20674700    1.30369300    0.80067400
```

P	3.61297600	1.92104200	-1.23857100
P	3.14309300	0.21489600	-2.44157000
N	-0.39834200	2.07567500	-0.67209600
N	-1.94765100	-2.64656300	0.90498600
N	-3.94505000	-0.81891700	-0.17353700
N	-0.25077800	2.19733300	1.47159700
C	6.36551700	-0.09937200	-1.29835000
C	-0.67701400	2.28860600	-2.10080800
C	-5.08635500	1.31678800	-0.63470900
C	5.54409400	-1.76287800	0.09162600
C	6.35580300	0.40603900	0.04339500
C	-4.35009700	-0.12131200	-2.48946000
C	5.86709700	-1.44325900	-1.26857100
C	-3.02451500	-3.40810100	1.07825700
C	-4.77234200	-1.78574600	0.25828600
C	-0.63751000	0.89804500	-2.72694100
H	0.34735700	0.42825900	-2.57595200
H	-0.82108800	0.96182000	-3.80811700
H	-1.41931300	0.25501400	-2.29296300
C	-0.66133700	-3.27948900	0.84443300
C	-4.34501000	-2.93265400	0.93529800
H	-5.13026000	-3.62248700	1.24006500
C	0.35719500	1.31979000	3.63125700
H	0.47571600	1.54447200	4.70117100
H	1.30792200	0.91238600	3.25806400
H	-0.42919000	0.55661300	3.53674100
C	-0.27215400	2.92676000	0.35105000
C	5.84302200	-0.62449000	0.89923700
C	-5.16799800	1.65949300	0.83888700
H	-4.90512100	0.76353700	1.41841500
C	-1.20503500	5.24806800	0.46449400
H	-2.18595000	4.83128600	0.70124100
C	-0.28761300	-3.95474800	-0.33600900
C	-4.45488600	0.14482700	-1.10164000
C	-0.03033200	2.59024200	2.87899500
C	-0.12037800	4.39490300	0.24491100
C	0.19137200	-3.24744300	1.97196500
C	-4.90837000	0.79980900	-3.38105000
H	-4.84210300	0.61734100	-4.45404900
C	-5.54362000	1.95273800	-2.93247200
H	-5.97001500	2.65729700	-3.65051400
C	-1.33572100	3.14131600	3.45700200
H	-1.18729500	3.41225100	4.51328000
H	-2.13058700	2.38471100	3.39970100
H	-1.65704400	4.04540900	2.91978900
C	-6.24556200	-1.64902800	-0.00578700
H	-6.63694600	-0.77933200	0.54380700
H	-6.78973900	-2.54478900	0.31506900
H	-6.45085100	-1.46477600	-1.06939100
C	0.36889500	3.17771400	-2.77369100
H	0.30119000	4.21871200	-2.43163400
H	0.19666400	3.17174100	-3.86032600
H	1.38363900	2.80240500	-2.58265100
C	-5.62053000	2.20858800	-1.57143800
H	-6.10685800	3.12200600	-1.22142200
C	-2.07035100	2.89908700	-2.25757200
H	-2.83487200	2.26840400	-1.78379500
H	-2.32397100	2.99367800	-3.32371200
H	-2.11386900	3.90305000	-1.80989000
C	-4.13079200	2.72822600	1.18273500
H	-3.11075500	2.38798300	0.94819600
H	-4.15811100	2.96835800	2.25560900
H	-4.32089900	3.65317600	0.61319400
C	5.72493000	-2.36671800	-2.43181000
H	4.81325800	-2.97674700	-2.34217100
H	6.58595300	-3.05262600	-2.50594900
H	5.65050500	-1.80953800	-3.37590400
C	1.39074500	-3.96055500	1.90462800
H	2.06564900	-3.95482600	2.76099500
C	-3.65724600	-1.36885800	-3.01827600
H	-2.78760000	-1.54774500	-2.36428100
C	1.13970000	4.91810700	-0.06961400
H	1.97937900	4.23778500	-0.23697400
C	-6.56535400	2.09560400	1.27736400
H	-6.85784200	3.06155900	0.83612900
H	-6.59682500	2.21381900	2.37126900
H	-7.33176300	1.35757900	0.99433000
C	0.92816100	-4.64383600	-0.35102700

H	1.23980600	-5.15982700	-1.26187600
C	1.09551800	3.61702400	3.02167400
H	0.81124000	4.60467800	2.63563000
H	2.00307700	3.27333800	2.50219300
H	1.33166700	3.73393000	4.08983100
C	-3.14425000	-1.20279300	-4.44665000
H	-3.97164900	-1.16696900	-5.17263400
H	-2.51587700	-2.06079100	-4.72451000
H	-2.54321000	-0.29137500	-4.56834300
C	1.75301300	-4.66619000	0.76327300
H	2.69834000	-5.21222600	0.73611500
C	-0.17266200	-2.46852300	3.22357400
H	-0.62523700	-1.52277700	2.88409500
C	-1.11968500	-3.91001600	-1.60449100
H	-2.08971900	-3.44942300	-1.36241900
C	6.81514500	1.75343900	0.48976000
H	6.78678400	2.47735000	-0.33643400
H	7.84771000	1.71598300	0.87658000
H	6.16909300	2.14617300	1.28946000
C	-2.86436200	-4.87005900	1.38341800
H	-2.71827300	-5.42730200	0.44542800
H	-3.76669700	-5.26080500	1.87066300
H	-1.98647100	-5.06543900	2.01215300
C	0.22667800	7.15194200	0.06559400
H	0.36369400	8.23385500	-0.00295600
C	-0.43014000	-3.02452900	-2.64341700
H	-0.28581300	-2.00039700	-2.27145700
H	-1.01623100	-2.98100500	-3.57323400
H	0.57227500	-3.40683300	-2.88830700
C	-1.02848900	6.62766700	0.37116500
H	-1.87687600	7.29487700	0.53961600
C	1.03650800	-2.09640700	4.07481200
H	1.47440300	-2.97687700	4.57201900
H	0.73121700	-1.39784800	4.86801900
H	1.81534800	-1.60989800	3.46857400
C	1.30772900	6.29680100	-0.15423400
H	2.29224700	6.70451400	-0.39423700
C	5.04493000	-3.07514600	0.59584600
H	4.33066700	-2.93964400	1.42027200
H	5.87972000	-3.69686900	0.96379300
H	4.52390900	-3.63199800	-0.19409700
C	6.84290700	0.63189600	-2.50762800
H	6.30267900	0.30426300	-3.40706600
H	7.92054900	0.46554800	-2.67483600
H	6.67515700	1.71360700	-2.40764800
C	5.70288000	-0.55570900	2.38361500
H	5.57682100	0.48003000	2.72676200
H	6.59429000	-0.97574200	2.88114900
H	4.82581700	-1.12295300	2.72764100
C	-4.53862200	-2.62036400	-2.94564400
H	-4.77754800	-2.91218300	-1.91540900
H	-4.01812600	-3.47321900	-3.40893200
H	-5.48253600	-2.46617700	-3.49280700
C	-1.22610500	-3.17363300	4.08030600
H	-2.18517400	-3.27994200	3.55759400
H	-1.42579300	-2.58621000	4.98930800
H	-0.87606900	-4.17268300	4.38724200
C	-1.40438300	-5.29706600	-2.18127000
H	-0.48415000	-5.78539100	-2.53751000
H	-2.08694800	-5.22060900	-3.04221700
H	-1.86802600	-5.96709600	-1.44138700

VI.3.2 compound 1, As analogue

0 1

Ga	-2.82335600	-0.65302700	0.77103200
Fe	4.30207700	-0.32049700	-0.32777800
Cl	-3.69572000	-0.17950400	2.79247700
As	1.28584800	-0.54374900	0.92878800
Si	-0.75330800	0.59542800	0.55784300
As	2.26541700	-1.50899300	-1.03180800
As	2.97225100	1.13089400	1.16985800
As	3.62798800	1.95168100	-0.95575400
As	3.12574400	0.20046600	-2.43062500
N	-0.75038400	2.05044300	-0.55878500
N	-2.61006600	-2.60908700	0.87658100
N	-4.44308400	-0.69309900	-0.33657300
N	-0.72859200	2.13233100	1.59047400
C	6.25970400	-0.36337300	-0.92611300

C	-0.90836300	2.29626800	-2.00033200
C	-5.45997400	1.49148000	-0.85629600
C	5.25217500	-2.05292800	0.30006900
C	6.17602200	0.06681400	0.43855500
C	-4.64799500	0.03936300	-2.66792800
C	5.69208700	-1.67668200	-1.01182600
C	-3.72615600	-3.32768700	0.95393500
C	-5.33916400	-1.62744100	0.02310900
C	-0.85214400	0.91735100	-2.65044900
H	0.10890200	0.42204200	-2.43879500
H	-0.95543900	1.00591700	-3.74060000
H	-1.67712400	0.28361100	-2.28819700
C	-1.34647900	-3.28770300	0.91434700
C	-5.01151500	-2.79710100	0.71640700
H	-5.84484800	-3.45748100	0.95072700
C	-0.32273100	1.20314500	3.77447700
H	-0.27884000	1.40778000	4.85399100
H	0.63760200	0.76099500	3.47160700
H	-1.13010300	0.47551000	3.60700400
C	-0.65729400	2.88037500	0.48463900
C	5.54991200	-0.97930400	1.19271900
C	-5.63304600	1.82587900	0.61126800
H	-5.45105800	0.91481000	1.19819100
C	-1.52571200	5.22828800	0.55261700
H	-2.53477600	4.83928200	0.70145900
C	-0.88500700	-3.93843100	-0.24867500
C	-4.84404700	0.29827600	-1.28878700
C	-0.59723300	2.49830100	3.01508600
C	-0.45194700	4.34473100	0.41471400
C	-0.59713500	-3.31053900	2.11394000
C	-5.10405500	0.98844600	-3.58791100
H	-4.96681300	0.81200000	-4.65516700
C	-5.72440600	2.16236600	-3.17426700
H	-6.06961700	2.88879800	-3.91380100
C	-1.91592600	3.10139200	3.50466900
H	-1.83400800	3.35323700	4.57286600
H	-2.73757500	2.38289900	3.37784700
H	-2.15540700	4.02540000	2.95870500
C	-6.78178700	-1.42751100	-0.34841900
H	-7.17669000	-0.54444600	0.17675600
H	-7.38519800	-2.30094300	-0.07553000
H	-6.89927700	-1.23027400	-1.42300400
C	0.21082200	3.16890600	-2.56789500
H	0.13938000	4.20645100	-2.21642300
H	0.13208600	3.18226000	-3.66520100
H	1.19680000	2.76457800	-2.29935000
C	-5.88885600	2.41123300	-1.81967800
H	-6.36226300	3.34105700	-1.49616000
C	-2.26891000	2.94648600	-2.25436400
H	-3.08404100	2.32815000	-1.85457400
H	-2.43463700	3.06728300	-3.33506100
H	-2.32225300	3.94290200	-1.79122900
C	-4.57806300	2.84547100	1.03979600
H	-3.55956300	2.46436300	0.87003100
H	-4.66853800	3.07501200	2.11157300
H	-4.69017100	3.78362500	0.47118200
C	5.62299600	-2.53512800	-2.23056600
H	4.70840700	-3.14699100	-2.23660400
H	6.48640500	-3.22043600	-2.28240200
H	5.61446000	-1.92869500	-3.14704100
C	0.59323300	-4.04189400	2.12779500
H	1.19004600	-4.07628400	3.03964200
C	-3.96346200	-1.22855200	-3.15734600
H	-3.15196500	-1.44381600	-2.44234700
C	0.84452800	4.83393300	0.21426400
H	1.67562100	4.13092600	0.10954800
C	-7.03815500	2.31901900	0.95384900
H	-7.25694400	3.29986000	0.50283900
H	-7.14253500	2.43073100	2.04390700
H	-7.81326500	1.61689700	0.60972500
C	0.32532100	-4.63562200	-0.18449700
H	0.70873000	-5.12573200	-1.08214000
C	0.55803800	3.47269400	3.25623100
H	0.34373300	4.47711400	2.86849100
H	1.48671600	3.10129500	2.79648400
H	0.72256100	3.56370900	4.34021900
C	-3.33987100	-1.06905700	-4.54178400
H	-4.10918700	-0.99639900	-5.32649100

H	-2.72382500	-1.94694900	-4.78261200
H	-2.69897300	-0.17929500	-4.60795500
C	1.05191700	-4.70424300	0.99500800
H	1.99471900	-5.25472300	1.02747100
C	-1.05196500	-2.55248500	3.34890700
H	-1.44120200	-1.58463800	2.99423800
C	-1.62421600	-3.87417300	-1.57287800
H	-2.59723400	-3.39006600	-1.39810200
C	6.69747800	1.34726500	1.00003500
H	6.75740600	2.12747100	0.22839100
H	7.70583000	1.21148700	1.42719100
H	6.04345700	1.72794100	1.79892000
C	-3.64985500	-4.79941000	1.24470600
H	-3.48042700	-5.34880900	0.30587800
H	-4.59504500	-5.15411200	1.67514400
H	-2.81872700	-5.04591000	1.91711200
C	-0.01115700	7.09261700	0.29802000
H	0.16229300	8.17055200	0.25353500
C	-0.84848100	-3.01251400	-2.56866700
H	-0.69782300	-1.99127900	-2.19104000
H	-1.37734400	-2.95427200	-3.53126700
H	0.15450000	-3.42446100	-2.75599400
C	-1.30199000	6.60293800	0.49149500
H	-2.14199600	7.29333300	0.59662300
C	0.08274600	-2.24292300	4.31953300
H	0.43953000	-3.14904500	4.83522200
H	-0.27220700	-1.54885500	5.09589900
H	0.93606100	-1.77567600	3.80564400
C	1.05927700	6.20757300	0.15980900
H	2.07199900	6.58742600	0.00738300
C	4.68058100	-3.37299000	0.70003400
H	3.92472700	-3.25896600	1.49022200
H	5.47373800	-4.04000400	1.08115900
H	4.19242500	-3.87415100	-0.14692600
C	6.88721600	0.39391900	-2.04796700
H	6.40679700	0.15455000	-3.00724000
H	7.96107300	0.15553300	-2.13426800
H	6.79012400	1.47867600	-1.89935600
C	5.33662600	-1.00218400	2.67016800
H	5.26368100	0.01273700	3.08364600
H	6.17332100	-1.51659900	3.17461600
H	4.40883000	-1.53037100	2.93341500
C	-4.89148500	-2.44796600	-3.16336300
H	-5.21941300	-2.73714400	-2.15710200
H	-4.36747500	-3.31624100	-3.59300300
H	-5.78447100	-2.25654600	-3.77986500
C	-2.20321900	-3.23817800	4.08741300
H	-3.11553400	-3.29038300	3.48004800
H	-2.45996100	-2.66795200	4.99303000
H	-1.92074500	-4.25867800	4.39331600
C	-1.90067400	-5.25832800	-2.16163000
H	-0.96887800	-5.76743400	-2.45295600
H	-2.52275300	-5.17225600	-3.06644200
H	-2.42572200	-5.91457700	-1.45119800

VI.3.3 compound 2, P

0 1

Ga	-0.09266300	-2.05613900	0.64454900
Fe	-2.04969800	3.04536900	-0.70467200
Cl	0.78665300	-1.93575400	2.69494100
P	-0.09919200	-0.30480400	-0.85488600
P	0.21282500	3.35381800	-0.70815400
P	-2.05883500	0.75422300	-0.55971800
Si	1.12216000	1.39880200	-0.27175100
P	-2.27322300	1.62257200	-2.52358000
P	-0.75137000	3.16079800	-2.64531900
N	-1.77295000	-3.02788800	0.92486000
N	2.16146900	1.62684900	1.24174300
N	0.89107400	-3.56019800	-0.15027000
N	2.90441600	1.43834600	-0.76481200
C	-2.58394800	5.03809500	-0.47236800
C	-1.69799500	-4.33353900	1.19351200
C	0.59713900	-4.79867300	0.24300600
C	-3.61162700	4.31392300	-1.15087000
C	-4.06014000	3.26285200	-0.28432700
C	-0.55578200	-5.12431400	0.97504900
H	-0.64184300	-6.16582800	1.27976000
C	3.25043400	1.77543200	0.47696000

C	-3.30588100	3.34027200	0.93219100
C	-3.05333200	-2.38164700	0.99384800
C	-3.24302400	-2.66814300	-1.54201800
H	-2.17622000	-2.38509500	-1.53619500
C	1.67444300	-3.28549900	-2.45162900
C	-3.80241400	-2.23694000	-0.19629400
C	-3.54034700	-1.90506400	2.22651100
C	0.26435100	-3.44959400	-2.98670700
H	-0.42163700	-3.34689600	-2.13313500
C	-4.80805200	-1.31295500	2.25523000
H	-5.19699200	-0.93059600	3.20220100
C	-2.39780700	4.43572900	0.81589000
C	1.96327400	-3.34013200	-1.06958800
C	1.84857100	2.07901300	2.60579500
C	4.55631600	2.32975300	0.91001500
C	3.28410900	-3.18830100	-0.59703900
C	3.63317000	1.41201100	-2.04005100
C	-1.50667500	4.96473700	1.88907700
H	-1.22832900	4.18634400	2.61133800
H	-2.01750000	5.76872600	2.44633700
H	-0.57990800	5.38361700	1.47218300
C	1.52760300	-5.92044500	-0.12137500
H	1.74281800	-5.92133100	-1.19921500
H	1.11005800	-6.89297300	0.16373900
H	2.49385700	-5.78507700	0.38705900
C	-5.57544100	-1.20275900	1.10454800
H	-6.56562900	-0.74237000	1.14615300
C	3.61780900	-3.17906400	0.88254100
H	2.71288400	-3.46064200	1.43999900
C	2.77438800	0.58731500	-2.99971500
H	1.79062200	1.05857800	-3.15543500
H	2.61242700	-0.42913100	-2.61370100
H	3.27339200	0.51225400	-3.97691100
C	6.05482100	4.22302000	1.03325500
H	6.26758500	5.27360900	0.82277900
C	-3.88366500	-1.93988900	-2.71905300
H	-4.92699500	-2.25658700	-2.87891500
H	-3.33359200	-2.16879400	-3.64391500
H	-3.86045700	-0.84975700	-2.57874700
C	-4.15394000	4.62296600	-2.50482100
H	-3.38417500	5.07338800	-3.14744900
H	-5.00111200	5.32607500	-2.43779700
H	-4.50181700	3.71084700	-3.00992900
C	4.83797600	3.67372400	0.63716500
H	4.09108500	4.28851900	0.12986600
C	-2.91405600	-5.03423300	1.73110500
H	-3.16854800	-4.63850700	2.72472900
H	-2.74571200	-6.11444700	1.81006200
H	-3.78838500	-4.84941300	1.09095300
C	0.37227700	1.74061600	2.80702000
H	0.02936500	2.09294400	3.79088800
H	0.22913300	0.65326400	2.76450300
H	-0.25623200	2.21179500	2.03226500
C	-2.72111200	-1.95527500	3.50177200
H	-1.81869200	-2.55263100	3.30699200
C	-3.51266700	2.47778600	2.13181800
H	-3.76743100	1.44719500	1.84546900
H	-4.33361600	2.87010500	2.75671500
H	-2.61041400	2.43011100	2.75628700
C	-1.85463600	6.23661100	-0.98021100
H	-0.79822900	6.21859700	-0.67227200
H	-2.30396300	7.16807700	-0.59598000
H	-1.87222400	6.27753700	-2.07806600
C	2.06138000	3.58892800	2.74287500
H	1.51235800	4.12543800	1.95418000
H	3.12517300	3.85743000	2.67823500
H	1.68792900	3.93051000	3.72004500
C	-5.06943600	-1.65675700	-0.10893700
H	-5.66613100	-1.53125700	-1.01285800
C	-5.16046800	2.29273900	-0.55802200
H	-5.30872500	2.15189400	-1.63799200
H	-6.11215400	2.64586500	-0.12531800
H	-4.93796400	1.30568600	-0.12597700
C	2.68585400	1.31084100	3.62926000
H	2.36031000	1.57852300	4.64585600
H	3.75374600	1.55648900	3.54460700
H	2.54846400	0.22784900	3.49624600
C	-3.32496500	-4.18172700	-1.75894900

H	-2.70602500	-4.74805100	-1.05018900
H	-2.97559500	-4.43935100	-2.77077800
H	-4.36580900	-4.53189800	-1.66665200
C	5.49391700	1.54492500	1.58716900
H	5.27002900	0.50008300	1.80324700
C	-2.25236400	-0.54685600	3.86663900
H	-1.76988500	-0.06172400	3.00810700
H	-1.52664500	-0.57599300	4.69386100
H	-3.10172800	0.08641100	4.17012500
C	6.71253100	2.09853800	1.97386500
H	7.44479300	1.47932300	2.49699000
C	4.30912000	-3.01455000	-1.53294200
H	5.33823600	-2.90145000	-1.18239600
C	2.73610200	-3.11696400	-3.34578400
H	2.52909700	-3.08323800	-4.41784600
C	6.99532700	3.43558200	1.69717700
H	7.95106000	3.86729200	2.00367800
C	3.98677200	-1.76395900	1.32408600
H	4.89772200	-1.42465200	0.80431000
H	4.17049200	-1.72816900	2.40940400
H	3.17712000	-1.05379900	1.10352400
C	-0.10264800	-2.36937300	-4.00235200
H	0.50257000	-2.44294200	-4.91982200
H	0.02844900	-1.36471600	-3.57379600
H	-1.15699900	-2.47214600	-4.30047400
C	0.06217800	-4.84978600	-3.57092100
H	-0.96123500	-4.96354600	-3.96075300
H	0.21983300	-5.63525800	-2.81675300
H	0.76107000	-5.03532500	-4.40254200
C	4.04505400	-2.98795300	-2.89693800
H	4.86061700	-2.85552200	-3.61201700
C	3.78445400	2.83356300	-2.59069400
H	4.19266600	2.79770200	-3.61204400
H	4.47196000	3.43073200	-1.97553700
H	2.80667100	3.33804500	-2.62191400
C	4.99640400	0.74181200	-1.87091700
H	4.87783000	-0.26563000	-1.44592500
H	5.66776600	1.32632000	-1.22679300
H	5.47744600	0.64199300	-2.85531900
C	-3.46659400	-2.59847400	4.67117700
H	-4.34270600	-2.00358200	4.97414900
H	-2.80456700	-2.67617400	5.54765800
H	-3.82587900	-3.61083500	4.42988500
C	4.72645600	-4.16642100	1.24780000
H	4.49562500	-5.18898500	0.91206000
H	4.86872900	-4.19323800	2.33929100
H	5.69162200	-3.88415100	0.79780700

VI.3.4 compound 2, As analogue

0 1

Ga	2.13330700	-1.12598400	0.66273700
Fe	-3.64857200	-0.16696700	-0.18456700
Cl	2.54486300	-0.31443900	2.70566000
As	0.41650200	-0.36182400	-0.83797500
As	-2.63294700	2.00184600	-0.44759300
As	-1.61282300	-1.47726100	0.04203800
Si	-0.36517000	1.67810500	-0.15352500
As	-2.74927800	-1.48795500	-2.03732900
As	-3.21338400	0.80692800	-2.42445700
N	2.18171900	-3.06866000	0.97318900
N	0.09717600	2.67688800	1.34354900
N	3.89656200	-1.02806100	-0.21612000
N	0.52458600	3.21628100	-0.69141800
C	-5.57014900	0.53359700	0.17800200
C	3.35874700	-3.65073500	1.19619800
C	4.84308500	-1.89860900	0.13915600
C	-5.60942900	-0.78090100	-0.38014800
C	-4.90702500	-1.66224400	0.50715400
C	4.59647300	-3.05502600	0.89639300
H	5.47584900	-3.63916400	1.16302400
C	0.50573300	3.68037500	0.55743600
C	-4.43168400	-0.88625000	1.61348900
C	0.97573200	-3.84065000	1.03096400
C	1.28113800	-4.30393400	-1.46423100
H	1.94218400	-3.43016900	-1.36151800
C	3.93157600	-0.11928100	-2.49076300
C	0.50757100	-4.42973900	-0.16453800
C	0.26796000	-3.98247800	2.24029100

C	3.25134700	-1.36672200	-3.02354700
H	2.62501200	-1.75662100	-2.20762800
C	-0.91846100	-4.72316000	2.22905900
H	-1.48466000	-4.83552800	3.15734400
C	-4.84153100	0.46616500	1.41152400
C	4.21858100	0.03648400	-1.11472700
C	-0.34322100	2.65209600	2.74704400
C	0.74713000	5.08292000	0.97884400
C	4.81907200	1.21748700	-0.62896600
C	0.87417900	3.82872200	-1.97948500
C	-4.68616300	1.58102600	2.39095700
H	-3.77874300	1.46690400	2.99832500
H	-5.54779700	1.60502300	3.08041000
H	-4.63286400	2.55766700	1.88983500
C	6.26182500	-1.65291800	-0.29358600
H	6.31551000	-1.41615900	-1.36553200
H	6.89628300	-2.52176300	-0.08332500
H	6.67062800	-0.78115600	0.23834200
C	-1.39037300	-5.31300000	1.06353500
H	-2.32117100	-5.88538100	1.07541700
C	5.03949700	1.46686500	0.85080500
H	4.82573400	0.53561600	1.39477700
C	1.04439500	2.67282100	-2.96608100
H	0.10976400	2.09765100	-3.06660600
H	1.84177400	1.98962100	-2.63983500
H	1.31027800	3.06433900	-3.95884200
C	-0.07946100	7.34889700	1.15649200
H	-0.87777000	8.07732900	0.99702300
C	0.38333500	-4.05845200	-2.67277000
H	-0.26175200	-4.92386300	-2.89084700
H	0.99732200	-3.88452400	-3.56937900
H	-0.26508500	-3.18312600	-2.52041400
C	-6.32278700	-1.17848400	-1.62789800
H	-6.32542000	-0.36072600	-2.36258200
H	-7.37017200	-1.44803400	-1.41021400
H	-5.83891900	-2.04129800	-2.10719400
C	-0.26875200	6.02402200	0.77146700
H	-1.21344100	5.70709600	0.32368500
C	3.39099600	-5.02396300	1.80601000
H	3.17765000	-4.93790600	2.88322300
H	4.37389900	-5.49387600	1.68296600
H	2.61579000	-5.67654900	1.38347800
C	-0.82773900	1.22392400	2.98994100
H	-1.21846900	1.12183600	4.01305700
H	0.00722300	0.52084200	2.87322800
H	-1.62772200	0.94522500	2.28303500
C	0.73032200	-3.33919300	3.53260000
H	1.69915100	-2.85483500	3.34186200
C	-3.74663600	-1.43176100	2.82184500
H	-3.11600000	-2.29645700	2.57113800
H	-4.48767900	-1.75905000	3.57169500
H	-3.09851500	-0.68246800	3.29564200
C	-6.23014400	1.75113700	-0.37800200
H	-5.64455200	2.65784200	-0.16517300
H	-7.23496000	1.88982200	0.05624600
H	-6.33819600	1.68284600	-1.46951500
C	-1.48952800	3.63975700	2.98122700
H	-2.30071600	3.46812000	2.25796400
H	-1.15361700	4.68238300	2.89350400
H	-1.89612100	3.50322900	3.99467700
C	-0.67778200	-5.16654400	-0.12111700
H	-1.05944900	-5.62323200	-1.03629400
C	-4.77225600	-3.14354200	0.37235100
H	-4.89472400	-3.46403000	-0.67153700
H	-5.53476500	-3.66102500	0.97939200
H	-3.78308100	-3.49239800	0.70709700
C	0.82999700	2.95009200	3.68222900
H	0.50965200	2.81434100	4.72627400
H	1.18213200	3.98527600	3.57321000
H	1.66062500	2.25787300	3.48372300
C	2.17981100	-5.52259900	-1.69053400
H	2.91200500	-5.65124100	-0.88058700
H	2.74109100	-5.42107200	-2.63287000
H	1.57867100	-6.44429100	-1.75124500
C	1.94613600	5.47568100	1.57998400
H	2.73437600	4.74140000	1.74505700
C	-0.24208700	-2.24001100	3.95787900
H	-0.44449900	-1.55278400	3.12580700

H	0.17005500	-1.65405300	4.79372300
H	-1.20738800	-2.66446400	4.27760400
C	2.13237300	6.80414000	1.95633300
H	3.07416400	7.10649000	2.41995400
C	5.17719000	2.20951100	-1.54818600
H	5.64947100	3.12650600	-1.18665300
C	4.31292100	0.90089900	-3.36754300
H	4.10675400	0.79407200	-4.43382600
C	1.12253300	7.74194300	1.74472300
H	1.27090500	8.78256600	2.04281600
C	4.03735800	2.50948100	1.34498400
H	4.20975100	3.47286400	0.83762400
H	4.13420600	2.66423200	2.43093600
H	3.00278300	2.19335400	1.14766000
C	2.31939000	-1.07772300	-4.19653300
H	2.87040100	-0.78302900	-5.10373600
H	1.60190700	-0.28198300	-3.94719500
H	1.74027100	-1.97750000	-4.44855900
C	4.26389000	-2.45766100	-3.37765700
H	3.74809200	-3.34286600	-3.78194300
H	4.83851400	-2.78534000	-2.49944900
H	4.97567000	-2.10284600	-4.14053900
C	4.94158800	2.05241200	-2.90771900
H	5.23276000	2.83660600	-3.61076900
C	-0.25946400	4.73987100	-2.46059600
H	-0.05932000	5.07554500	-3.48938300
H	-0.35085600	5.63394400	-1.82846100
H	-1.21746100	4.19782500	-2.44886300
C	2.18925100	4.60084000	-1.87075700
H	2.98718800	3.94807200	-1.48697500
H	2.09910500	5.47959900	-1.21748900
H	2.48870500	4.95361000	-2.86896100
C	0.92349800	-4.35816400	4.65633900
H	-0.02974200	-4.83039000	4.94267000
H	1.32981200	-3.86630500	5.55404600
H	1.61425200	-5.16535500	4.36864800
C	6.46912100	1.89453100	1.18270200
H	7.21459300	1.17909600	0.80334200
H	6.59954900	1.97125200	2.27319500
H	6.71304200	2.87949500	0.75385200

VI.3.5 compound 3, P

0 1

Ga	2.68473800	-0.15364700	-0.39192200
Fe	-1.97196900	2.27685200	-0.94416000
Cl	3.28580700	1.02847200	-2.16440300
P	-0.66423200	-1.03283000	-1.01446100
P	-1.03617800	0.72209400	-2.51463700
P	0.14727800	2.37282500	-1.88674400
P	0.01731200	2.08240400	0.25351400
P	0.56323500	-0.05867000	0.52747200
Si	-2.35232400	0.24113500	-0.24772800
N	3.31165200	-1.96747300	-0.77740900
N	4.06882000	0.28484400	0.92298600
N	-3.05031500	-0.36237900	1.40414600
N	-3.87695300	-0.85859400	-0.53361600
C	-2.79848100	3.85374500	0.16006600
C	-2.08434900	4.34937300	-0.97074300
C	-2.68504600	3.79820000	-2.15570300
C	-3.76284100	2.96206700	-1.75187500
C	-3.82182000	2.97473400	-0.31565400
C	-2.55748400	4.29872300	1.56498800
H	-2.74656300	5.38103900	1.65708800
H	-1.51824000	4.11221800	1.87658700
H	-3.22339300	3.79093300	2.27518600
C	-0.99014800	5.36247000	-0.90190700
H	-1.41079200	6.37188800	-0.75428400
H	-0.38878900	5.37324700	-1.82063800
H	-0.30772800	5.15579800	-0.06388600
C	-2.30758800	4.10143700	-3.56683500
H	-2.94984300	4.89677400	-3.98122600
H	-2.41181600	3.21248400	-4.20611300
H	-1.26219600	4.43062900	-3.63899800
C	-4.74264500	2.31262600	-2.66723300
H	-5.54430600	3.02008200	-2.94062200
H	-5.21661000	1.44082900	-2.19813900
H	-4.26487400	1.97840100	-3.59875400
C	-4.90693700	2.36283700	0.50855200

H	-5.75726300	3.05857000	0.60792100
H	-4.55549200	2.11453400	1.51820400
H	-5.28216300	1.43699800	0.04975200
C	-2.76460200	-0.22271300	2.84432200
C	-1.98150000	-1.44682100	3.32666600
H	-1.65052000	-1.29937800	4.36593400
H	-1.09192200	-1.59175100	2.69825400
H	-2.59410600	-2.35813400	3.29506800
C	-4.03690500	-0.04300100	3.67986900
H	-3.74990200	0.21564800	4.70973700
H	-4.64851800	-0.95248600	3.72751000
H	-4.65990000	0.77497400	3.28784200
C	-1.89159800	1.01615400	3.02283600
H	-1.69964800	1.18642200	4.09211700
H	-2.37413900	1.90731400	2.60580200
H	-0.92095200	0.89180300	2.52358300
C	-3.98839200	-1.07012800	0.77952100
C	-5.00371300	-1.92920300	1.44361200
C	-4.67269200	-3.20227000	1.91767800
H	-3.66493900	-3.59263600	1.76165000
C	-5.63063500	-3.97405200	2.57191000
H	-5.36673000	-4.96970200	2.93576900
C	-6.91993600	-3.47772400	2.76136200
H	-7.66823200	-4.08255500	3.27897100
C	-7.25367700	-2.20915500	2.28690600
H	-8.26230600	-1.81603800	2.43336600
C	-6.30091000	-1.43788300	1.62659400
H	-6.55507100	-0.43983000	1.26280200
C	-4.42281600	-1.68381300	-1.63234400
C	-3.78361200	-1.21473000	-2.93645600
H	-4.25702800	-1.73023200	-3.78481600
H	-2.71010400	-1.44962200	-2.96217100
H	-3.89573100	-0.13426000	-3.08064100
C	-4.05507600	-3.16087500	-1.44055300
H	-4.32291600	-3.72797400	-2.34494700
H	-4.58826100	-3.61622200	-0.59575400
H	-2.97010700	-3.26233600	-1.28193700
C	-5.94255400	-1.51955600	-1.73373300
H	-6.31702400	-2.06631600	-2.61213800
H	-6.21514200	-0.46017700	-1.85237400
H	-6.45909000	-1.91618400	-0.84999800
C	2.41507900	-2.93935600	-1.32642400
C	1.66031600	-3.73820400	-0.43605100
C	0.79964000	-4.69806300	-0.97287500
H	0.21239000	-5.32892400	-0.30401200
C	0.65689200	-4.85134000	-2.34763100
H	-0.02659600	-5.60466100	-2.74728800
C	1.36548100	-4.02488600	-3.20707300
H	1.22502300	-4.12227800	-4.28638900
C	2.25030700	-3.05507400	-2.72221900
C	1.74909500	-3.53970700	1.06699400
H	1.88397600	-2.45821900	1.23091400
C	0.46309900	-3.92826200	1.78997600
H	0.50471700	-3.59932500	2.83859600
H	0.30509300	-5.01876500	1.79798100
H	-0.41106300	-3.45401300	1.31844900
C	2.95457300	-4.24862300	1.68643700
H	2.96730800	-4.10285800	2.77852000
H	3.90586300	-3.86196000	1.29552800
H	2.91645000	-5.33241400	1.49010400
C	2.93852500	-2.13410600	-3.71122700
H	3.64015700	-1.49540300	-3.15523600
C	1.91202400	-1.20655100	-4.36562600
H	2.41389600	-0.46655600	-5.00746100
H	1.33338900	-0.65039800	-3.61484500
H	1.20096300	-1.77664100	-4.98547500
C	3.73270300	-2.89545700	-4.77377700
H	4.27621500	-2.18918100	-5.42038300
H	3.07472400	-3.49424100	-5.42353100
H	4.46963500	-3.58368800	-4.33121900
C	5.14257700	-3.51602700	-1.23149100
H	6.18439300	-3.68725300	-0.93631800
H	5.08561100	-3.47815400	-2.32928100
H	4.53010200	-4.37390400	-0.91887900
C	4.61199300	-2.23569200	-0.65020000
C	5.52900900	-1.39783400	0.00895900
H	6.56668600	-1.72887300	-0.01198600
C	5.26772300	-0.27506000	0.81834100

C	6.42718000	0.30925600	1.57545100
H	7.15692300	-0.46331000	1.84929400
H	6.10125700	0.84592700	2.47560300
H	6.93530000	1.03864900	0.92372800
C	3.74411700	1.25805000	1.91807300
C	3.91603900	2.63450200	1.66847800
C	3.49802700	3.53980200	2.65027200
H	3.61953900	4.61073800	2.46956100
C	2.92682900	3.10667500	3.83872800
H	2.60192300	3.83256400	4.58825600
C	2.76542200	1.74461500	4.07093600
H	2.31591300	1.40995000	5.00803000
C	3.16382000	0.79914700	3.12358900
C	4.53504100	3.16412400	0.38958500
H	4.77553000	2.30326400	-0.25132900
C	3.54966000	4.03592500	-0.38904600
H	3.98396000	4.33452900	-1.35551400
H	3.29749700	4.95282800	0.16859700
H	2.61613600	3.49507400	-0.59553400
C	5.83324300	3.92405900	0.67129600
H	6.31080000	4.23144700	-0.27237100
H	6.55366900	3.31281100	1.23573200
H	5.64547900	4.83690300	1.25940400
C	3.01968800	-0.68429600	3.40864200
H	2.98277500	-1.19608300	2.43508400
C	1.73290200	-1.02827400	4.14979200
H	1.62048500	-2.12071800	4.22654300
H	0.85863700	-0.63108200	3.61570900
H	1.72673800	-0.63282700	5.17796300
C	4.24260500	-1.22125700	4.15620800
H	4.14272300	-2.30304600	4.33920300
H	4.35605800	-0.71916600	5.13073700
H	5.17067000	-1.06379000	3.58891900

VI.3.6 compound 3, As analogue (= compound 5)

0 1

As	-0.55074800	0.74071300	0.65220600
Ga	-2.70012600	0.56921000	-0.43472000
As	0.02130400	-1.59615400	1.13727200
As	0.79395700	1.07595600	-1.31655900
As	0.96599100	-1.29399800	-2.23602900
As	-0.36427700	-2.69010000	-0.91829700
Fe	1.94992300	-2.31276400	-0.15396600
Cl	-2.77318400	0.03206200	-2.58057300
Si	2.43968100	-0.16091700	-0.17371200
N	-4.20136200	-0.40432900	0.37479000
N	4.04256400	0.65053500	-0.84337800
N	-3.54765200	2.34825100	-0.34932400
N	3.29608000	0.87709300	1.17558000
C	-5.43389100	0.09413500	0.31831200
C	2.87042300	-3.40572600	1.37412700
C	-3.92286400	-1.70536000	0.89974100
C	-1.24402700	5.06530400	-1.44520000
H	-0.87212100	5.52115300	-2.36625400
C	3.85143800	-2.83871100	0.49856300
C	2.08051500	0.32870800	3.20313200
H	2.45070200	-0.70017200	3.12858100
H	1.09503400	0.37750700	2.72119600
H	1.94215000	0.57835300	4.26508500
C	-2.19771800	4.04396700	-1.52988700
C	-2.66055300	3.46679600	-0.32981500
C	4.65274000	0.96712600	-2.15077700
C	-5.74316500	1.39826000	-0.10888800
H	-6.80598300	1.63689700	-0.14888500
C	-2.16458600	-0.70565900	4.16479400
H	-2.51287500	-1.38122300	4.96286600
H	-1.96465500	0.27101800	4.63070800
H	-1.21556700	-1.09614000	3.76797000
C	-2.72471000	3.31866700	2.22034800
H	-3.04191700	2.28902500	1.99241300
C	-0.76136700	5.50483000	-0.22002300
H	-0.01243700	6.29982200	-0.17888800
C	7.65891700	2.51732000	1.32919500
H	8.62861200	2.09922200	1.60900000
C	4.24633400	1.25869300	0.32371700
C	5.36269400	2.19042500	0.63920700
C	6.61109900	1.66504700	0.99044700
H	6.75196600	0.58214400	1.01385600

C	-6.02117300	-3.61325900	-1.32878300
H	-6.52490400	-3.47880300	-2.29902700
H	-6.71918500	-3.31174800	-0.53454400
H	-5.83191300	-4.69145600	-1.20355600
C	-5.49343300	3.81210300	-0.62467200
H	-4.81723600	4.64046800	-0.37768300
H	-6.43848300	3.93330000	-0.07973200
H	-5.71595800	3.87635500	-1.70201700
C	-4.09730500	-2.85494300	0.09926500
C	-4.86971100	2.47209500	-0.34737300
C	-1.23467400	4.93171600	0.95670800
H	-0.85165600	5.28353800	1.91664800
C	-3.38790200	-1.79352900	2.20722800
C	2.49514000	-4.22829000	-0.75859500
C	2.81111600	-3.28138200	2.86045400
H	3.49176500	-2.50432100	3.23265900
H	3.11118800	-4.23165800	3.33347800
H	1.79587600	-3.04111300	3.21084900
C	-2.18432400	3.90840500	0.92910900
C	4.33237700	1.33216000	3.40440100
H	4.06360400	1.50844800	4.45637700
H	5.03142700	2.12321200	3.10733800
C	-3.96790100	4.07683000	2.69339700
H	-3.72411400	5.12997800	2.90800900
H	-4.36959800	3.62496300	3.61438500
H	-4.76819400	4.06505600	1.94114100
C	-4.71151000	-2.81768400	-1.29049400
H	-4.93038400	-1.76795300	-1.53806200
C	-3.75762700	-3.33376700	-2.36742700
H	-3.46390300	-4.37910900	-2.18040300
H	-2.84820100	-2.72229100	-2.42026200
H	-4.24540800	-3.29211900	-3.35404300
C	-3.03407700	-3.05373300	2.69336100
H	-2.60980200	-3.14485700	3.69394100
C	-6.60329800	-0.75838100	0.73090400
H	-7.07631400	-1.17883100	-0.16990000
H	-7.35804600	-0.15376900	1.25077100
H	-6.29987800	-1.59472700	1.37274400
C	1.98519500	-5.04632500	-1.89786900
H	0.95558700	-5.38575400	-1.72334600
H	2.62050800	-5.93587200	-2.04871100
H	1.98399100	-4.47062400	-2.83520600
C	4.52175200	2.46052000	-2.47774100
H	5.17743500	3.08403400	-1.85667800
H	3.47925900	2.78725700	-2.34213600
H	4.80030100	2.63223300	-3.52849700
C	-1.59720400	3.11130200	-3.80103700
H	-2.01577400	2.76076800	-4.75712900
H	-1.06451000	2.26784200	-3.34195100
H	-0.86405800	3.90353300	-4.02388400
C	-3.20523200	-0.54905300	3.06085500
H	-2.83787300	0.24407600	2.38709100
C	3.62669700	-3.36864100	-0.81720300
C	6.12660900	0.54865000	-2.18528800
H	6.53971400	0.72601700	-3.18968500
H	6.23874400	-0.52186300	-1.95914400
H	6.73196000	1.12119900	-1.47058700
C	2.40072100	2.70548500	2.55676700
H	2.08861300	2.98008200	3.57619300
H	1.50924600	2.70710600	1.91152900
H	3.09822000	3.47600800	2.20152700
C	2.02361900	-4.25158900	0.59937500
C	-1.68960100	3.23882900	3.33802600
H	-0.78572800	2.70939200	3.00304900
H	-2.10772800	2.69280700	4.19789000
H	-1.39733300	4.23624500	3.70368800
C	3.89140100	0.19377800	-3.22338000
H	2.86822800	0.57890700	-3.33971000
H	3.82683600	-0.87377100	-2.98515000
H	4.39978400	0.30435600	-4.19230500
C	-2.71501600	3.62225300	-2.89292700
C	4.50101600	-3.19719300	-2.01188700
H	5.17469500	-4.06420300	-2.12274100
H	5.12929400	-2.30167800	-1.93177200
H	3.91221700	-3.11562700	-2.93680300
C	3.05089100	1.31650500	2.56228000
C	0.93594400	-5.10813000	1.15970500
H	0.23002100	-5.42902900	0.38167100

H	0.35508600	-4.57198800	1.92540000
H	1.36200700	-6.01078000	1.63038800
C	7.46908500	3.89907500	1.31472800
H	8.29133900	4.56736400	1.58120900
C	-4.52990200	-0.05957000	3.65158900
H	-5.26423300	0.19510700	2.87622100
H	-4.36773500	0.84453300	4.26022400
H	-4.97328200	-0.83094200	4.30163100
C	5.17705400	3.57611400	0.62120300
H	4.20860900	3.98804600	0.33046300
C	5.04487500	-2.05076200	0.92965100
H	5.42705300	-1.42514200	0.11252800
H	5.85685700	-2.72539800	1.24985300
H	4.80642000	-1.38590700	1.77060900
C	6.22865400	4.42623400	0.95700700
H	6.07697600	5.50792900	0.93757900
C	-3.71471600	-4.09084000	0.63386100
H	-3.83192500	-4.99074900	0.02508600
C	-3.18910400	-4.19540800	1.91380000
H	-2.89127600	-5.17065500	2.30681700
C	-3.47449200	4.76797400	-3.56810800
H	-2.80049600	5.60663200	-3.80672300
H	-3.92536500	4.42671100	-4.51332400
H	-4.27740300	5.16520000	-2.92972100
H	-3.41270500	2.78473100	-2.74314000
H	4.85512800	0.36498400	3.34754500

VI.3.7 compound 4, P analogue

0 1

P	0.12056200	-0.81268200	1.81734100
P	0.06827000	-1.50230400	-0.80430100
P	-0.46369500	0.48673300	0.07790700
P	2.23425900	-0.59395300	2.19171000
P	2.17879900	-1.41873200	-1.26885700
Ga	-2.77675400	0.26924200	0.30778400
Fe	1.40991200	-2.44589600	0.81129900
Cl	-3.55499900	-1.15563000	1.82570600
Si	2.93195100	0.00159400	0.21842600
N	3.50794700	1.74334300	-0.24044000
N	-3.60783000	1.98592100	0.74336000
N	4.79083100	0.04676300	0.07574700
N	-3.92295300	-0.11467900	-1.25423100
C	0.17084700	-4.04409200	1.13253100
C	1.07029900	-4.33434100	0.05816200
C	-1.31556400	-4.06664500	1.05580700
H	-1.76832200	-3.33148000	1.73497900
H	-1.70364900	-5.06534500	1.31884800
H	-1.66184500	-3.82630100	0.04152200
C	0.95308800	-3.79742100	2.30510300
C	2.40670700	-4.29877800	0.57713300
C	2.33272500	-3.97571800	1.96205400
C	1.85095500	3.31544100	0.51321000
H	1.13592500	2.49341600	0.66366900
H	1.26993100	4.21650400	0.27073600
H	2.38639100	3.48740400	1.45904800
C	4.76388600	1.32058500	-0.31962400
C	2.83997700	2.99657900	-0.60996200
C	-2.82997500	2.99991900	1.38031300
C	-5.60166700	1.45286300	-0.50012000
H	-6.63488800	1.75562900	-0.66875100
C	-2.59003200	2.95602100	2.76894700
C	2.11431200	2.74708600	-1.93511400
H	2.83745900	2.48143600	-2.72189500
H	1.56793800	3.64597400	-2.25470000
H	1.39631500	1.92065300	-1.83399900
C	5.93413800	2.08794900	-0.81144100
C	0.44170400	-3.53197600	3.68184900
H	1.06539800	-2.79075400	4.20463600
H	0.44667300	-4.45746100	4.28307900
H	-0.58549500	-3.14359600	3.66242800
C	3.61317200	-4.69320200	-0.20890100
H	3.65439300	-4.15955200	-1.16975400
H	3.58394300	-5.77377500	-0.42830300
H	4.54639700	-4.49039200	0.33048000
C	0.70013700	-4.72794100	-1.33358300
H	-0.29799200	-4.35810000	-1.60723500
H	0.69871000	-5.82634300	-1.43985900
H	1.41278900	-4.32000000	-2.06629500

C	-4.88370100	2.21747100	0.42545900
C	3.44449000	-3.95164800	2.95925500
H	4.41713300	-4.16459500	2.49842900
H	3.26909800	-4.71883500	3.73120700
H	3.51178000	-2.97753500	3.46658100
C	6.69574500	2.87205300	0.05879800
H	6.42466400	2.92775300	1.11553400
C	-2.45383800	-0.79807000	-3.07683700
C	-2.01574800	0.64433800	-3.26124700
H	-2.02864100	1.11944700	-2.26620500
C	-3.45644500	-1.13715200	-2.13881600
C	-1.21505100	3.93772100	-1.69667900
H	-1.40383600	3.90918800	-2.78132200
H	-0.70071500	3.01075000	-1.40764500
H	-0.52975300	4.77832600	-1.50144900
C	-5.11675300	0.45075600	-1.36758000
C	-2.27452200	4.02144500	0.57581000
C	-1.90184300	-1.81625900	-3.85567300
H	-1.11590600	-1.57893200	-4.57356800
C	-3.91651100	-2.46662600	-2.00483700
C	-6.04621100	0.04729800	-2.47957600
H	-5.54685600	-0.57020000	-3.23560000
H	-6.46693700	0.94116800	-2.96081900
H	-6.88731300	-0.52711400	-2.06272500
C	6.27624100	2.00826800	-2.16445300
H	5.67203100	1.39837000	-2.84054200
C	-5.06438800	-2.87180000	-1.09263400
H	-5.38467600	-1.98268500	-0.52900700
C	-0.59987800	0.79190500	-3.80667000
H	0.12443600	0.21116300	-3.21558900
H	-0.29563900	1.84852200	-3.77733300
H	-0.52888400	0.46461000	-4.85637200
C	7.79707300	3.57256300	-0.42452600
H	8.39242300	4.18421100	0.25726900
C	3.79259400	4.18176500	-0.76483500
H	4.37428000	4.35858000	0.15103800
H	3.18635300	5.07965800	-0.95546300
H	4.49024200	4.06554900	-1.60461900
C	-3.01457100	1.40685700	-4.13573000
H	-3.07567800	0.95499700	-5.13885800
H	-2.70542800	2.45748800	-4.25449500
H	-4.02469500	1.40373000	-3.70337300
C	5.86859900	-0.94832100	0.11186500
C	-1.46562900	4.98295500	1.18613300
H	-1.02929800	5.77965100	0.57737000
C	-1.75916200	3.93325300	3.32811400
H	-1.55460000	3.90490900	4.40135500
C	-3.22086400	1.90942100	3.66697800
H	-3.86111800	1.27102400	3.04072600
C	-1.19831800	4.93833700	2.55033000
H	-0.55288700	5.69188300	3.00838600
C	-5.57652300	3.39035800	1.05819000
H	-5.49523100	3.32677700	2.15319000
H	-6.63481100	3.43080300	0.77441100
H	-5.09378500	4.33397300	0.76670100
C	-2.52042300	4.09647600	-0.92194800
H	-3.16718800	3.25150100	-1.20113300
C	-3.31825200	-3.44856300	-2.80381600
H	-3.65238400	-4.48484900	-2.70833300
C	8.14056400	3.49362900	-1.77472400
H	9.00568000	4.04453600	-2.15123200
C	7.37929800	2.71239600	-2.64353300
H	7.64444200	2.65037900	-3.70148500
C	-2.16888800	1.00309300	4.30439800
H	-1.55459900	0.49461500	3.54662100
H	-2.65428100	0.22012200	4.90720300
H	-1.49403200	1.57248200	4.96431600
C	5.45398100	-1.95702700	1.17755200
H	5.42726700	-1.48595400	2.17132400
H	6.16135500	-2.79911800	1.20562100
H	4.44694000	-2.34134600	0.96639100
C	-6.25065600	-3.38667100	-1.91698400
H	-6.54274000	-2.69249800	-2.71728700
H	-7.12615500	-3.55287800	-1.26949200
H	-6.00754800	-4.34944300	-2.39423300
C	-4.66259800	-3.92164000	-0.05805600
H	-4.28661900	-4.84025800	-0.53622000
H	-5.53473800	-4.19865500	0.55471300

H	-3.89149400	-3.53374000	0.61586000
C	-2.31835100	-3.13520500	-3.71406800
H	-1.86091200	-3.92153600	-4.31937100
C	-4.10927200	2.55270000	4.73438500
H	-3.52136200	3.16416700	5.43765600
H	-4.62391700	1.77610900	5.32143300
H	-4.87685700	3.20701800	4.29222800
C	7.22225700	-0.35185700	0.50267200
H	7.65807800	0.27502100	-0.28577200
H	7.92344100	-1.17724900	0.69676100
H	7.14000700	0.24603500	1.42263800
C	5.96852800	-1.63201200	-1.25545600
H	4.99626100	-2.05813900	-1.54508200
H	6.71332700	-2.44215800	-1.22761300
H	6.27625500	-0.91212800	-2.02904000
C	-3.24136700	5.38349200	-1.32581700
H	-2.62899500	6.27252500	-1.10548700
H	-4.19952000	5.50324900	-0.79860300
H	-3.45098200	5.38428800	-2.40717900

VI.3.8 compound 4, As

0 1

As	0.02710500	-0.78906000	1.88200000
As	-0.03706500	-1.48905000	-0.87779000
As	-0.67266300	0.70015300	0.04571800
As	2.34319300	-0.42076600	2.22867200
As	2.26183300	-1.26624700	-1.42458100
Ga	-3.03557100	0.24259900	0.23373800
Fe	1.52641600	-2.38194800	0.77591900
Cl	-3.68629300	-1.33971000	1.65900000
Si	2.95336000	0.26261000	0.14022400
N	3.41726700	2.04539600	-0.30753300
N	-4.03408200	1.85054400	0.73236700
N	4.80891600	0.42787400	-0.03310100
N	-4.10876600	-0.14963500	-1.38147100
C	0.40840200	-4.06421600	1.15654700
C	1.26232000	-4.29129200	0.03030200
C	-1.07488500	-4.20936300	1.17130100
H	-1.55771900	-3.48347300	1.84069400
H	-1.36009000	-5.22278700	1.50156300
H	-1.49575900	-4.05372200	0.16976100
C	1.23693700	-3.76767900	2.28434800
C	2.62044800	-4.16115200	0.47274700
C	2.60391700	-3.84593600	1.86129200
C	1.73382500	3.51783500	0.58749000
H	1.08160200	2.65234300	0.77314400
H	1.08524400	4.38512600	0.39443900
H	2.31685800	3.70992500	1.50079300
C	4.69691000	1.70590100	-0.40174000
C	2.66856400	3.27326700	-0.60043000
C	-3.34499700	2.87562700	1.44758700
C	-5.93837000	1.22552200	-0.59947500
H	-6.98933700	1.44689300	-0.78419400
C	-3.19124300	2.80059500	2.84647800
C	1.87556600	3.02534400	-1.88667300
H	2.55988500	2.82144500	-2.72475700
H	1.26605000	3.90478400	-2.14088500
H	1.20573200	2.16104000	-1.77275200
C	5.81322900	2.55839600	-0.88012000
C	0.78853800	-3.56780800	3.69416300
H	1.38625600	-2.79608000	4.20297200
H	0.89500100	-4.50292700	4.27075000
H	-0.26495100	-3.26038300	3.74574500
C	3.81124900	-4.47877300	-0.37017600
H	3.72935500	-4.02703700	-1.36917500
H	3.90055900	-5.57069400	-0.50186500
H	4.74578400	-4.12308200	0.08072400
C	0.84459500	-4.73030600	-1.33475400
H	-0.19663700	-4.45407100	-1.55313700
H	0.93102000	-5.82601900	-1.43400200
H	1.47484900	-4.27519800	-2.11393900
C	-5.31482600	1.99575200	0.38868800
C	3.76999100	-3.77291400	2.79166800
H	4.72728500	-3.83696000	2.25991900
H	3.73118300	-4.61522500	3.50263600
H	3.76816200	-2.84204500	3.37757900
C	6.53962900	3.35377800	0.00999400
H	6.28037500	3.35384300	1.07121000

C	-2.55917200	-0.56730800	-3.22142900
C	-2.24762000	0.91686300	-3.30091400
H	-2.30515300	1.31462800	-2.27414500
C	-3.52907000	-1.06219900	-2.31770400
C	-1.59176700	4.20253500	-1.51159100
H	-1.73001300	4.19492900	-2.60406300
H	-0.90715600	3.38550800	-1.24525400
H	-1.10438000	5.15579900	-1.25086100
C	-5.34587000	0.31381300	-1.49942800
C	-2.77088400	3.93312600	0.70444400
C	-1.91187900	-1.47450700	-4.06260000
H	-1.15210800	-1.11593400	-4.75798000
C	-3.85130000	-2.43677800	-2.27149300
C	-6.21140300	-0.11836500	-2.65186900
H	-5.63932000	-0.63449200	-3.43208800
H	-6.72064900	0.75143400	-3.08939500
H	-6.99020700	-0.80362900	-2.28391200
C	6.14082100	2.55033300	-2.23900700
H	5.56325700	1.93280100	-2.93127500
C	-4.93294800	-3.01395800	-1.37284200
H	-5.33470500	-2.19819700	-0.75319700
C	-0.84373700	1.21699500	-3.81464800
H	-0.08077600	0.64945900	-3.25995600
H	-0.62219900	2.28791200	-3.69853700
H	-0.73893600	0.97930700	-4.88540100
C	7.59071400	4.13644200	-0.45901700
H	8.15787200	4.75708300	0.23852500
C	3.55008700	4.50877300	-0.78092200
H	4.16800900	4.70355600	0.10681800
H	2.88941100	5.37622300	-0.92628900
H	4.20929900	4.44013100	-1.65631200
C	-3.29976000	1.65750200	-4.12980500
H	-3.31765900	1.27858500	-5.16436400
H	-3.07675300	2.73582700	-4.16642900
H	-4.30884300	1.54109500	-3.71076900
C	5.94713600	-0.49881300	-0.04884700
C	-2.05138000	4.91388400	1.39168500
H	-1.60690800	5.74218600	0.83374100
C	-2.45124200	3.80156300	3.48532100
H	-2.31650100	3.75317400	4.56887900
C	-3.79732900	1.67868700	3.66687600
H	-4.36202500	1.02889000	2.98168600
C	-1.88607500	4.85077500	2.77139500
H	-1.31224600	5.62205100	3.29108400
C	-6.13036500	3.04789800	1.08507600
H	-6.24729900	2.76979800	2.14414400
H	-7.12410000	3.15384200	0.63415900
H	-5.62138400	4.02151000	1.07560800
C	-2.93296400	4.03565700	-0.80295500
H	-3.36899800	3.08830600	-1.15419400
C	-3.16408000	-3.30170600	-3.13182700
H	-3.39504800	-4.36964500	-3.10492900
C	7.92003500	4.12787900	-1.81501500
H	8.74590800	4.74280400	-2.18039900
C	7.19423400	3.33549300	-2.70378900
H	7.44792200	3.32862400	-3.76635400
C	-2.71306100	0.81519500	4.31092700
H	-2.02308800	0.40682400	3.55861800
H	-3.16499900	-0.03871400	4.83856400
H	-2.12012300	1.39279000	5.03875600
C	5.60877400	-1.58631700	0.96582500
H	5.56418400	-1.17177900	1.98385700
H	6.37071200	-2.37980800	0.94305600
H	4.62682700	-2.02755100	0.74414900
C	-6.07512500	-3.60801700	-2.20472200
H	-6.46629100	-2.90050700	-2.94924700
H	-6.90748300	-3.91450900	-1.55165500
H	-5.73941500	-4.50371000	-2.75146700
C	-4.38849900	-4.06756400	-0.40994400
H	-3.94970000	-4.92202700	-0.94987400
H	-5.19979900	-4.45591600	0.22545300
H	-3.62710900	-3.63725400	0.24997800
C	-2.20175900	-2.83376000	-4.01500500
H	-1.67201600	-3.52963100	-4.66998800
C	-4.77159000	2.21037400	4.71996500
H	-4.25549400	2.82138600	5.47788000
H	-5.25987400	1.37525900	5.24608000
H	-5.55860600	2.83778300	4.27343900

C	7.26149700	0.16532200	0.36820100
H	7.65408000	0.85143000	-0.39315900
H	8.01510400	-0.62029100	0.52794900
H	7.14209700	0.71775100	1.31218800
C	6.08929700	-1.11107100	-1.44615100
H	5.15714000	-1.61334800	-1.74616900
H	6.90398800	-1.85136000	-1.45928200
H	6.32252000	-0.33521500	-2.19084400
C	-3.89957900	5.15628000	-1.19153600
H	-3.52282500	6.13648800	-0.85704800
H	-4.89515100	5.01229300	-0.74743300
H	-4.02414700	5.19809300	-2.28534000

VI.3.9 compound 7, As/Ge

0 1

As	-0.55074800	0.74071300	0.65220600
Ga	-2.70012600	0.56921000	-0.43472000
As	0.02130400	-1.59615400	1.13727200
As	0.79395700	1.07595600	-1.31655900
As	0.96599100	-1.29399800	-2.23602900
As	-0.36427700	-2.69010000	-0.91829700
Fe	1.94992300	-2.31276400	-0.15396600
Cl	-2.77318400	0.03206200	-2.58057300
Si	2.43968100	-0.16091700	-0.17371200
N	-4.20136200	-0.40432900	0.37479000
N	4.04256400	0.65053500	-0.84337800
N	-3.54765200	2.34825100	-0.34932400
N	3.29608000	0.87709300	1.17558000
C	-5.43389100	0.09413500	0.31831200
C	2.87042300	-3.40572600	1.37412700
C	-3.92286400	-1.70536000	0.89974100
C	-1.24402700	5.06530400	-1.44520000
H	-0.87212100	5.52115300	-2.36625400
C	3.85143800	-2.83871100	0.49856300
C	2.08051500	0.32870800	3.20313200
H	2.45070200	-0.70017200	3.12858100
H	1.09503400	0.37750700	2.72119600
H	1.94215000	0.57835300	4.26508500
C	-2.19771800	4.04396700	-1.52988700
C	-2.66055300	3.46679600	-0.32981500
C	4.65274000	0.96712600	-2.15077700
C	-5.74316500	1.39826000	-0.10888800
H	-6.80598300	1.63689700	-0.14888500
C	-2.16458600	-0.70565900	4.16479400
H	-2.51287500	-1.38122300	4.96286600
H	-1.96465500	0.27101800	4.63070800
H	-1.21556700	-1.09614000	3.76797000
C	-2.72471000	3.31866700	2.22034800
H	-3.04191700	2.28902500	1.99241300
C	-0.76136700	5.50483000	-0.22002300
H	-0.01243700	6.29982200	-0.17888800
C	7.65891700	2.51732000	1.32919500
H	8.62861200	2.09922200	1.60900000
C	4.24633400	1.25869300	0.32371700
C	5.36269400	2.19042500	0.63920700
C	6.61109900	1.66504700	0.99044700
H	6.75196600	0.58214400	1.01385600
C	-6.02117300	-3.61325900	-1.32878300
H	-6.52490400	-3.47880300	-2.29902700
H	-6.71918500	-3.31174800	-0.53454400
H	-5.83191300	-4.69145600	-1.20355600
C	-5.49343300	3.81210300	-0.62467200
H	-4.81723600	4.64046800	-0.37768300
H	-6.43848300	3.93330000	-0.07973200
H	-5.71595800	3.87635500	-1.70201700
C	-4.09730500	-2.85494300	0.09926500
C	-4.86971100	2.47209500	-0.34737300
C	-1.23467400	4.93171600	0.95670800
H	-0.85165600	5.28353800	1.91664800
C	-3.38790200	-1.79352900	2.20722800
C	2.49514000	-4.22829000	-0.75859500
C	2.81111600	-3.28138200	2.86045400
H	3.49176500	-2.50432100	3.23265900
H	3.11118800	-4.23165800	3.33347800
H	1.79587600	-3.04111300	3.21084900
C	-2.18432400	3.90840500	0.92910900
C	4.33237700	1.33216000	3.40440100
H	4.06360400	1.50844800	4.45637700

H	5.03142700	2.12321200	3.10733800
C	-3.96790100	4.07683000	2.69339700
H	-3.72411400	5.12997800	2.90800900
H	-4.36959800	3.62496300	3.61438500
H	-4.76819400	4.06505600	1.94114100
C	-4.71151000	-2.81768400	-1.29049400
H	-4.93038400	-1.76795300	-1.53806200
C	-3.75762700	-3.33376700	-2.36742700
H	-3.46390300	-4.37910900	-2.18040300
H	-2.84820100	-2.72229100	-2.42026200
H	-4.24540800	-3.29211900	-3.35404300
C	-3.03407700	-3.05373300	2.69336100
H	-2.60980200	-3.14485700	3.69394100
C	-6.60329800	-0.75838100	0.73090400
H	-7.07631400	-1.17883100	-0.16990000
H	-7.35804600	-0.15376900	1.25077100
H	-6.29987800	-1.59472700	1.37274400
C	1.98519500	-5.04632500	-1.89786900
H	0.95558700	-5.38575400	-1.72334600
H	2.62050800	-5.93587200	-2.04871100
H	1.98399100	-4.47062400	-2.83520600
C	4.52175200	2.46052000	-2.47774100
H	5.17743500	3.08403400	-1.85667800
H	3.47925900	2.78725700	-2.34213600
H	4.80030100	2.63223300	-3.52849700
C	-1.59720400	3.11130200	-3.80103700
H	-2.01577400	2.76076800	-4.75712900
H	-1.06451000	2.26784200	-3.34195100
H	-0.86405800	3.90353300	-4.02388400
C	-3.20523200	-0.54905300	3.06085500
H	-2.83787300	0.24407600	2.38709100
C	3.62669700	-3.36864100	-0.81720300
C	6.12660900	0.54865000	-2.18528800
H	6.53971400	0.72601700	-3.18968500
H	6.23874400	-0.52186300	-1.95914400
H	6.73196000	1.12119900	-1.47058700
C	2.40072100	2.70548500	2.55676700
H	2.08861300	2.98008200	3.57619300
H	1.50924600	2.70710600	1.91152900
H	3.09822000	3.47600800	2.20152700
C	2.02361900	-4.25158900	0.59937500
C	-1.68960100	3.23882900	3.33802600
H	-0.78572800	2.70939200	3.00304900
H	-2.10772800	2.69280700	4.19789000
H	-1.39733300	4.23624500	3.70368800
C	3.89140100	0.19377800	-3.22338000
H	2.86822800	0.57890700	-3.33971000
H	3.82683600	-0.87377100	-2.98515000
H	4.39978400	0.30435600	-4.19230500
C	-2.71501600	3.62225300	-2.89292700
C	4.50101600	-3.19719300	-2.01188700
H	5.17469500	-4.06420300	-2.12274100
H	5.12929400	-2.30167800	-1.93177200
H	3.91221700	-3.11562700	-2.93680300
C	3.05089100	1.31650500	2.56228000
C	0.93594400	-5.10813000	1.15970500
H	0.23002100	-5.42902900	0.38167100
H	0.35508600	-4.57198800	1.92540000
H	1.36200700	-6.01078000	1.63038800
C	7.46908500	3.89907500	1.31472800
H	8.29133900	4.56736400	1.58120900
C	-4.52990200	-0.05957000	3.65158900
H	-5.26423300	0.19510700	2.87622100
H	-4.36773500	0.84453300	4.26022400
H	-4.97328200	-0.83094200	4.30163100
C	5.17705400	3.57611400	0.62120300
H	4.20860900	3.98804600	0.33046300
C	5.04487500	-2.05076200	0.92965100
H	5.42705300	-1.42514200	0.11252800
H	5.85685700	-2.72539800	1.24985300
H	4.80642000	-1.38590700	1.77060900
C	6.22865400	4.42623400	0.95700700
H	6.07697600	5.50792900	0.93757900
C	-3.71471600	-4.09084000	0.63386100
H	-3.83192500	-4.99074900	0.02508600
C	-3.18910400	-4.19540800	1.91380000
H	-2.89127600	-5.17065500	2.30681700
C	-3.47449200	4.76797400	-3.56810800

H	-2.80049600	5.60663200	-3.80672300
H	-3.92536500	4.42671100	-4.51332400
H	-4.27740300	5.16520000	-2.92972100
H	-3.41270500	2.78473100	-2.74314000
H	4.85512800	0.36498400	3.34754500

VI.4 Optimized structures: Model compounds and transition states

VI.4.1 gallasilylene

0 1

Ga	0.47982900	-0.30574100	-0.05176400
Cl	0.50087300	-1.92843500	1.50767600
Si	-1.51113400	-0.34949000	-1.47296000
N	-2.68326500	-0.76624800	-0.02283800
N	0.99371700	1.30826400	0.97298100
N	2.23254200	-0.49144700	-0.95258700
N	-2.32526100	1.22507500	-0.72662100
C	2.17871300	1.87125200	0.88000500
C	3.23183700	0.33990500	-0.76220400
C	3.24029400	1.46997400	0.06351800
H	4.15521200	2.06008900	0.10039600
C	-3.06602800	0.48934500	0.09220900
H	-3.88242700	0.86080900	0.73310400
H	2.35343000	2.75145800	1.51962900
H	4.16326700	0.12065100	-1.30849900
C	0.03202400	1.80361000	1.92996800
H	-0.90569400	2.08241900	1.42232200
H	-0.20919200	1.01723200	2.66486200
H	0.41572300	2.68348600	2.47251000
C	2.40850300	-1.65541200	-1.78973800
H	2.33352800	-2.57512400	-1.18540300
H	1.61857800	-1.69952400	-2.55819600
H	3.38819200	-1.64701800	-2.29522600
C	-2.53053100	2.60316500	-1.05350900
H	-3.23642100	3.07243600	-0.34787200
H	-1.58172200	3.16198300	-1.00222600
H	-2.93659200	2.72780300	-2.07189700
C	-3.11716600	-1.88999300	0.75193700
H	-3.91261700	-1.59371900	1.45536200
H	-3.51399900	-2.68462100	0.10016500
H	-2.27295900	-2.30470700	1.32693400

VI.4.2 gallagermylene

0 1

Ga	0.66177000	-0.27524500	0.07217600
Cl	0.75882200	-1.70104300	1.81054500
Ge	-1.45445600	-0.48611500	-1.26577000
N	-2.54769500	-0.65001700	0.44424200
N	1.23327300	1.44344400	0.87284100
N	2.37223300	-0.58571600	-0.88101200
N	-2.23671200	1.26494200	-0.53596900
C	2.40761100	1.98780700	0.64132300
C	3.37598500	0.26188200	-0.85302100
C	3.42186200	1.48874000	-0.18197300
H	4.33384500	2.07785700	-0.27081800
C	-2.86877600	0.62285500	0.43125300
H	-3.57948300	1.09549700	1.13299200
H	2.61642700	2.93744900	1.15987400
H	4.27946100	-0.02879200	-1.41286900
C	0.33170000	2.05167400	1.82362900
H	-0.63065700	2.28730800	1.34171600
H	0.12759100	1.35097100	2.65054400
H	0.75378700	2.97836600	2.24631400
C	2.51495600	-1.85267600	-1.55912500
H	2.45935100	-2.68194800	-0.83397500
H	1.69905600	-1.99585500	-2.28769600
H	3.47575200	-1.92001800	-2.09556900
C	-2.49356200	2.60890200	-0.95153500
H	-3.12608700	3.13744900	-0.21672600
H	-1.55331400	3.17626700	-1.05339300
H	-3.01034600	2.64830400	-1.92650200
C	-2.92225300	-1.62053900	1.42738700
H	-3.61088000	-1.18193600	2.17002400
H	-3.42955900	-2.48014300	0.95968600

H	-2.02999400	-1.99520700	1.95600600

VI.4.3 $CpFeP_5$

0 1

Fe	-0.42158700	0.00044500	0.00079500
P	1.11714400	-1.80191800	0.15295600
P	1.11859000	-0.41098600	1.76018400
P	1.11591500	-0.70286900	-1.66632900
P	1.11761600	1.36689600	-1.18348600
P	1.11924600	1.54732500	0.93419000
C	-2.08734600	1.19001100	-0.22122200
C	-2.08708200	-0.83181500	0.87911000
C	-2.08705300	0.15707700	-1.19951000
C	-2.08745200	0.57878900	1.06343000
C	-2.08689100	-1.09243200	-0.51946800
H	-2.05089300	1.09926000	2.01902000
H	-2.05025800	-1.57979500	1.66939100
H	-2.04964000	-2.07515000	-0.98664500
H	-2.05000200	0.29793700	-2.27846900
H	-2.05067000	2.25969700	-0.42075300

VI.4.4 $CpFeAs_5$

0 1

Fe	-0.00000500	0.00109800	-0.88894200
As	-0.39957900	-1.93899900	0.68023000
As	-1.96726200	-0.21984100	0.68151700
As	1.72007800	-0.97972200	0.68124000
As	1.46259000	1.33251900	0.68368100
As	-0.81627100	1.80210600	0.68400700
C	0.36318800	1.15727100	-2.55799300
C	-0.97155200	-0.71776800	-2.56034800
C	1.21037200	0.01460400	-2.55896600
C	-0.98534100	0.70461500	-2.55876400
C	0.38544500	-1.14420500	-2.56047700
H	-1.87182600	1.33584200	-2.53108800
H	-1.84583000	-1.36583900	-2.53404000
H	0.73151600	-2.17600800	-2.53439200
H	2.29859700	0.02490400	-2.53132700
H	0.68965500	2.19538800	-2.52959700

VI.4.5 $Int1^M$ – P/Si

0 1

Ga	-2.48776900	-0.56646600	-0.05792900
Fe	3.13584600	-0.23321300	0.06654600
Cl	-4.51389500	0.32605500	-0.33999000
P	0.63596000	0.84573900	1.73525600
Si	-1.04166100	1.28909200	0.38652300
P	0.98758800	-0.97156100	0.51782200
P	2.49142800	1.80724400	1.00615200
P	2.48312000	1.60655500	-1.15172200
P	1.42370100	-0.23674400	-1.50023400
N	-1.08374500	2.46831500	-1.04725600
N	-2.55539200	-1.88629900	1.35918000
N	-2.17957300	-1.76638300	-1.54341900
N	-2.14832900	2.74883200	0.80384600
C	4.80909100	-0.83779800	-0.93724700
C	4.04965900	-1.85027600	0.98470900
C	5.16640900	-0.01077400	0.16690800
C	4.12544800	-1.97983200	-0.43154100
C	-2.35735300	-3.16427000	1.10891500
C	-2.04506800	-3.06276200	-1.35162400
C	-2.12302600	-3.74977500	-0.13736500
H	-1.98494900	-4.82970300	-0.16470400
C	-1.98098500	3.21105000	-0.41673800
C	4.69083200	-0.63672600	1.35706400
H	-2.52364000	4.05651700	-0.86618800
H	3.70136600	-2.78797900	-1.02513600
H	3.55889600	-2.54596500	1.66306000
H	-2.38003800	-3.83848600	1.97810300
H	-1.85328200	-3.66679700	-2.25084700
H	4.78104900	-0.24325200	2.36780000
H	5.68028400	0.94749800	0.10883600
H	5.00345200	-0.62052700	-1.98657900
C	-2.74404700	-1.42657600	2.71649500
H	-1.90652100	-0.77488900	3.02269900
H	-3.67776100	-0.84674200	2.79862400

H	-2.79581600	-2.27149000	3.42123500
C	-2.03940100	-1.20979200	-2.87082800
H	-2.85835800	-0.50133000	-3.07193000
H	-1.07596200	-0.67796400	-2.96190000
H	-2.06686000	-1.99939200	-3.63810900
C	-3.18420600	3.09334000	1.73556700
H	-3.51970300	4.13000000	1.57647100
H	-4.05081500	2.42078000	1.62099300
H	-2.80104900	3.01139000	2.76276100
C	-0.60672600	2.66236600	-2.38920700
H	-1.26829600	3.36350800	-2.92176700
H	0.42200500	3.05317900	-2.39444700
H	-0.59715100	1.70658800	-2.93107300

VI.4.6 Int2^{M} – P/Si

0 1

Ga	2.09933100	-0.02545800	0.07664700
Fe	-1.83989400	-1.44256700	-0.12138300
Cl	3.56827700	1.58062300	-0.27614900
P	0.00912900	0.95589600	0.44116900
Si	0.33000200	3.23022900	0.97732100
P	-0.90243400	-0.49245600	1.78700700
P	-1.09367200	0.41708200	-1.36111000
P	-3.13379300	0.41228600	-0.64284500
P	-3.00624800	-0.14251200	1.42921700
N	-1.44929800	3.62488100	0.41581600
N	2.28176000	-1.34748600	-1.32481600
N	2.66213000	-1.12402900	1.57114000
N	0.25130700	3.58731700	-0.89008700
C	-3.09358300	-3.03705600	-0.36128800
C	-0.81422700	-3.22797000	-0.06500200
C	-2.46419700	-2.73955500	-1.60320500
C	-2.07810600	-3.34522700	0.58819500
C	2.63544100	-2.58666600	-1.04554900
C	2.94202600	-2.39972900	1.41262400
C	2.92461900	-3.12056700	0.21300800
H	3.19012300	-4.17586600	0.25884700
C	-1.05058900	3.81707600	-0.82638000
C	-1.05690100	-2.85513800	-1.41496700
H	-1.68888800	4.14241400	-1.66315900
H	-2.23774000	-3.59537400	1.63594900
H	0.16409900	-3.38106500	0.38774600
H	2.71447400	-3.27130700	-1.90321000
H	3.22639200	-2.95205800	2.32068300
H	-0.29713800	-2.66210600	-2.16970100
H	-2.96758600	-2.44383100	-2.52209300
H	-4.16416700	-3.00765300	-0.16380500
C	2.08003100	-0.93856100	-2.69943600
H	1.05222300	-0.56284300	-2.83914100
H	2.77757000	-0.12556000	-2.95873100
H	2.24877900	-1.77930500	-3.39066000
C	2.73855200	-0.51012600	2.88065200
H	3.40375400	0.36725100	2.84948000
H	1.73807200	-0.17427800	3.20141500
H	3.12405600	-1.21977600	3.62909000
C	1.05935100	3.51075500	-2.07140600
H	0.73070000	4.24881200	-2.82145600
H	2.10863700	3.70817500	-1.81611800
H	1.00605200	2.50626600	-2.52741900
C	-2.75879700	3.84161000	0.95638200
H	-3.46453800	4.11507900	0.15627200
H	-3.13376500	2.92342000	1.43408700
H	-2.75160300	4.64946600	1.70616900

VI.4.7 Int3^{M} – P/Si

0 1

Ga	2.90676900	-0.18665100	0.04138500
Fe	-1.32130400	0.89519100	0.36378100
Cl	2.49538500	0.49189400	2.10669100
P	-0.33194700	-1.15754100	-0.05648800
P	-2.04525100	-0.54479300	-1.19404300
P	-1.70917800	1.46019900	-1.87906900
P	0.30333700	1.61424400	-1.09204300
P	1.17445000	-0.39871200	-1.50756800
Si	-4.05462600	-1.70539300	-1.44986900
N	4.37467200	0.92002200	-0.61548400
N	3.91341400	-1.85256900	0.21014700

N	-5.06836700	-0.35910600	-0.55320000
N	-4.14466500	-2.02765400	0.42977200
C	-0.65275200	2.12168600	1.89214300
C	-1.83545000	2.65770400	1.30692200
C	-2.87330300	1.69248700	1.44861700
C	-2.33303900	0.56436100	2.13466100
C	-0.95947200	0.82952800	2.39855000
C	-4.92438100	-0.97805200	0.60197000
C	5.56805300	0.41565400	-0.84568600
C	5.97494200	-0.91058600	-0.66387200
H	7.00484500	-1.15725400	-0.91871400
C	5.17685900	-1.93649700	-0.14753700
H	6.32904100	1.11927100	-1.21722900
H	5.65491700	-2.92033200	-0.02127600
H	-5.39197600	-0.67592300	1.55460600
H	-0.24539700	0.16159100	2.87564700
H	-2.86110100	-0.34836900	2.40189700
H	-3.89617800	1.80865300	1.09553300
H	-1.92430300	3.62187100	0.80878500
H	0.32944500	2.58828400	1.92531400
C	-3.65382200	-2.94043100	1.41757500
H	-2.55478100	-2.87497500	1.48828500
H	-4.08071900	-2.70852300	2.40681900
H	-3.91957400	-3.97898800	1.16474100
C	-5.78740200	0.84727800	-0.82904500
H	-6.30112600	1.20991600	0.07601100
H	-5.09866700	1.63601900	-1.17540100
H	-6.54582200	0.68766200	-1.61173700
C	4.13286900	2.33604900	-0.78920800
H	3.25625300	2.50290200	-1.43620900
H	3.91262600	2.80678800	0.18323400
H	5.00605700	2.83826200	-1.23559900
C	3.23275300	-2.99420500	0.77792600
H	2.93382000	-2.78219500	1.81786500
H	2.31298400	-3.21644800	0.21136900
H	3.87527900	-3.88934100	0.77065900

VI.4.8 Int4^{M} – P/Si

0 1

Ga	2.78048300	0.00941600	0.00038800
Fe	-1.82363100	-1.41181700	-0.00072300
Cl	2.74174500	-2.19865600	-0.00030900
Si	-2.49686200	1.35553000	-0.00031600
N	-2.42346000	3.23835100	-0.00005900
N	3.94784100	0.56100300	-1.46283600
N	-4.22403600	2.06420200	0.00041700
N	3.94841400	0.55970100	1.46362100
C	-1.18127000	-3.34137400	-0.00330100
C	-1.98334500	-3.09970000	1.14914900
C	-1.98721700	-3.09766900	-1.15259000
C	-3.28474700	-2.71466600	0.70913700
C	-3.28716300	-2.71330600	-0.70749700
C	-3.73974300	3.29252800	0.00089700
C	5.69815000	1.39796200	0.00041900
H	6.68358800	1.86218100	0.00043200
C	5.12235700	1.11102400	-1.24225600
C	5.12288500	1.10984000	1.24305600
H	5.71546500	1.36703100	2.13486900
H	5.71453100	1.36912800	-2.13407600
H	-4.34456100	4.21384800	0.00203500
H	-4.12121700	-2.43111700	-1.34750500
H	-1.66096300	-3.17051200	-2.18927600
H	-0.12432400	-3.60653300	-0.00526800
H	-1.65355500	-3.17439200	2.18458100
H	-4.11656400	-2.43345300	1.35248000
P	0.68265200	1.01948200	0.00077000
P	-0.21278000	-0.51005000	-1.38930800
P	-0.21343200	-0.51097100	1.38935100
P	-2.21639800	0.18948000	1.80713200
P	-2.21562800	0.19019600	-1.80806300
C	-5.58696200	1.62912900	0.00518000
H	-5.79631900	1.01859600	0.89800100
H	-6.27218800	2.49154100	0.00483800
H	-5.80091600	1.01434400	-0.88356800
C	-1.46853400	4.30431200	-0.00273300
H	-0.82444600	4.24321900	-0.89360200
H	-1.97400500	5.28315300	0.00268300
H	-0.81483500	4.23822600	0.88067000

C	3.50485900	0.28220800	2.81204700
H	4.24076200	0.62890700	3.55537500
H	2.54020200	0.77747900	3.01082200
H	3.34734400	-0.80051500	2.94510600
C	3.50351200	0.28519400	-2.81135200
H	2.53947200	0.78193800	-3.00948400
H	4.23968800	0.63145100	-3.55461600
H	3.34447600	-0.79720200	-2.94520700

VI.4.9 Int5^{M} – P/Si

0 1

Fe	-0.84541700	2.03462600	0.09161100
P	0.35794600	1.31925900	-1.72320600
P	-1.66367300	2.00770100	-2.12066300
P	-2.74218900	1.03720800	-0.54568400
P	-1.11021700	-0.23302600	0.45920700
P	0.05822000	-0.84841400	-1.34190100
Ga	2.02739700	-1.08392300	-0.08680900
Cl	2.59080800	-3.20918900	0.12142900
Si	-2.75044700	-1.53134400	-0.90321300
N	-2.11248000	-3.10029400	0.02575400
C	-3.18746200	-3.10669200	0.78510100
N	-3.87230000	-1.99588500	0.58490100
C	-1.10263700	-4.11120300	-0.07952300
H	-1.40491000	-5.02414300	0.46060800
H	-0.13802200	-3.76810600	0.32866600
H	-0.93180100	-4.37467800	-1.13421900
H	-3.48937400	-3.93666100	1.44727400
C	-5.15564800	-1.64816400	1.11744600
H	-5.26425600	-0.55361600	1.11081000
H	-5.98845200	-2.07186500	0.52905400
H	-5.25927300	-1.99273200	2.15946000
C	0.72201900	3.04872200	0.98618100
H	1.77864400	2.86382200	0.79945500
C	-0.12059300	3.94508400	0.26598400
H	0.17605500	4.56293300	-0.58035200
C	-1.43282800	3.85608900	0.81492800
H	-2.30791200	4.40166000	0.46450600
C	-1.40271400	2.91423400	1.88344100
H	-2.24974900	2.61060600	2.49659000
C	-0.07385100	2.41187900	1.97852300
H	0.26859300	1.64968200	2.67595900
N	2.25894800	-0.34482400	1.70328100
C	3.14018300	0.60497400	1.94397300
C	3.99680000	1.21768500	1.02585400
C	4.13056600	0.85231300	-0.31908900
N	3.46300800	-0.08690100	-0.95140800
C	1.53991900	-0.95646900	2.80072600
H	1.82176000	-2.01829700	2.89102500
H	0.45325000	-0.91032700	2.61838100
H	1.76373200	-0.44932000	3.75300600
H	3.21010500	0.94689600	2.98796700
H	4.64635500	2.00909800	1.39766600
H	4.88050600	1.39957200	-0.91000200
C	3.71759800	-0.34971700	-2.35087100
H	4.56455500	0.24915200	-2.72096400
H	3.94715500	-1.41635700	-2.50224800
H	2.82747200	-0.09895500	-2.95282000

VI.4.10 Int6^{M} – P/Si

0 1

Ga	2.27247600	-0.01888500	-0.05301800
Fe	-2.00642100	-1.43393800	-0.03220700
Cl	1.97093600	1.35497500	-1.78708300
P	-1.05074500	0.54756700	0.09803600
P	-2.86365700	0.33060900	1.26245500
P	-2.27990600	-1.48287400	2.27588900
P	-0.28508100	-1.84223400	1.50648700
P	0.57877700	0.25098400	1.52444200
Si	-1.08577200	2.36239200	-1.41259900
N	2.73226900	-1.75088600	-0.79297200
N	4.02361500	0.38188000	0.71154900
N	-0.27092700	3.55587800	-0.16958600
N	-2.39882000	3.35371600	-0.39105100
C	-1.76166800	-3.15212000	-1.16117200
C	-2.99331400	-3.21786500	-0.45055900
C	-3.77982400	-2.09790200	-0.83765000

C	-3.04080200	-1.34283500	-1.79239100
C	-1.78736600	-1.99649300	-1.99277800
C	-1.44423000	4.04070200	0.19715900
C	3.92036900	-2.29237600	-0.63078000
C	5.01065600	-1.73658100	0.04651200
H	5.92426900	-2.32719000	0.09912100
C	5.02255900	-0.47585000	0.64778900
H	4.06592400	-3.28722000	-1.07837800
H	5.96477500	-0.16140000	1.12213000
H	-1.59360400	4.90810200	0.86279000
H	-0.99628800	-1.66071700	-2.66112200
H	-3.36700700	-0.42230700	-2.27508500
H	-4.76246900	-1.84197200	-0.44440900
H	-3.27212800	-3.97248700	0.28262900
H	-0.94169300	-3.86212300	-1.06798000
C	-3.80894300	3.59512300	-0.33224400
H	-4.33128200	2.72244500	0.09301300
H	-4.03085100	4.46964800	0.30115400
H	-4.21963400	3.78757400	-1.33666900
C	1.01621400	3.95055800	0.31635100
H	0.96933800	4.95182400	0.77604700
H	1.38850600	3.23971100	1.07493800
H	1.74324000	3.97110500	-0.50730700
C	1.71988400	-2.41952000	-1.58041400
H	0.74656200	-2.32884000	-1.07512700
H	1.63005800	-1.94615900	-2.57279700
H	1.95529900	-3.48710100	-1.71528900
C	4.20883100	1.66546900	1.35049000
H	4.08994500	2.48119100	0.61799100
H	3.45450400	1.81142800	2.14140300
H	5.20966100	1.74750300	1.80357000

VI.4.11 Int7^{M} – P/Si

0 1

Ga	2.17535300	-0.52404300	-0.01360300
Fe	-2.51874200	-0.87742800	0.14397400
Cl	1.62547400	-0.37427400	2.13191100
P	0.76370900	0.55127300	-1.52069800
P	-1.77764800	0.97505900	1.27570800
P	-0.90830900	-0.98329600	-1.47105100
Si	-0.17341900	1.77643400	0.04013300
P	-2.73273400	0.03385800	-1.99743400
P	-3.28513700	1.25688400	-0.28259500
N	2.58234900	-2.40039800	-0.34866900
N	0.91203800	3.02576800	0.92562600
N	4.00050800	0.15397900	-0.20737600
N	-0.49658700	3.49490200	-0.63284600
C	-3.93042300	-1.47648600	1.54812700
C	3.79376800	-2.79524500	-0.67756500
C	4.99589900	-0.62743900	-0.57474400
C	-4.23561800	-2.01001900	0.26582100
C	-3.14034400	-2.81734600	-0.14994700
C	4.93610300	-2.00011400	-0.82190200
H	5.85660800	-2.49702200	-1.12541300
C	0.36050500	4.00576400	0.21962400
C	-2.15139300	-2.77842000	0.87847000
C	-2.63857800	-1.94932300	1.92208800
H	0.58440600	5.07794000	0.33795300
H	5.97737000	-0.14389900	-0.69653700
H	3.91855500	-3.87460400	-0.85254400
H	-4.55623100	-0.79733400	2.12508100
H	-5.13277600	-1.80362700	-0.31595100
H	-3.05948300	-3.34715200	-1.09801900
H	-1.18606000	-3.27844500	0.86267900
H	-2.10116100	-1.69769700	2.83472000
C	1.52790700	-3.37831700	-0.17233200
H	1.16876000	-3.35685400	0.86967800
H	0.67409000	-3.14235600	-0.82937700
H	1.88843000	-4.39380000	-0.40008600
C	4.24592100	1.55153100	0.06461200
H	3.43861800	2.16905200	-0.36142200
H	4.27160100	1.74243500	1.15093900
H	5.20322300	1.88422900	-0.36788400
C	-1.21431700	4.12978500	-1.69766100
H	-2.27811200	3.85375700	-1.64193600
H	-1.12252400	5.22497800	-1.62991800
H	-0.83101900	3.79978700	-2.67651700
C	1.59950800	3.16576100	2.18142800

H	2.22629000	4.07222700	2.18122300
H	0.89078500	3.22456000	3.02433200
H	2.23477500	2.28763500	2.35081800

VI.4.12 Int8^{M} – P/Si

0 1

Fe	2.89314600	-0.48299900	0.03594000
P	2.66767500	1.60319600	-1.08384900
P	3.16970800	-0.10149900	-2.27162400
P	2.16091700	-1.90631200	-1.67283100
P	0.68518100	-1.36694700	-0.19877200
P	-0.72615100	-0.00815600	-1.37934800
Si	0.70216900	1.19626800	-0.21993900
Ga	-2.59370100	-0.11936900	0.00721100
Cl	-3.03615000	1.45248200	1.52932200
N	0.32879600	1.48982000	1.56768000
C	-0.18718300	2.69452600	1.32517000
N	-0.05430100	2.96965900	0.05874200
C	0.22189400	0.75423700	2.79434500
H	0.20641700	-0.31938900	2.56341300
H	1.07088900	0.94254600	3.47315400
H	-0.71895800	1.00025800	3.31061500
H	-0.66479900	3.33197400	2.08195600
C	-0.48456100	4.13079900	-0.65297700
H	-1.27739200	3.87135800	-1.37407700
H	0.35376900	4.56705400	-1.21906000
H	-0.88056100	4.89708000	0.03247100
C	3.05430400	-1.09292800	2.00230100
H	2.22052500	-1.35546500	2.64948900
C	3.74930700	-1.99421200	1.14969200
H	3.54043600	-3.05635700	1.03491000
C	4.75418400	-1.25508100	0.45845500
H	5.43356900	-1.64757600	-0.29634100
C	4.67329000	0.09590900	0.88173700
H	5.27954500	0.91871300	0.50661300
C	3.61274200	0.20437200	1.83163300
H	3.28754400	1.11878600	2.32486000
N	-4.14720600	-0.08066900	-1.18361000
C	-5.01834300	-1.06495700	-1.22455200
C	-5.00173900	-2.22916200	-0.45015900
C	-4.06289600	-2.52258200	0.54247500
N	-3.01482100	-1.80528900	0.89429600
C	-4.31488900	1.08231500	-2.02435600
H	-3.42293000	1.22947100	-2.65673800
H	-4.44168900	1.98595600	-1.40509200
H	-5.19405200	0.98127500	-2.68067200
H	-5.84748400	-0.95553700	-1.94054700
H	-5.79968600	-2.95234700	-0.61320400
H	-4.21621600	-3.45716300	1.10328800
C	-2.19401600	-2.23290300	2.00787000
H	-2.22056700	-1.47672500	2.80993700
H	-2.55352000	-3.18888300	2.42077600
H	-1.14752200	-2.35740700	1.68373400

VI.4.13 Int9^{M} – P/Si

0 1

Ga	-2.60351000	0.07056000	-0.05287000
Fe	2.52917400	-0.82628200	0.17241900
Cl	-2.50479000	2.23143600	0.45830500
P	0.25204700	0.92640400	-1.97439800
P	2.30019300	-0.21571200	-2.14540200
P	2.00407600	-2.27188300	-1.53097500
P	0.48850400	-1.89879400	-0.01775300
P	-0.92577800	-0.84279700	-1.38172900
Si	1.38662900	0.98067300	-0.06146500
N	-3.10705400	-0.93616000	1.54281700
N	-4.31778300	-0.09801100	-0.98432500
N	0.86133100	2.07418000	1.37984900
N	2.26550100	2.64295300	-0.14877700
C	2.93496400	-1.06476300	2.16954900
C	3.44982600	-2.16036400	1.42782600
C	4.39815500	-1.64972300	0.48610200
C	4.46865300	-0.24475100	0.64464800
C	3.54933100	0.12645300	1.67210800
C	1.63580400	3.04747700	0.93321100
C	-4.32892400	-1.40943700	1.70157500
C	-5.40135000	-1.31036400	0.81432000

H	-6.34365100	-1.76637300	1.11523000
C	-5.35492300	-0.69211600	-0.44163000
H	-4.51707500	-1.95012900	2.64175300
H	-6.27888900	-0.71118900	-1.04018900
H	1.74072200	4.03854900	1.40326800
H	3.40100900	1.13248000	2.06179400
H	5.07730400	0.43630200	0.05226700
H	4.94728700	-2.23893800	-0.24621200
H	3.16069300	-3.20403300	1.54238800
H	2.18305200	-1.12148900	2.95502500
C	3.03791800	3.40984400	-1.07868300
H	2.46713500	3.60226300	-2.00247300
H	3.33368500	4.37707900	-0.64173400
H	3.94650400	2.85623500	-1.35875600
C	0.16921500	2.02571900	2.63427900
H	0.41361500	2.90973600	3.24427600
H	-0.91875200	2.00528300	2.47265800
H	0.46534900	1.12817000	3.20092100
C	-2.11730700	-1.15145900	2.57567900
H	-1.22525600	-1.64838200	2.15601900
H	-1.79769200	-0.19185000	3.01378600
H	-2.51814800	-1.78273200	3.38475900
C	-4.41324400	0.49741900	-2.29795500
H	-4.23891700	1.58426500	-2.23701900
H	-3.64382000	0.07186300	-2.96373900
H	-5.40357400	0.32244300	-2.74787600

VI.4.14 TS1^{M} – P/Si

0 1

Ga	3.07190500	-0.68638500	-0.33893100
Fe	-3.68110100	-0.00303600	-0.01916000
Cl	4.88269500	-0.84127200	-1.55668900
P	-0.77523700	1.46852300	-0.34447600
Si	1.85330500	1.39073100	-0.27025400
P	-1.98729100	0.29310900	-1.75393400
P	-1.80427600	0.64317000	1.41674900
P	-2.25610300	-1.45250300	1.15350200
P	-2.37692700	-1.68653800	-0.97399600
N	2.04880700	2.32335900	1.32199500
N	1.71480300	-1.97800700	-0.85280400
N	3.36501900	-1.31707500	1.47074000
N	2.58869100	3.03973900	-0.63044200
C	-5.53458800	-0.80048700	0.14999500
C	-5.11094600	1.26266500	-0.78743700
C	-5.30696400	0.12658900	1.20917400
C	-5.41645600	-0.09833400	-1.08536500
C	1.16648600	-2.78064200	0.03292400
C	2.58299000	-2.24692600	2.00158600
C	1.54234400	-2.92590600	1.37717900
H	0.97336500	-3.63487500	1.97657900
C	2.48143600	3.37743100	0.65043600
C	-5.04391300	1.40070400	0.62546200
H	2.68925600	4.37225000	1.07164900
H	-5.50487600	-0.53321800	-2.07956700
H	-4.91594300	2.04750700	-1.51620800
H	0.32861400	-3.39777200	-0.32005000
H	2.78465600	-2.50346800	3.05245900
H	-4.78704500	2.30979500	1.16653400
H	-5.29716000	-0.10677300	2.27254700
H	-5.73027400	-1.86583500	0.26355500
C	1.20148900	-1.92577900	-2.20568800
H	0.72175800	-0.94916600	-2.39663000
H	2.02091900	-2.06520300	-2.92815400
H	0.43571000	-2.69824700	-2.37058600
C	4.42873200	-0.72547900	2.24989700
H	5.40841300	-0.91779500	1.78277700
H	4.30276700	0.36970000	2.31199700
H	4.44554400	-1.12952800	3.27469400
C	3.06445200	3.83559300	-1.72603100
H	3.37068800	4.83070700	-1.36942100
H	3.93200900	3.35840500	-2.20772600
H	2.27630400	3.96902100	-2.48286100
C	1.56722600	2.25965600	2.67548300
H	1.77082700	3.20595600	3.19950300
H	0.48098300	2.06708900	2.69063300
H	2.06352200	1.44268500	3.22076300

VI.4.15 TS2^{M} – P/Si

```
0 1
 Ga                 2.11212100   -0.91628800   -0.21770800
 Fe                -2.91099600   -0.22693400   -0.03993900
 Cl                 3.57118000   -0.51755900   -1.84426800
 P                  0.00233200    0.50671300   -0.77453000
 Si                 1.58899000    1.57226400    0.28622000
 P                 -0.84188600   -0.32862800    1.07767100
 P                 -1.88997700    0.97603500   -1.75383400
 P                 -2.87869700    2.10215100   -0.18547700
 P                 -2.26318200    1.20367200    1.66982500
 N                  1.20912200    3.23284400    1.04666500
 N                  1.20434300   -2.62442200   -0.54060500
 N                  3.15651000   -1.54202500    1.31829000
 N                  2.47849800    2.91813400   -0.66309700
 C                 -4.87803100   -0.61429600    0.35058000
 C                 -3.28728700   -2.25806800    0.09913300
 C                 -4.61356400   -0.75885300   -1.04097500
 C                 -4.06390500   -1.54526700    1.05660900
 C                  1.29300300   -3.63720000    0.29630300
 C                  2.96455700   -2.72233500    1.87307600
 C                  2.09413300   -3.72108600    1.43740500
 H                  2.05030300   -4.64156800    2.01792900
 C                  1.98041700    3.82833300    0.15116400
 C                 -3.62376800   -1.77583600   -1.19540300
 H                  2.18257200    4.91017300    0.10493200
 H                 -4.01691500   -1.66430000    2.13773100
 H                 -2.54132500   -3.01828000    0.32508700
 H                  0.67114700   -4.51481100    0.06372100
 H                  3.56495300   -2.94308600    2.76871700
 H                 -3.19233100   -2.11006000   -2.13752800
 H                 -5.06438000   -0.17581700   -1.84266300
 H                 -5.56406200    0.10319200    0.79851200
 C                  0.27531300   -2.70558100   -1.64859200
 H                 -0.62139600   -2.09231200   -1.44609000
 H                  0.74396000   -2.32428900   -2.56803000
 H                 -0.04037900   -3.74701300   -1.81874100
 C                  4.13973000   -0.64343800    1.87405100
 H                  4.89683900   -0.38933300    1.11435800
 H                  3.66221600    0.29899000    2.19355100
 H                  4.64664000   -1.09358800    2.74209300
 C                  3.34959800    3.09956400   -1.78893800
 H                  3.81695000    4.09652300   -1.76065200
 H                  4.13463700    2.33075600   -1.78161100
 H                  2.79626300    2.99480500   -2.73586900
 C                  0.41306000    3.83674700    2.07769300
 H                  0.68868800    4.89580500    2.20299700
 H                 -0.65845300    3.76920300    1.83263500
 H                  0.57055900    3.32006000    3.03556700
```

VI.4.16 TS3^{M} – P/Si

```
0 1
 Fe                -1.89712100    1.67058900    0.04184200
 P                 -0.46266300    0.86951300   -1.53039300
 P                 -2.45694100   -0.06866400   -1.47388200
 P                 -2.77913000   -0.28987900    0.71001900
 P                 -0.83995800    0.22364300    1.53870000
 P                  0.31308700   -0.63021000   -0.13836300
 Ga                 2.55571800   -0.19897200    0.29325000
 Cl                 3.22947800   -1.18246800    2.13131400
 Si                -1.13737000   -2.43738100   -1.12231300
 N                 -0.93148000   -3.40271800    0.49824000
 C                 -2.19467900   -3.80138100    0.53006900
 N                 -2.86478900   -3.19600600   -0.41568400
 C                  0.10413500   -3.67711200    1.44872700
 H                 -0.18742500   -4.50238700    2.11904500
 H                  0.32698900   -2.79145100    2.06920000
 H                  1.03658200   -3.96794000    0.94086100
 H                 -2.59876100   -4.55755400    1.22514300
 C                 -4.21660800   -3.43003100   -0.81567200
 H                 -4.71045700   -4.16432100   -0.15672400
 H                 -4.79181600   -2.49013800   -0.77843600
 H                 -4.26585300   -3.81128000   -1.84885700
 C                 -2.54261200    3.35270800   -0.95962200
 H                 -2.60328900    3.43941900   -2.04356400
 C                 -3.56680300    2.86572800   -0.10006900
 H                 -4.54794300    2.51090100   -0.41261400
```

C	-3.07616400	2.89500600	1.23669300
H	-3.61794700	2.57364900	2.12477300
C	-1.73937800	3.38306900	1.20096000
H	-1.07951500	3.49625500	2.05947200
C	-1.41094600	3.67035700	-0.15283400
H	-0.45547900	4.04772400	-0.51322100
N	2.90125000	1.71104300	0.28482000
C	3.79516700	2.24056600	-0.52330400
C	4.59060900	1.56623600	-1.45651500
C	4.52558700	0.19850900	-1.73474400
N	3.74614500	-0.69290100	-1.15527200
C	2.08340900	2.54971900	1.13611700
H	2.21831000	2.27351700	2.19418600
H	1.01666300	2.40956300	0.88712200
H	2.34237500	3.61334300	1.01216700
H	3.91800000	3.33266200	-0.46302900
H	5.29253500	2.16200700	-2.03846400
H	5.18778200	-0.17866600	-2.52867100
C	3.77235700	-2.07746300	-1.57320600
H	4.49129200	-2.23404200	-2.39279600
H	4.05529400	-2.72665700	-0.72843700
H	2.77433100	-2.39390800	-1.92129900

VI.4.17 TS4^{M} – P/Si

0 1

Fe	-0.90200100	1.88746900	0.13793500
P	-0.08274700	0.69743900	-1.67405100
P	-2.21725700	0.94738100	-1.41429300
P	-2.52507700	0.37731600	0.90727300
P	-0.40154000	0.01471000	1.30920300
P	0.10947900	-1.18406800	-0.52055500
Ga	2.42328900	-1.12811000	-0.14216000
Cl	3.38310100	-3.10101100	-0.18092000
Si	-2.66120300	-1.35920200	-0.73898900
N	-2.86518300	-2.71249100	0.54005300
C	-4.18333600	-2.64351000	0.46614400
N	-4.50188300	-1.65525800	-0.34714100
C	-2.03000700	-3.52635600	1.36538200
H	-1.24451000	-4.00608800	0.76122200
H	-2.61906500	-4.31316500	1.86346200
H	-1.53426100	-2.91381800	2.13825600
H	-4.89156300	-3.32233900	0.96621800
C	-5.80235600	-1.24062300	-0.77332600
H	-6.58474200	-1.85995800	-0.30577800
H	-5.98356000	-0.18941800	-0.49616200
H	-5.90680300	-1.32341800	-1.86708300
C	0.03113600	3.63165800	-0.45671700
H	0.64736800	3.72395100	-1.34968900
C	-1.37122300	3.86873900	-0.38256700
H	-2.01290000	4.19090800	-1.20112800
C	-1.78719900	3.58574800	0.94687300
H	-2.80829500	3.63930400	1.32202600
C	-0.64351100	3.18883500	1.69734400
H	-0.63941200	2.89673800	2.74663700
C	0.48810800	3.21910100	0.82621600
H	1.51316300	2.95104800	1.07640500
N	3.00425600	-0.24316300	1.49572800
C	3.61499700	0.92234900	1.45818700
C	3.98620200	1.64488400	0.31950300
C	3.86229300	1.19058000	-0.99856600
N	3.31788500	0.06205600	-1.39899400
C	2.78012200	-0.90892300	2.76168700
H	3.24151500	-1.90931400	2.74572300
H	1.69892400	-1.02670700	2.94350800
H	3.21396800	-0.33231600	3.59402000
H	3.87373500	1.36562200	2.43204300
H	4.47582400	2.60572700	0.47350400
H	4.27969000	1.83571000	-1.78656700
C	3.30840900	-0.29106900	-2.80192900
H	3.87701700	0.43889300	-3.39952600
H	3.75501200	-1.28802100	-2.94350300
H	2.27286500	-0.31822200	-3.18200500

VI.4.18 TS5^{M} – P/Si

0 1

Fe	2.36758900	-0.53030000	0.03282400
P	1.13699600	-0.77409300	-1.89995400

P	2.80595300	0.61340800	-1.93028600
P	2.44410600	1.76501700	-0.13700800
P	0.63185800	0.75106300	0.72330400
P	-0.50930400	0.51497600	-1.18680200
Ga	-2.06456900	-0.96408700	-0.25513600
Cl	-4.06764700	-0.72679200	-1.11897800
Si	0.04982700	2.90210900	-0.88255400
N	-1.79545500	3.09744300	-0.25363500
C	-1.39298800	3.83943400	0.76380000
N	-0.08376600	3.80465000	0.83956300
C	-3.11315800	3.07937400	-0.82509400
H	-3.86237500	3.40639500	-0.08477600
H	-3.37690400	2.06002700	-1.14657800
H	-3.19146100	3.74271200	-1.70322900
H	-2.05641000	4.43692700	1.41317600
C	0.76215200	4.30741400	1.87500000
H	1.60763900	4.86514500	1.44511100
H	0.20964300	4.98048300	2.55215200
H	1.18049900	3.47642300	2.46947400
C	2.53694400	-2.55891500	0.42001100
H	1.92417400	-3.33638500	-0.03276800
C	3.75792200	-2.04676700	-0.10388600
H	4.24206700	-2.36134800	-1.02711000
C	4.21301100	-1.01731800	0.77085500
H	5.11031100	-0.41502400	0.63572600
C	3.28001800	-0.90289200	1.84107800
H	3.33742400	-0.19580700	2.66749000
C	2.23941600	-1.85269300	1.61783900
H	1.35778100	-2.00564800	2.23883900
N	-2.22453500	-0.80471600	1.67309500
C	-1.82861900	-1.77425600	2.47068400
C	-1.33091300	-3.02455400	2.08994900
C	-1.22204700	-3.48425400	0.77317000
N	-1.50549300	-2.82068800	-0.32872300
C	-2.74678600	0.42886800	2.21620200
H	-3.75226900	0.62362200	1.80996200
H	-2.09149900	1.27072100	1.93420700
H	-2.80955300	0.38501300	3.31480900
H	-1.90908800	-1.57908300	3.55058600
H	-1.04907600	-3.71456700	2.88425500
H	-0.87196300	-4.51873900	0.63796600
C	-1.38887800	-3.46387700	-1.62176600
H	-1.08680300	-4.51723800	-1.51221400
H	-2.35449000	-3.42783700	-2.15094500
H	-0.63673900	-2.94512300	-2.23989100

VI.4.19 TS6^{M} – P/Si

0 1

Ga	2.64050100	-0.37523000	0.02549200
Fe	-1.24967100	1.63992000	0.24445300
Cl	2.43569400	0.70599900	1.94496700
P	-0.64614600	-0.55744300	0.15739800
P	-2.43527200	0.16859300	-0.94348800
P	-1.62295500	1.80063900	-2.10627200
P	0.40013900	1.74289900	-1.34994500
P	0.83937700	-0.43771700	-1.46380600
Si	-2.78932600	-2.17727300	-0.85988400
N	4.29546100	0.26304100	-0.78772300
N	3.26163000	-2.17323800	0.46803200
N	-4.75071100	-2.01889300	-0.67458800
N	-3.36167500	-2.19921200	0.95778600
C	-0.30859200	2.94344400	1.53521600
C	-1.34733800	3.61340400	0.82752000
C	-2.57368300	2.94702500	1.10773700
C	-2.29591000	1.87686100	2.01045100
C	-0.89768900	1.87081800	2.26553500
C	-4.64206700	-2.19838800	0.61734900
C	5.34900700	-0.51590700	-0.90946100
C	5.46471600	-1.84988900	-0.50362400
H	6.41334400	-2.35016400	-0.69418700
C	4.47145600	-2.58379300	0.15277800
H	6.23609800	-0.06345600	-1.37906500
H	4.72660200	-3.61538800	0.44096700
H	-5.47961700	-2.35848900	1.31929700
H	-0.34564300	1.15671100	2.87372100
H	-3.02166700	1.16219100	2.39600400
H	-3.54790100	3.19969900	0.69164800
H	-1.22046100	4.45696200	0.15052300

H	0.75422200	3.17498200	1.51279400
C	-2.81067000	-2.48039400	2.25088500
H	-1.91398700	-1.86179200	2.40730500
H	-3.54046400	-2.24654600	3.04293600
H	-2.51308300	-3.53814700	2.35660600
C	-5.94792700	-1.91595800	-1.44776800
H	-6.84356800	-2.06194400	-0.82074100
H	-6.02175200	-0.92377300	-1.92404500
H	-5.96583500	-2.67248000	-2.24861800
C	4.35560900	1.64772800	-1.20268500
H	3.52090100	1.88457300	-1.88253500
H	4.26017300	2.31209300	-0.32793100
H	5.30540600	1.87063300	-1.71457000
C	2.35441200	-3.04009400	1.18538500
H	2.10611700	-2.60391300	2.16712200
H	1.40909100	-3.15498000	0.62892400
H	2.79366000	-4.03829300	1.34300700

VI.4.20 TS7^{M} – P/Si

0 1

Ga	-1.84542400	1.38429500	-0.13235700
Fe	0.44856200	-2.10708100	0.12490500
Cl	-2.24337100	3.54777700	-0.08444900
P	1.23580600	0.03826300	0.31448300
P	2.59382700	-1.42525200	-0.56794400
P	1.29814600	-2.26570900	-2.05538300
P	-0.57441700	-1.23169500	-1.74639000
P	0.06599000	0.87794300	-1.40135000
Si	2.04051600	2.23057700	0.50797800
N	-2.08220700	0.77190100	1.70671100
N	-3.42175600	0.50152900	-0.88135900
N	3.32714600	2.00878300	-0.86634600
N	3.79623300	1.86980500	1.22673600
C	-1.24755600	-2.88106300	0.99904300
C	-0.56696400	-3.87700300	0.23503100
C	0.74481900	-4.02660600	0.77141300
C	0.87861000	-3.13467000	1.87314000
C	-0.34930300	-2.42636100	2.00373500
C	4.30319300	1.88221000	0.00905900
C	-3.08618100	-0.00990700	2.04825800
C	-4.07244200	-0.53930900	1.21245000
H	-4.82283900	-1.18359300	1.66885800
C	-4.20335100	-0.26301100	-0.15456300
H	-3.15587900	-0.26877200	3.11612600
H	-5.05609500	-0.72542200	-0.67486300
H	5.37722400	1.82688300	-0.23839800
H	-0.55270000	-1.63598300	2.72434900
H	1.77031800	-2.99664100	2.48204300
H	1.51918400	-4.68639700	0.38278000
H	-0.96662600	-4.40800700	-0.62770800
H	-2.26103200	-2.51793400	0.83765800
C	4.51560500	1.89345200	2.46385100
H	4.18361300	1.07456400	3.12207500
H	5.59720200	1.77056600	2.29078500
H	4.36349600	2.84293200	3.00386100
C	3.39656200	1.88597600	-2.29205800
H	4.44196400	1.95564000	-2.63438000
H	2.98174500	0.91711900	-2.61822100
H	2.81093500	2.68165400	-2.77432300
C	-1.19979500	1.29610200	2.72536700
H	-0.17117600	0.92799200	2.56965800
H	-1.17605900	2.39654600	2.67526400
H	-1.53214300	0.99647300	3.73242100
C	-3.70372700	0.71353100	-2.28375600
H	-3.79603400	1.79149800	-2.49210700
H	-2.88329600	0.30957200	-2.90099900
H	-4.63918800	0.21454200	-2.58264000

VI.4.21 TS8^{M} – P/Si

0 1

Ga	2.27155400	-0.07956400	0.16388400
Fe	-1.86948700	-1.57263500	0.15294700
Cl	1.78280800	-0.88866600	2.14921900
P	0.53928300	0.71094100	-1.19193400
P	-1.50373900	0.54225800	0.92453000
P	-0.50698100	-1.16309900	-1.61879900
Si	-0.45901200	2.37239300	0.10853000

P	-2.58376600	-0.81784100	-1.95149200
P	-3.31185000	0.23362000	-0.15134500
N	3.35224500	-1.41691900	-0.76004900
N	-1.60095700	3.69299300	0.92122200
N	3.67755800	1.25049900	0.41337500
N	-1.59071200	3.16731200	-1.15694800
C	-2.85807400	-2.46420200	1.73974900
C	4.57876700	-1.14410500	-1.15465800
C	4.85478300	1.11257600	-0.15845700
C	-3.14722800	-3.12687700	0.50927200
C	-1.92299000	-3.61358800	-0.02876700
C	5.29382100	0.03759400	-0.93821900
H	6.29997600	0.09652500	-1.35130500
C	-2.14805900	3.94538700	-0.25026200
C	-0.87244600	-3.23083700	0.85730200
C	-1.45362300	-2.52519400	1.94689600
H	-2.93234100	4.69293000	-0.44937100
H	5.57493400	1.92798600	0.01012600
H	5.10104700	-1.94463200	-1.70066500
H	-3.58148000	-1.96627600	2.38326300
H	-4.12940600	-3.22244100	0.04842900
H	-1.80804400	-4.14296200	-0.97348600
H	0.19054600	-3.42160300	0.72788200
H	-0.89599600	-2.06315600	2.75956600
C	2.80240300	-2.73937300	-0.96803700
H	2.62651800	-3.23321500	0.00204800
H	1.83501100	-2.67721300	-1.49444400
H	3.48837600	-3.36571600	-1.56025200
C	3.41611600	2.38078800	1.27856600
H	2.51476600	2.91889000	0.94103300
H	3.22597300	2.03377600	2.30759600
H	4.26967600	3.07740200	1.29137500
C	-1.84792100	3.09135800	-2.56346200
H	-2.20150400	2.08170600	-2.82904900
H	-2.61933400	3.82125400	-2.85609300
H	-0.93318700	3.29469000	-3.14189700
C	-1.99159800	4.13493400	2.22082400
H	-2.88812800	4.77345800	2.17041400
H	-2.22820800	3.26479200	2.85781800
H	-1.18711400	4.70647900	2.71175800

VI.4.22 TS9^{M} – P/Si

0 1

Ga	2.63647400	-0.01722400	-0.13363200
Fe	-3.04049900	-0.29241200	0.05849300
Cl	2.84575100	2.06631000	-0.89896800
P	0.66572900	-1.18617600	-0.64826100
P	-1.92870100	-0.73402400	-1.82655100
P	-0.20817700	-1.10036100	1.37859500
Si	-0.84769100	0.51512000	-0.10588200
P	-2.17937200	-2.12290200	1.22377800
P	-2.69738100	-2.46093400	-0.84663500
N	3.43674100	0.00084600	1.64381600
N	-0.32647300	2.06861800	0.84027300
N	4.06515200	-1.01831200	-1.02395000
N	-0.51905400	2.00002700	-1.29007900
C	-4.24764900	1.22117400	-0.65366300
C	4.56975900	-0.62375100	1.89740900
C	5.10036800	-1.49092100	-0.36562100
C	-5.00492300	0.05172800	-0.36353100
C	-4.83429200	-0.26238900	1.01547300
C	5.36108000	-1.34521100	1.00107000
H	6.26641200	-1.80751200	1.39215300
C	-0.20641900	2.76885100	-0.27638200
C	-3.96571900	0.71285700	1.58833300
C	-3.59953500	1.62230800	0.55306800
H	0.10500600	3.82063900	-0.34376100
H	5.83939700	-2.05494900	-0.95528800
H	4.93266000	-0.56032500	2.93456400
H	-4.15929300	1.71032300	-1.62198500
H	-5.57853100	-0.53210300	-1.08198300
H	-5.26462000	-1.11830400	1.53300300
H	-3.62762100	0.74502700	2.62265400
H	-2.95972200	2.49583000	0.66781600
C	2.77925100	0.75115600	2.69000800
H	2.67143200	1.80549500	2.38753900
H	1.77184800	0.34349400	2.87604700
H	3.35448700	0.71366300	3.62870300

C	3.95560800	-1.21369800	-2.45246800
H	3.00620300	-1.71786700	-2.69803300
H	3.96343600	-0.24081900	-2.97118400
H	4.78706000	-1.82461400	-2.83861400
C	-0.25226900	2.24668500	-2.67708800
H	0.76177500	1.90767100	-2.94727700
H	-0.98275900	1.70408000	-3.29263000
H	-0.32687600	3.32232900	-2.90493100
C	-0.33916800	2.53687400	2.19183500
H	-1.25953300	3.09425500	2.44220500
H	-0.28881400	1.66183200	2.85631200
H	0.52763800	3.18329900	2.40629600

VI.4.23 TS10^{M} – P/Si

0 1

Ga	2.64050100	-0.37523000	0.02549200
Fe	-1.24967100	1.63992000	0.24445300
Cl	2.43569400	0.70599900	1.94496700
P	-0.64614600	-0.55744300	0.15739800
P	-2.43527200	0.16859300	-0.94348800
P	-1.62295500	1.80063900	-2.10627200
P	0.40013900	1.74289900	-1.34994500
P	0.83937700	-0.43771700	-1.46380600
Si	-2.78932600	-2.17727300	-0.85988400
N	4.29546100	0.26304100	-0.78772300
N	3.26163000	-2.17323800	0.46803200
N	-4.75071100	-2.01889300	-0.67458800
N	-3.36167500	-2.19921200	0.95778600
C	-0.30859200	2.94344400	1.53521600
C	-1.34733800	3.61340400	0.82752000
C	-2.57368300	2.94702500	1.10773700
C	-2.29591000	1.87686100	2.01045100
C	-0.89768900	1.87081800	2.26553500
C	-4.64206700	-2.19838800	0.61734900
C	5.34900700	-0.51590700	-0.90946100
C	5.46471600	-1.84988900	-0.50362400
H	6.41334400	-2.35016400	-0.69418700
C	4.47145600	-2.58379300	0.15277800
H	6.23609800	-0.06345600	-1.37906500
H	4.72660200	-3.61538800	0.44096700
H	-5.47961700	-2.35848900	1.31929700
H	-0.34564300	1.15671100	2.87372100
H	-3.02166700	1.16219100	2.39600400
H	-3.54790100	3.19969900	0.69164800
H	-1.22046100	4.45696200	0.15052300
H	0.75422200	3.17498200	1.51279400
C	-2.81067000	-2.48039400	2.25088500
H	-1.91398700	-1.86179200	2.40730500
H	-3.54046400	-2.24654600	3.04293600
H	-2.51308300	-3.53814700	2.35660600
C	-5.94792700	-1.91595800	-1.44776800
H	-6.84356800	-2.06194400	-0.82074100
H	-6.02175200	-0.92377300	-1.92404500
H	-5.96583500	-2.67248000	-2.24861800
C	4.35560900	1.64772800	-1.20268500
H	3.52090100	1.88457300	-1.88253500
H	4.26017300	2.31209300	-0.32793100
H	5.30540600	1.87063300	-1.71457000
C	2.35441200	-3.04009400	1.18538500
H	2.10611700	-2.60391300	2.16712200
H	1.40909100	-3.15498000	0.62892400
H	2.79366000	-4.03829300	1.34300700

VI.4.24 Int1^{M} – As/Si

0 1

Ga	-2.92866700	0.41658900	0.09728800
Fe	2.73243500	0.67848300	0.01894400
Cl	-4.88752600	-0.62052200	0.29886200
As	0.22151400	-1.05121800	-1.89279500
Si	-1.08129700	-1.10754700	0.07996700
As	0.71903400	1.19836400	-1.04055000
As	2.44719500	-1.54388700	-0.99135100
As	2.22309300	-1.20041900	1.34345100
As	0.55625400	0.57753500	1.34008500
N	-1.20602200	-2.30074700	1.49812300
N	-3.02936100	1.60912200	-1.44366100
N	-2.89704600	1.80610600	1.46714400

N	-2.13798400	-2.75723400	-0.38312000
C	3.79099700	1.96467200	1.25942700
C	3.95291300	1.93899900	-1.03877400
C	4.63134400	0.87788800	0.89015200
C	3.37614500	2.62818600	0.07171800
C	-2.94284000	2.91588800	-1.31506900
C	-2.83794200	3.08475900	1.15842400
C	-2.83482100	3.64017500	-0.12382100
H	-2.76948800	4.72460000	-0.20083100
C	-1.98662500	-3.16186200	0.83976700
C	4.72151700	0.85482500	-0.53042400
H	-2.44401300	-4.05343300	1.29751700
H	2.72498600	3.49992500	0.01960200
H	3.82186300	2.18788500	-2.09043300
H	-2.96408300	3.49869000	-2.24845800
H	-2.79270200	3.78788400	2.00410300
H	5.26890100	0.12617700	-1.12563600
H	5.10925500	0.17841600	1.57377600
H	3.49622500	2.22619900	2.27475400
C	-3.15203200	1.01254800	-2.75454300
H	-2.28120400	0.36937800	-2.97116400
H	-4.05688600	0.38519900	-2.80443300
H	-3.21541200	1.78189500	-3.54039200
C	-2.93603200	1.38924100	2.84930100
H	-3.85125700	0.80750600	3.04624000
H	-2.06800100	0.74821900	3.08077400
H	-2.91368000	2.25462800	3.53066300
C	-3.01881000	-3.28103100	-1.38056900
H	-3.26488700	-4.33835400	-1.18703000
H	-3.95940800	-2.70489900	-1.40684800
H	-2.53899200	-3.21391000	-2.36913700
C	-0.76513300	-2.41689100	2.85764500
H	-1.55108300	-2.86870900	3.48464100
H	0.15506100	-3.01781100	2.95213100
H	-0.54688400	-1.41723200	3.26094100

VI.4.25 Int2^{M} – As/Si

0 1

Ga	-2.61069200	-0.34084100	-0.04852900
Fe	1.72330900	-1.36235200	0.34402200
Cl	-4.29849500	1.04156400	0.27454000
As	-0.58158500	0.90931600	-0.48871600
Si	-1.16835700	3.23391700	-1.07366500
As	0.62469600	-0.73618600	-1.75170200
As	0.66086900	0.54515900	1.52862400
As	2.90545500	0.73251300	0.79407400
As	2.87085200	-0.06758100	-1.42213700
N	0.54454900	3.80858200	-0.46545700
N	-2.60695700	-1.64229200	1.39059500
N	-3.00676200	-1.56164500	-1.50778100
N	-1.17523600	3.59036800	0.79401700
C	3.12101200	-2.80048000	0.75384500
C	0.88206500	-3.24456700	0.42148700
C	2.42520500	-2.46182600	1.94874900
C	2.17212800	-3.28937200	-0.18841100
C	-2.72863400	-2.93128700	1.14258100
C	-3.04888800	-2.86313200	-1.31932000
C	-2.90182700	-3.54014700	-0.10339300
H	-2.97239500	-4.62687400	-0.12315800
C	0.09903900	3.95195300	0.76790400
C	1.04227000	-2.73420000	1.73836900
H	0.68105300	4.33320500	1.62158600
H	2.39169800	-3.61959400	-1.20266500
H	-0.06061600	-3.53696000	-0.03864700
H	-2.69657100	-3.59717700	2.01800200
H	-3.22768200	-3.47937900	-2.21314900
H	0.24339800	-2.56363700	2.45760700
H	2.86861400	-2.04714400	2.85246100
H	4.19024200	-2.68526000	0.58213600
C	-2.50351500	-1.17063800	2.75532600
H	-1.54634300	-0.64356900	2.90871000
H	-3.31966600	-0.46327800	2.97409800
H	-2.56316000	-2.00743700	3.46900200
C	-3.19090900	-1.00404200	-2.83064500
H	-4.00639700	-0.26367200	-2.82114500
H	-2.27018200	-0.49518700	-3.16328600
H	-3.43491400	-1.78938000	-3.56289700
C	-2.01671400	3.44624400	1.94591600

H	-1.86585200	4.27554100	2.65645500
H	-3.06888500	3.43765100	1.63271000
H	-1.81705400	2.49612000	2.47272100
C	1.85665100	4.09935500	-0.96276800
H	2.50318900	4.46653900	-0.15033500
H	2.32194900	3.19038800	-1.37535200
H	1.82050200	4.86632500	-1.75314000

VI.4.26 Int3^{M} – As/Si

0 1

Fe	1.09416400	-1.68404000	0.61919200
As	-0.27929900	-1.57403100	-1.36323900
As	2.06952200	-1.80708200	-1.67803400
As	2.85927300	-0.28354200	-0.07633400
As	0.73127700	0.73714700	0.76510600
As	-0.55500300	0.84794900	-1.33353900
Ga	-2.61189200	0.67890400	-0.03021900
Cl	-3.69624200	2.60829200	0.00833900
Si	2.04669000	2.30202900	-0.80093400
N	0.96336900	3.74922500	-0.11031800
C	1.95914700	4.15638200	0.64862400
N	2.93395000	3.26871400	0.61119100
C	-0.25940700	4.44209200	-0.39281800
H	-0.27116900	5.42736200	0.10274900
H	-1.13751100	3.87221200	-0.04710000
H	-0.37740100	4.60077200	-1.47610900
H	1.99058300	5.11663700	1.19265500
C	4.20459500	3.33826700	1.26405900
H	4.35780000	2.46291700	1.91650300
H	5.02955000	3.35546300	0.53319600
H	4.28055700	4.24640200	1.88493600
C	-0.22354500	-2.96333200	1.58036600
H	-1.27198700	-3.10620700	1.32332400
C	0.88435300	-3.68344400	1.04648400
H	0.83619500	-4.47139900	0.29626900
C	2.07307500	-3.16484100	1.63585500
H	3.08788700	-3.49484100	1.41796800
C	1.70339000	-2.13091900	2.54446100
H	2.38356500	-1.53279100	3.14895000
C	0.28575300	-2.00485100	2.49985400
H	-0.30690700	-1.28480800	3.06130800
N	-2.72539900	0.03528900	1.81364300
C	-3.28790900	-1.12002400	2.10580000
C	-3.88874500	-2.01733500	1.21924900
C	-4.10812900	-1.77461100	-0.14204100
N	-3.73729300	-0.71291300	-0.82236600
C	-2.28444600	0.90886100	2.87996800
H	-2.84856600	1.85504000	2.84829200
H	-1.21518400	1.15281200	2.76335000
H	-2.43511700	0.43921500	3.86526700
H	-3.29448000	-1.39999600	3.17050600
H	-4.28102100	-2.94527000	1.63353800
H	-4.66254100	-2.54412800	-0.70046200
C	-4.06184800	-0.59594900	-2.22636300
H	-4.68650000	-1.43799800	-2.56385400
H	-4.60466900	0.34392400	-2.41500200
H	-3.14069200	-0.58417500	-2.83391000

VI.4.27 Int4^{M} – As/Si

0 1

Ga	3.18358700	0.76032500	-0.00025100
Fe	-1.41652600	-1.59617700	0.00023000
Cl	4.67157600	2.38222800	-0.00070800
Si	-2.50838800	1.18712400	0.00009700
N	-2.63900000	3.06676700	0.00001400
N	3.63921300	-0.46420900	1.45797500
N	-4.30697400	1.70996600	-0.00006100
N	3.63906800	-0.46488600	-1.45795500
C	-0.52012400	-3.42622900	0.00079700
C	-1.34738700	-3.29280300	1.15293000
C	-1.34667800	-3.29321300	-1.15189900
C	-2.68668900	-3.08239300	0.70854300
C	-2.68624500	-3.08266400	-0.70841400
C	-3.95376200	2.98226400	-0.00018500
C	3.93251100	-2.38513000	0.00044100
H	4.12445900	-3.45739400	0.00068000
C	3.86276400	-1.74223100	1.24147800

C	3.86265600	-1.74280400	-1.24088700
H	4.02475700	-2.36757300	-2.13277300
H	4.02492900	-2.36659000	2.13363800
H	-4.65106200	3.83571200	-0.00041000
H	-3.55201000	-2.92211300	-1.34803400
H	-1.01409600	-3.33550100	-2.18842100
H	0.55985500	-3.57154900	0.00115300
H	-1.01544600	-3.33471400	2.18967300
H	-3.55285100	-2.92162200	1.34757000
As	0.85158900	1.45194200	-0.00027700
As	0.17113600	-0.43857400	-1.44675700
As	0.17135000	-0.43826700	1.44671800
As	-2.12041300	-0.01630400	1.89450100
As	-2.12068000	-0.01660100	-1.89418800
C	-5.61905800	1.13936700	-0.00188500
H	-5.77024400	0.50746200	0.88789000
H	-6.38727700	1.92878400	-0.00119900
H	-5.76908300	0.51008100	-0.89373700
C	-1.80755700	4.23301400	0.00136300
H	-1.15495300	4.24321000	-0.88506400
H	-2.42136000	5.14776700	0.00113400
H	-1.15672500	4.24250100	0.88911400
C	3.64670200	0.06151200	-2.80334300
H	3.90583400	-0.71836300	-3.53711000
H	2.65236000	0.46371200	-3.06397500
H	4.37729000	0.88232000	-2.88415600
C	3.64688700	0.06279200	2.80312600
H	2.65249700	0.46492600	3.06368100
H	3.90623900	-0.71670600	3.53721600
H	4.37733600	0.88376700	2.88349500

VI.4.28 Int5^{M} – As/Si

0 1

Ga	-3.18104400	0.28742400	0.14344200
Fe	1.22708800	-0.58311100	0.86548000
Cl	-2.64431400	0.29511700	2.29781100
As	0.15207300	1.29884200	-0.14820900
As	2.03693700	0.36163000	-1.25209700
As	1.77347800	-1.97592800	-1.05286000
As	-0.47206300	-1.87743000	-0.27362300
As	-1.42420500	0.02292400	-1.50978000
Si	4.26129300	1.36200500	-1.47960300
N	-4.65959700	-0.98084000	-0.03436100
N	-4.23502900	1.91356300	-0.13488300
N	5.12425200	0.35084300	-0.11272900
N	4.19270100	2.25775300	0.20424800
C	0.56861600	-1.24751400	2.71362800
C	1.77680000	-1.90937700	2.35558800
C	2.78429600	-0.91879800	2.17177700
C	2.20130300	0.35485100	2.43445400
C	0.83066800	0.14883800	2.76170800
C	4.92141200	1.31278100	0.76665400
C	-5.88590100	-0.58371100	-0.29931700
C	-6.32623700	0.73016600	-0.49034600
H	-7.38242000	0.87685400	-0.71270000
C	-5.52574800	1.87219700	-0.38647400
H	-6.64736400	-1.37549300	-0.37406000
H	-6.02695600	2.84271100	-0.52585900
H	5.31422100	1.33368300	1.79767300
H	0.09178700	0.91236800	2.99621300
H	2.69820200	1.32092900	2.38729100
H	3.81570700	-1.11568700	1.88943500
H	1.90514500	-2.98245600	2.22226200
H	-0.39974900	-1.70739500	2.89922500
C	3.67320100	3.44920900	0.80356300
H	2.57007500	3.42736800	0.81618700
H	4.02907700	3.54984900	1.84187000
H	3.98971300	4.34443800	0.24546600
C	5.86123500	-0.86388600	0.05787800
H	6.28664200	-0.92328200	1.07286900
H	5.20499500	-1.73732300	-0.09302800
H	6.69056700	-0.93205700	-0.66412200
C	-4.37856200	-2.38217300	0.18801600
H	-3.60192800	-2.73894900	-0.50840000
H	-3.99525700	-2.53611500	1.21005800
H	-5.28270400	-2.99740600	0.05367000
C	-3.55353900	3.18167500	-0.00837200
H	-3.15423200	3.30017000	1.01256100

H	-2.69888000	3.23267200	-0.70364200
H	-4.23011800	4.02472500	-0.22220300

VI.4.29 Int6^{M} – As/Si

0 1

Ga	2.65951700	0.07098700	-0.02310000
Fe	-1.66380400	-0.86365000	0.88773800
Cl	2.03284500	1.59376500	1.51039200
Si	-0.23442400	3.09338400	-0.53816000
N	-0.94137300	3.48366100	1.19250600
N	3.68152900	-1.23656300	1.00199400
N	-2.09633000	3.57562200	-0.61594700
N	4.18211700	0.90978500	-0.92332000
C	-1.20668600	-1.68909600	2.72368500
C	-1.01970800	-0.27888400	2.73275700
C	-2.56940600	-1.96069700	2.40670800
C	-2.27885700	0.32553300	2.42452600
C	-3.22980300	-0.71445800	2.22068500
C	-2.10200800	3.84344900	0.67372400
C	5.83046200	-0.56513200	0.07400900
H	6.89579800	-0.79035000	0.10145000
C	4.99220600	-1.32760300	0.89093600
C	5.41496900	0.48876700	-0.74745800
H	6.19970700	1.02581400	-1.30241500
H	5.47729400	-2.08881500	1.52087000
H	-2.92510900	4.32935100	1.22501900
H	-4.27424600	-0.58118400	1.94312500
H	-3.02101400	-2.94589800	2.30589300
H	-0.43765600	-2.43653200	2.91165900
H	-0.07765800	0.24151200	2.90265000
H	-2.47218900	1.39322000	2.34048000
As	0.99370400	-0.59637400	-1.67177000
As	-0.06245600	-2.33302800	-0.24597100
As	-0.65275300	0.70109600	-0.50561300
As	-2.80964500	-0.03718700	-1.17425500
As	-2.33082800	-2.33706600	-0.96022700
C	-3.14192600	3.81182800	-1.56521800
H	-3.44108200	2.86942800	-2.05243000
H	-4.02963600	4.23699200	-1.06956600
H	-2.81564200	4.51460400	-2.34872700
C	-0.50469900	3.65950600	2.54624900
H	0.42911600	4.24085100	2.58441300
H	-1.27103000	4.19184200	3.13333100
H	-0.30602800	2.68888100	3.02510100
C	3.90699900	2.04344000	-1.77805900
H	4.83031700	2.43496700	-2.23409300
H	3.21103700	1.75716800	-2.58426400
H	3.42616600	2.85067700	-1.20122000
C	2.98190300	-2.05547400	1.96886300
H	2.18813200	-2.64291000	1.47808000
H	3.67220100	-2.74812000	2.47603400
H	2.50195600	-1.41873200	2.73063300

VI.4.30 Int7^{M} – As/Si

0 1

Ga	2.72279700	-0.44215300	0.11323400
Fe	-2.18846100	-1.10879900	0.44531200
Cl	2.29437200	-0.06846900	2.26438000
As	1.19408000	0.50378300	-1.51026900
As	-1.29921000	0.80005600	1.63619700
As	-0.55603700	-1.26262600	-1.31577700
Si	0.15611200	1.73476100	0.13567200
As	-2.61405500	-0.19023100	-1.81041700
As	-3.12984800	1.11174300	0.11975000
N	3.15563200	-2.34341200	0.00072900
N	1.16547600	3.12910300	0.89401400
N	4.53629000	0.22497800	-0.22055400
N	-0.34304800	3.37844700	-0.62076500
C	-3.62025400	-1.74810700	1.82498500
C	4.36118500	-2.76080100	-0.32294700
C	5.53029400	-0.58210500	-0.52871000
C	-3.82987000	-2.35480900	0.55561900
C	-2.66204700	-3.09403200	0.21925700
C	5.48253900	-1.97556200	-0.61146700
H	6.40011300	-2.49468700	-0.88522200
C	0.51408900	4.01039700	0.14969000
C	-1.71970100	-2.93569700	1.28046700

C	-2.31534000	-2.10556400	2.26845400
H	0.66688700	5.10125900	0.17613300
H	6.50078900	-0.10573200	-0.73736700
H	4.50038200	-3.85198800	-0.36163700
H	-4.32402500	-1.10652000	2.35275500
H	-4.71771300	-2.24744500	-0.06558300
H	-2.51071800	-3.66666800	-0.69508500
H	-0.72314400	-3.36867800	1.32888600
H	-1.84704900	-1.79064100	3.19948100
C	2.12978400	-3.30356900	0.35066800
H	1.76799000	-3.10840100	1.37336300
H	1.26810600	-3.21586300	-0.33209400
H	2.51787900	-4.33337100	0.30372100
C	4.76526800	1.64693000	-0.11353300
H	3.97268900	2.20194500	-0.64226200
H	4.74736600	1.96714200	0.94212500
H	5.73768800	1.93291500	-0.54586800
C	-1.11518200	3.88566600	-1.71614500
H	-2.14751300	3.51274700	-1.64436900
H	-1.12884900	4.98682200	-1.70299600
H	-0.70066000	3.54658300	-2.67961300
C	1.92790600	3.40657800	2.07989100
H	2.37511700	4.41210300	2.02257700
H	1.29760700	3.35028400	2.98293700
H	2.72529700	2.66138300	2.19356000

VI.4.31 Int8^{M} – As/Si

0 1

Fe	2.61966500	-0.28256800	0.63716700
As	2.36482900	1.80135100	-0.72464200
As	3.16223200	-0.13017100	-1.79059900
As	2.11476100	-2.07977800	-0.98316500
As	0.34434900	-1.35383200	0.40983000
As	-1.08556200	-0.15064900	-1.26625100
Si	0.24301300	1.29042700	-0.04133700
Ga	-3.12240300	-0.07193300	0.04889500
Cl	-3.64988000	1.60962900	1.42478100
N	-0.29882900	1.75909400	1.66679800
C	-0.84858700	2.89995000	1.25176300
N	-0.63365300	3.03995100	-0.02510300
C	-0.43358700	1.18651500	2.97466100
H	-0.43104900	0.09070800	2.89108200
H	0.39097400	1.47616500	3.64795700
H	-1.39260900	1.48511800	3.42566700
H	-1.40884400	3.59097000	1.89650500
C	-1.09012800	4.07489200	-0.89629300
H	-1.80895800	3.67379300	-1.63056400
H	-0.24645100	4.50862600	-1.45651000
H	-1.58809300	4.88139200	-0.33443800
C	2.59461900	-0.59856300	2.67952100
H	1.70909600	-0.79641700	3.27955800
C	3.39516400	-1.58554400	2.03916300
H	3.23225000	-2.66143000	2.07099100
C	4.44543500	-0.91303300	1.34710200
H	5.21125800	-1.38308300	0.73235100
C	4.28944500	0.48027500	1.55951400
H	4.91666700	1.26326000	1.13675100
C	3.13616700	0.68112700	2.37797200
H	2.74340000	1.64233600	2.70498300
N	-4.59770900	-0.09353500	-1.24454900
C	-5.48126200	-1.06754900	-1.27894600
C	-5.54230300	-2.17358200	-0.42607100
C	-4.69631700	-2.39650200	0.66450200
N	-3.66718000	-1.66664500	1.04208100
C	-4.70014300	1.01873200	-2.16066200
H	-3.77157400	1.12251900	-2.74754700
H	-4.85159600	1.95862300	-1.60394700
H	-5.54030100	0.88771200	-2.86138700
H	-6.25714000	-0.99710700	-2.05701000
H	-6.33837200	-2.89684500	-0.59781800
H	-4.91853500	-3.27629200	1.28772600
C	-2.96045200	-1.99556000	2.26135500
H	-3.03658100	-1.16142200	2.97867700
H	-3.37949000	-2.89891800	2.73265100
H	-1.89191700	-2.17005800	2.05285900

VI.4.32 Int9^{M} – As/Si

0 1

Ga	-2.92456900	0.03689400	-0.12875100
Fe	2.37621500	-0.99992200	0.14943300
Cl	-2.69995400	-0.54034700	-2.23839300
As	0.14814300	1.82325500	-1.03908000
As	1.19912100	-0.30875400	-1.95339800
As	0.40284100	-2.12991900	-0.69497100
As	0.30170400	-1.00101300	1.41327900
As	-1.00041200	1.04409000	0.95949700
Si	1.99310700	1.12924500	0.19978400
N	-4.41579800	1.31586900	-0.09777800
N	-3.84856400	-1.40997300	0.80809500
N	2.36172200	2.21870800	1.68744700
N	3.39859200	2.34085900	-0.19250300
C	3.59315600	-1.63272500	1.69609600
C	3.30069900	-2.71377700	0.82355100
C	3.76998100	-2.36962400	-0.48260500
C	4.35338600	-1.07892700	-0.41439800
C	4.22968000	-0.61084200	0.93213900
C	3.29091200	2.86626800	1.01127800
C	-5.55712400	1.04762200	0.49490600
C	-5.89524500	-0.13561500	1.16101200
H	-6.88874000	-0.19712700	1.60342700
C	-5.07824500	-1.26573300	1.25817600
H	-6.32779700	1.83348600	0.45481800
H	-5.51247300	-2.14350200	1.76132800
H	3.87535300	3.72046700	1.39048800
H	4.61579700	0.32999900	1.32159900
H	4.78915200	-0.53144600	-1.24840300
H	3.67484500	-2.98316700	-1.37696700
H	2.79472900	-3.63837000	1.09659700
H	3.34042300	-1.57852400	2.75381800
C	4.16178800	2.81886400	-1.30387900
H	3.49985900	3.18043700	-2.10819200
H	4.82226600	3.64761200	-1.00193000
H	4.78706500	2.01473500	-1.72226700
C	1.94272300	2.40319600	3.04399500
H	2.49351500	3.23346900	3.51454900
H	0.86450300	2.62402200	3.08387100
H	2.11789900	1.48891800	3.63389100
C	-4.22739100	2.56451200	-0.79944100
H	-3.35551700	3.10630300	-0.39511900
H	-4.03031500	2.37366400	-1.86718500
H	-5.11393400	3.21343000	-0.71265300
C	-3.17829000	-2.68613000	0.94576800
H	-2.85782800	-3.05486700	-0.04212600
H	-2.27257500	-2.58725900	1.56638800
H	-3.84439900	-3.43510700	1.40357100

VI.4.33 Int1^{M} – P/Ge

0 1

Ga	-2.42249600	0.99451200	0.02548300
Fe	3.47522300	-0.14722200	-0.05043900
Cl	-4.62526400	1.08382100	-0.13150800
P	0.80564800	-1.74542300	-0.68826500
Ge	-1.65551000	-1.29948000	-0.39560800
P	1.89049100	-0.24878900	-1.86039700
P	1.68079700	-1.15828100	1.23066000
P	1.93625800	0.99270200	1.30675900
P	2.05911900	1.59124300	-0.73905000
N	-2.16238100	-2.48278900	1.09382100
N	-1.60442000	2.26340700	-1.18610000
N	-1.77962700	1.75358700	1.68249300
N	-3.15696100	-2.50101400	-0.83930700
C	5.25934200	0.75220200	0.30047800
C	5.01528900	-1.15116300	-0.97718100
C	5.09251800	-0.35341300	1.18469400
C	5.21535800	0.26003900	-1.03628900
C	-1.04047400	3.36576300	-0.73336700
C	-1.18656900	2.93463800	1.69981400
C	-0.89313700	3.74434800	0.60364700
H	-0.40900300	4.69924600	0.80208200
C	-3.12516900	-3.02317100	0.37463400
C	4.93962900	-1.52792400	0.39087300
H	-3.81081100	-3.80747500	0.73406900
H	5.28233200	0.86070200	-1.94189600

H	4.89737400	-1.81611600	-1.83089800
H	-0.62291800	4.04422600	-1.49118100
H	-0.87468600	3.30367000	2.68770500
H	4.75024700	-2.53199300	0.76658000
H	5.05021900	-0.30349900	2.27143300
H	5.36772000	1.79535700	0.59406000
C	-1.52447000	1.93956300	-2.59423200
H	-0.77082200	1.14857800	-2.76313200
H	-2.50106400	1.59036700	-2.96476100
H	-1.22406100	2.81756200	-3.18710400
C	-1.83211800	0.96657000	2.89592400
H	-2.79431600	0.43635500	2.96785800
H	-1.01482100	0.22315800	2.90776700
H	-1.72281100	1.60415700	3.78736700
C	-4.22755700	-2.58986800	-1.79091300
H	-4.86499500	-3.46237400	-1.57375100
H	-4.85592600	-1.68362700	-1.76290100
H	-3.82689500	-2.70766200	-2.80851800
C	-1.66023100	-2.92382500	2.36464000
H	-2.16170800	-3.85370100	2.67703400
H	-0.57597900	-3.10679000	2.30540700
H	-1.82509700	-2.16048600	3.14100900

VI.4.34 Int2^{M} – P/Ge

0 1

Ga	0.08574800	2.06744400	-0.03271900
Fe	-1.91060900	-1.59067600	0.07377900
Cl	1.91638100	3.25578700	0.31410600
P	0.76381200	-0.13864200	-0.39303700
Ge	3.17772000	-0.09695900	-0.82726900
P	-0.75829500	-0.81989500	-1.79363000
P	-0.00386900	-1.15022800	1.37887000
P	-0.30452100	-3.16437900	0.65196000
P	-0.75641400	-2.95210800	-1.43697000
N	3.25962700	-1.99983300	-0.11883400
N	-1.19261500	2.46459100	1.36534700
N	-0.90015100	2.81174900	-1.52756200
N	3.35246400	-0.25911000	1.17909600
C	-3.69615700	-2.56880600	0.24813000
C	-3.50137100	-0.28758300	-0.03106000
C	-3.34278600	-2.00233800	1.50560000
C	-3.80110400	-1.51230200	-0.70074400
C	-2.35603300	3.01786700	1.08370400
C	-2.11146300	3.30112600	-1.37162400
C	-2.83013400	3.39739800	-0.17467200
H	-3.82689600	3.83375200	-0.22222200
C	3.35315500	-1.57942200	1.12318800
C	-3.21994700	-0.59423700	1.32803800
H	3.43099400	-2.24121900	2.00233400
H	-4.03779800	-1.62399300	-1.75778700
H	-3.47761200	0.70531000	-0.47723600
H	-3.02186300	3.20404000	1.93958300
H	-2.60437100	3.67928500	-2.27967500
H	-2.92962000	0.12076500	2.09534400
H	-3.16474800	-2.55172000	2.42846200
H	-3.83533000	-3.62884700	0.04086200
C	-0.83143400	2.18896900	2.74067300
H	-0.63762000	1.11138300	2.87591900
H	0.08722800	2.73605900	3.00797200
H	-1.63466800	2.49540300	3.42912500
C	-0.27619700	2.79557200	-2.83440600
H	0.69957000	3.30517000	-2.79399800
H	-0.11162700	1.75564000	-3.16341100
H	-0.90754800	3.30134000	-3.58140900
C	3.25260100	0.53708000	2.36528300
H	3.78116700	0.05852700	3.20726200
H	3.69484300	1.52741700	2.19173100
H	2.19974400	0.68745400	2.66552400
C	3.27422000	-3.35947900	-0.56755500
H	3.35088100	-4.05107000	0.28767200
H	2.34488100	-3.60063900	-1.10761000
H	4.12644800	-3.54899500	-1.24118200

VI.4.35 Int3^{M} – P/Ge

0 1

Ga	0.08574800	2.06744400	-0.03271900
Fe	-1.91060900	-1.59067600	0.07377900

Cl	1.91638100	3.25578700	0.31410600
P	0.76381200	-0.13864200	-0.39303700
Ge	3.17772000	-0.09695900	-0.82726900
P	-0.75829500	-0.81989500	-1.79363000
P	-0.00386900	-1.15022800	1.37887000
P	-0.30452100	-3.16437900	0.65196000
P	-0.75641400	-2.95210800	-1.43697000
N	3.25962700	-1.99983300	-0.11883400
N	-1.19261500	2.46459100	1.36534700
N	-0.90015100	2.81174900	-1.52756200
N	3.35246400	-0.25911000	1.17909600
C	-3.69615700	-2.56880600	0.24813000
C	-3.50137100	-0.28758300	-0.03106000
C	-3.34278600	-2.00233800	1.50560000
C	-3.80110400	-1.51230200	-0.70074400
C	-2.35603300	3.01786700	1.08370400
C	-2.11146300	3.30112600	-1.37162400
C	-2.83013400	3.39739800	-0.17467200
H	-3.82689600	3.83375200	-0.22222200
C	3.35315500	-1.57942200	1.12318800
C	-3.21994700	-0.59423700	1.32803800
H	3.43099400	-2.24121900	2.00233400
H	-4.03779800	-1.62399300	-1.75778700
H	-3.47761200	0.70531000	-0.47723600
H	-3.02186300	3.20404000	1.93958300
H	-2.60437100	3.67928500	-2.27967500
H	-2.92962000	0.12076500	2.09534400
H	-3.16474800	-2.55172000	2.42846200
H	-3.83533000	-3.62884700	0.04086200
C	-0.83143400	2.18896900	2.74067300
H	-0.63762000	1.11138300	2.87591900
H	0.08722800	2.73605900	3.00797200
H	-1.63466800	2.49540300	3.42912500
C	-0.27619700	2.79557200	-2.83440600
H	0.69957000	3.30517000	-2.79399800
H	-0.11162700	1.75564000	-3.16341100
H	-0.90754800	3.30134000	-3.58140900
C	3.25260100	0.53708000	2.36528300
H	3.78116700	0.05852700	3.20726200
H	3.69484300	1.52741700	2.19173100
H	2.19974400	0.68745400	2.66552400
C	3.27422000	-3.35947900	-0.56755500
H	3.35088100	-4.05107000	0.28767200
H	2.34488100	-3.60063900	-1.10761000
H	4.12644800	-3.54899500	-1.24118200

VI.4.36 Int4^{M} – P/Ge

0 1

Ga	-2.92334900	-0.92878600	-0.00000900
Fe	1.22041300	1.74213600	0.00005900
Cl	-4.12293500	-2.76717400	-0.00020700
Ge	2.46022300	-0.97570700	-0.00003600
N	2.84096700	-2.93698700	-0.00014700
N	-3.52907700	0.21372500	1.46044300
N	4.39848900	-1.41999100	-0.00024000
N	-3.52915400	0.21407100	-1.46016000
C	0.17980600	3.49081500	0.00033300
C	1.01639100	3.42613300	1.15158800
C	1.01600300	3.42628300	-1.15121500
C	2.36899900	3.32849700	0.70815900
C	2.36875500	3.32859600	-0.70825700
C	4.13647500	-2.71077000	-0.00029300
C	-4.11056700	2.06663200	0.00037700
H	-4.46246400	3.09752700	0.00050800
C	-3.93869500	1.44464000	1.24187000
C	-3.93876800	1.44493200	-1.24127200
H	-4.18397800	2.04156800	-2.13317000
H	-4.18384500	2.04107000	2.13392300
H	4.90776400	-3.49953600	-0.00049500
H	3.24349500	3.23420500	-1.34912900
H	0.68062700	3.43154000	-2.18754600
H	-0.90854500	3.54182300	0.00052000
H	0.68136900	3.43125800	2.18803400
H	3.24395800	3.23403300	1.34872000
P	-0.59935000	-1.23741600	-0.00008500
P	-0.13836100	0.48231500	-1.38365000
P	-0.13834300	0.48218000	1.38365300
P	1.97132900	0.28889500	1.79992200

P	1.97130500	0.28901300	-1.79991400
C	5.67723200	-0.77886200	-0.00094600
H	5.79719600	-0.13989300	0.88897700
H	6.49038400	-1.52340700	-0.00097000
H	5.79656800	-0.14051300	-0.89140600
C	2.14649800	-4.18779900	0.00039100
H	1.49826800	-4.27521400	-0.88573300
H	2.85641700	-5.03143700	-0.00144700
H	1.50143100	-4.27642800	0.88872300
C	-3.42745100	-0.29481400	-2.80915400
H	-3.84277500	0.41998200	-3.53730600
H	-2.36998300	-0.47639600	-3.06893000
H	-3.97481400	-1.24675000	-2.89614400
C	-3.42727000	-0.29547000	2.80931100
H	-2.36978200	-0.47711200	3.06896500
H	-3.84253800	0.41915700	3.53766100
H	-3.97462400	-1.24742800	2.89612400

VI.4.37 Int5^{M} – P/Ge

0 1

Ga	-3.15029500	0.22927700	0.06082200
Fe	1.00692900	-1.12612200	0.26744000
Cl	-2.84164200	-0.84219100	1.97164600
P	0.13583400	1.01976700	0.21105500
P	1.85484400	0.53005200	-0.98148900
P	1.43102000	-1.29423800	-2.03222600
P	-0.60923500	-1.47532800	-1.33010600
P	-1.36267800	0.62520500	-1.38516500
Ge	3.98440600	1.68078300	-1.00440300
N	-4.65283700	-0.65070400	-0.82261300
N	-4.07405200	1.88992200	0.51593200
N	4.94130200	0.07381800	-0.20872900
N	4.01183300	1.60674100	1.02374700
C	0.23242300	-2.58315300	1.51879300
C	1.41162200	-3.05721100	0.87571000
C	2.48327000	-2.18583700	1.22309600
C	1.96687700	-1.18052500	2.09375600
C	0.57512300	-1.42412700	2.26689500
C	4.70566500	0.48858100	1.01700700
C	-5.80940300	-0.04394200	-0.98270400
C	-6.15146900	1.24746500	-0.56693300
H	-7.15767500	1.59648900	-0.79546800
C	-5.31841100	2.11187500	0.15063000
H	-6.59366700	-0.62152200	-1.49611800
H	-5.74810700	3.08125900	0.44745800
H	5.04416400	-0.03830900	1.92749700
H	-0.12671300	-0.82297200	2.84103100
H	2.52243600	-0.35869100	2.53947000
H	3.51120400	-2.27968300	0.87884900
H	1.47727400	-3.91446400	0.20754300
H	-0.76904600	-3.00019100	1.43719300
C	3.47021900	2.28568400	2.16108800
H	2.36695300	2.25089200	2.14654600
H	3.81782900	1.81880200	3.09834400
H	3.77674800	3.34390600	2.17641000
C	5.62459700	-1.11898400	-0.60362200
H	6.00636900	-1.66301600	0.27699000
H	4.94659900	-1.79299000	-1.15413700
H	6.48188600	-0.89278100	-1.25843700
C	-4.48104500	-2.02234000	-1.25027600
H	-3.59158400	-2.11889800	-1.89403900
H	-4.32200900	-2.67644900	-0.37699900
H	-5.36298900	-2.38095800	-1.80484100
C	-3.35421000	2.86451000	1.30391000
H	-3.10258300	2.44559400	2.29232800
H	-2.40502900	3.13438300	0.81137600
H	-3.94819800	3.78112300	1.44951800

VI.4.38 Int6^{M} – P/Ge

0 1

Ga	2.34002800	0.17818200	-0.09474500
Fe	-1.49972500	-1.71351000	0.17029900
Cl	1.38994500	1.33593200	1.57883400
Ge	-1.05023300	2.56958600	-0.31155900
N	-1.98066900	2.37666700	1.47599900
N	3.47614500	-1.14230800	0.77016200
N	-3.10651800	2.52164900	-0.38248400

N	3.76707600	1.34514200	-0.74084000
C	-0.93915600	-2.84210800	1.80650000
C	-1.11682500	-1.47561900	2.15983800
C	-2.17027400	-3.33694800	1.28823900
C	-2.47132600	-1.12565700	1.86177200
C	-3.11527900	-2.27437900	1.32107200
C	-3.17527900	2.47876400	0.92739600
C	5.55355800	-0.02590100	0.15940800
H	6.63669200	-0.10243700	0.24487500
C	4.79022000	-1.02952900	0.76028900
C	5.03667200	1.07857800	-0.52589400
H	5.76388800	1.80100200	-0.92726600
H	5.34392400	-1.81887600	1.29074700
H	-4.11674900	2.53694700	1.50375000
H	-4.14255300	-2.32262000	0.96313600
H	-2.34819600	-4.34044000	0.90600400
H	-0.01542500	-3.41136800	1.89267300
H	-0.35137600	-0.80627800	2.55094000
H	-2.92168700	-0.14590400	2.00285200
P	0.91317300	-0.35545200	-1.87196000
P	0.31321400	-2.39699500	-1.11609900
P	-0.87324100	0.19836500	-0.73835700
P	-2.57780700	-0.74223200	-1.68631200
P	-1.67065500	-2.67813700	-1.94336300
C	-4.20605000	2.60801800	-1.29470700
H	-4.23259900	1.72633800	-1.95647200
H	-5.16553800	2.65446800	-0.75177200
H	-4.12940800	3.50804600	-1.92670200
C	-1.68057100	2.37888000	2.87556300
H	-1.07314300	3.25514100	3.15573000
H	-2.60817000	2.40073500	3.47282500
H	-1.10790300	1.48165700	3.15567900
C	3.37681300	2.54783600	-1.44274300
H	4.25632500	3.11064800	-1.79381300
H	2.75036800	2.29499000	-2.31430000
H	2.78090600	3.20025000	-0.78306400
C	2.85261900	-2.22859700	1.49710400
H	2.21046600	-2.81988700	0.82344600
H	3.61038400	-2.89227300	1.94259200
H	2.21696100	-1.83141700	2.30563400

VI.4.39 Int7^{M} – P/Ge

0 1

Ga	2.20441000	-0.67857400	-0.03974600
Fe	-2.58314700	-0.95167900	0.15365300
Cl	1.65555900	-0.42492900	2.10296400
P	0.75433900	0.34671300	-1.55047500
P	-1.92103000	0.95090900	1.21654400
P	-0.90355200	-1.17740000	-1.39628100
Ge	-0.13385600	1.67438800	0.05689200
P	-2.70691300	-0.19253100	-2.04883300
P	-3.30479700	1.16727900	-0.46332300
N	2.59445400	-2.57240400	-0.27168800
N	1.05819800	2.99602100	0.95792700
N	4.02987700	-0.02174400	-0.27472600
N	-0.34479700	3.53495700	-0.61485700
C	-3.92619200	-1.46197200	1.63846200
C	3.80627600	-2.99421400	-0.56442900
C	5.02252700	-0.83148100	-0.58424600
C	-4.36304800	-1.96739400	0.38383200
C	-3.36382200	-2.85218000	-0.10860900
C	4.95557200	-2.21668300	-0.74469900
H	5.87577400	-2.73726500	-1.00654400
C	0.53747200	3.98227900	0.24405600
C	-2.30505000	-2.89099300	0.84581100
C	-2.64709300	-2.03171900	1.92120500
H	0.80921100	5.04444800	0.36333100
H	6.00794200	-0.36246100	-0.72857800
H	3.92498600	-4.08290100	-0.67323400
H	-4.45882700	-0.74366200	2.26032100
H	-5.28201500	-1.69161000	-0.13134900
H	-3.38948200	-3.38221100	-1.05939300
H	-1.38289200	-3.46050700	0.75502800
H	-2.02833200	-1.82581800	2.79294000
C	1.52897100	-3.53021900	-0.05357300
H	1.13325900	-3.42225800	0.96956600
H	0.69904300	-3.34479000	-0.75585900
H	1.89208700	-4.56168900	-0.18515700

C	4.27885800	1.39083300	-0.09898200
H	3.51193900	1.98235600	-0.62495000
H	4.23497100	1.66691900	0.96779500
H	5.26834600	1.67594900	-0.49091000
C	-1.04707000	4.24761500	-1.63826000
H	-2.12329300	4.02357500	-1.57790300
H	-0.90557700	5.33521600	-1.52848100
H	-0.69851600	3.94749300	-2.64005200
C	1.80686100	3.13706100	2.17595900
H	2.55229700	3.94580800	2.08998400
H	1.15405000	3.35293800	3.03917800
H	2.32865800	2.19536000	2.39026000

VI.4.40 Int8^{M} – P/Ge

0 1

Fe	2.89282700	-0.62163200	0.05743500
P	2.75302800	1.51235100	-0.94374600
P	3.19466100	-0.15142900	-2.22707300
P	2.13498500	-1.95336900	-1.69847000
P	0.66492800	-1.44851600	-0.20809200
P	-0.77479000	-0.11509100	-1.38368700
Ge	0.61642600	1.30097600	-0.31419700
Ga	-2.64044900	-0.22620400	0.01767200
Cl	-3.15532000	1.40425100	1.43957000
N	0.21844800	1.65571400	1.55992900
C	-0.34921400	2.82772100	1.30556500
N	-0.25921300	3.14353800	0.04382500
C	0.19949200	0.95358100	2.80757400
H	0.03065800	-0.11753000	2.62586500
H	1.14948700	1.05439600	3.35945200
H	-0.62325100	1.31719800	3.44313000
H	-0.84748100	3.43712400	2.07423800
C	-0.82927600	4.28536400	-0.59981300
H	-1.63872300	3.98598200	-1.28698100
H	-0.06936400	4.82065500	-1.19118300
H	-1.25367700	4.99064500	0.13420500
C	2.98111100	-1.13901800	2.05974800
H	2.12134800	-1.25140700	2.71631000
C	3.54616100	-2.16728600	1.25397900
H	3.19811100	-3.19714600	1.19267600
C	4.63403700	-1.60191600	0.52526700
H	5.24958600	-2.11954700	-0.20882600
C	4.73715000	-0.23246000	0.87960700
H	5.44716200	0.48242500	0.46669600
C	3.70617200	0.05986400	1.82444400
H	3.50737300	1.03218000	2.27215500
N	-4.18248000	-0.35590700	-1.17999400
C	-4.98220300	-1.40019800	-1.17433800
C	-4.89281900	-2.51746700	-0.33846400
C	-3.94775200	-2.69030300	0.67639600
N	-2.95676600	-1.88279600	0.99666500
C	-4.42222600	0.74659900	-2.08276700
H	-3.53522800	0.92404900	-2.71423500
H	-4.62062600	1.67012700	-1.51381800
H	-5.28352700	0.54810400	-2.74045600
H	-5.80912400	-1.38734500	-1.90098900
H	-5.63655800	-3.30252900	-0.46813600
H	-4.04259900	-3.60109700	1.28694200
C	-2.11956400	-2.19051100	2.13719100
H	-2.18886300	-1.38350600	2.88517600
H	-2.43082200	-3.13341300	2.61421400
H	-1.06718200	-2.28495400	1.82079000

VI.4.41 Int9^{M} – P/Ge

0 1

Ga	-2.90399400	0.06645400	-0.16965600
Fe	2.16260800	-1.24667400	0.08993300
Cl	-2.83825600	-0.65538900	-2.24137700
P	0.11914300	1.39304100	-1.23530200
P	0.99427500	-0.65964700	-1.94067500
P	0.19625400	-2.18663100	-0.68302200
P	0.11738200	-1.08380500	1.19216200
P	-0.87502000	0.85502000	0.67524400
Ge	1.99998900	0.96950900	0.00505100
N	-4.24392800	1.49079100	-0.10890900
N	-3.87906100	-1.23010900	0.91144400
N	2.38904900	2.32404600	1.41122500

N	3.51195000	2.19811600	-0.44823600
C	3.32342400	-1.91983200	1.66627000
C	2.88750100	-3.00582900	0.86196700
C	3.37785900	-2.80111500	-0.46596000
C	4.11700200	-1.59133200	-0.48224600
C	4.07028500	-1.03616600	0.83511800
C	3.35392800	2.84776400	0.68689200
C	-5.35771100	1.36958000	0.57850200
C	-5.75993000	0.26032800	1.33023400
H	-6.71836900	0.32272800	1.84409200
C	-5.05161200	-0.94087000	1.43681700
H	-6.04583300	2.22899200	0.55215100
H	-5.52940500	-1.74358500	2.01934400
H	3.95098200	3.72520600	0.98831200
H	4.55793700	-0.11687600	1.15862100
H	4.60344800	-1.15045800	-1.35069200
H	3.19040300	-3.44854700	-1.32103500
H	2.27181500	-3.84094000	1.19217200
H	3.08935600	-1.76756200	2.71839000
C	4.42627200	2.49645100	-1.50713900
H	3.88759300	2.73486700	-2.43878000
H	5.06206200	3.35982300	-1.24962700
H	5.08588200	1.63806700	-1.71495300
C	1.88866100	2.75996100	2.67940300
H	2.37290100	3.69960200	2.99335500
H	0.80112100	2.92369300	2.62023800
H	2.06679100	2.00049800	3.45832000
C	-3.97906800	2.68245500	-0.88204800
H	-3.02166000	3.13510100	-0.57362400
H	-3.89329400	2.43073700	-1.95186000
H	-4.77887900	3.43000300	-0.75596500
C	-3.32017400	-2.55695700	1.07304400
H	-3.11919700	-3.00483100	0.08631600
H	-2.35983600	-2.50958400	1.61256600
H	-4.01233100	-3.21236500	1.62560700

VI.4.42 Int1^{M} – As/Ge

0 1

Ga	-2.61781100	0.81563700	0.00654200
Fe	2.84963800	0.31569700	0.15417900
Cl	-4.74418200	0.17226500	-0.00287500
As	0.56554600	-1.92703200	-1.46316300
Ge	-1.27266000	-1.22255400	-0.11442700
As	1.57404300	0.25975500	-1.94497000
As	1.78372500	-1.75411200	0.65669600
As	0.90699700	0.27179900	1.66589300
As	0.96099900	1.75516000	-0.19827000
N	-1.70303200	-2.37309600	1.41300100
N	-2.34481200	2.10681200	-1.40645200
N	-2.44196900	2.00338900	1.52194800
N	-2.75776300	-2.61911600	-0.47440900
C	4.14524900	1.58019700	1.11567900
C	4.69830800	0.39208600	-0.77986200
C	4.40896900	0.23539900	1.50280300
C	4.33427100	1.67946700	-0.29342100
C	-2.19435400	3.38688300	-1.13214800
C	-2.28600800	3.30041500	1.34797500
C	-2.18325900	3.98135000	0.13237100
H	-2.05245900	5.06163400	0.17501800
C	-2.66771800	-3.01290100	0.76563600
C	4.74642400	-0.49892400	0.32865000
H	-3.31304300	-3.77311800	1.23653900
H	4.19742300	2.57647800	-0.89534900
H	4.89029100	0.13085100	-1.81882500
H	-2.05280900	4.05354900	-1.99554800
H	-2.22972100	3.90762800	2.26363300
H	4.99488900	-1.55794500	0.28493800
H	4.34090400	-0.16537900	2.51318200
H	3.83996600	2.38878900	1.77835800
C	-2.23791900	1.63334100	-2.76872100
H	-1.30255900	1.05950200	-2.89918200
H	-3.09047900	0.98081100	-3.01542000
H	-2.22531500	2.47288000	-3.48133100
C	-2.53880900	1.44777300	2.85276900
H	-3.47683700	0.87944500	2.96025800
H	-1.69294600	0.76517400	3.04346300
H	-2.51856500	2.24047900	3.61695300
C	-3.76850100	-2.98130600	-1.42021500

H	-4.32759600	-3.87085100	-1.08390100
H	-4.48710200	-2.15610400	-1.55710700
H	-3.31197600	-3.21459800	-2.39491800
C	-1.24781700	-2.61743900	2.75009000
H	-1.90477700	-3.35183800	3.24449600
H	-0.21594600	-3.00329000	2.75523600
H	-1.25684400	-1.69151000	3.34620400

VI.4.43 Int2^{M} – As/Ge

0 1

Ga	-2.33347400	-1.10181400	-0.01766400
Fe	2.11254200	-1.04558700	0.28215800
Cl	-4.30230900	-0.14074900	0.27011000
As	-0.69154900	0.62850200	-0.43651200
Ge	-1.97515500	2.78680100	-0.88970100
As	0.86409800	-0.61753500	-1.77455600
As	0.63906100	0.49025900	1.55214200
As	2.75759500	1.25515500	0.81908000
As	2.88410300	0.56586200	-1.42978600
N	-0.38419100	3.78888000	-0.12169500
N	-2.04475900	-2.36195400	1.42977600
N	-2.42549400	-2.38943500	-1.47123500
N	-1.97509900	2.98637400	1.12117200
C	3.82186900	-2.13386700	0.57942200
C	1.72833000	-3.06962700	0.32541200
C	3.12840000	-1.99787200	1.81527500
C	2.96292900	-2.80034700	-0.33988800
C	-1.85860100	-3.64464900	1.18907400
C	-2.16673900	-3.66447800	-1.27489900
C	-1.87414700	-4.28284500	-0.05414600
H	-1.68869700	-5.35603700	-0.06752400
C	-0.82629200	3.64039100	1.10786100
C	1.83529700	-2.57364800	1.65341900
H	-0.31147600	4.01784000	2.00735100
H	3.20104900	-3.04339500	-1.37442800
H	0.85518000	-3.55928600	-0.10335100
H	-1.67925000	-4.28063300	2.06891500
H	-2.19350500	-4.31008100	-2.16550900
H	1.05544800	-2.61049400	2.41192000
H	3.51061400	-1.51825600	2.71475600
H	4.82676100	-1.77190300	0.36696000
C	-2.06540700	-1.87401400	2.79264200
H	-1.25776000	-1.13892800	2.95044600
H	-3.02550500	-1.37498400	3.00141700
H	-1.93535100	-2.69899300	3.51067000
C	-2.73192900	-1.89843800	-2.79783800
H	-3.69481800	-1.36349300	-2.79149600
H	-1.95076700	-1.19665200	-3.13630600
H	-2.79181700	-2.72435600	-3.52365200
C	-2.66457700	2.50536900	2.28025200
H	-2.48976400	3.16692300	3.14550800
H	-3.74536300	2.46054800	2.08741100
H	-2.33410000	1.48810200	2.55751300
C	0.83418500	4.42432800	-0.52438600
H	1.35751200	4.85044900	0.34743900
H	1.51501100	3.69840100	-0.99822300
H	0.64011200	5.23894700	-1.24119700

VI.4.44 Int3^{M} – As/Ge

0 1

Fe	0.59533600	-1.98209700	0.64532000
As	-0.68387500	-1.58773200	-1.36397100
As	1.56760100	-2.30443300	-1.63389500
As	2.63889800	-0.99676200	-0.00034000
As	0.77254800	0.46423400	0.78354300
As	-0.45964600	0.84009100	-1.31805100
Ga	-2.53007100	1.09779600	-0.05506100
Cl	-3.23772100	3.19407200	-0.07452400
Ge	2.42440900	1.83357100	-0.77960600
N	1.54995800	3.50262500	0.06432600
C	2.56539200	3.66305100	0.88213300
N	3.42489200	2.66926000	0.81677200
C	0.47788100	4.42645300	-0.15663200
H	0.57156800	5.30243400	0.50883800
H	-0.50371400	3.96092100	0.03059500
H	0.47138200	4.79115700	-1.19709500
H	2.68868500	4.54314900	1.54135200

C	4.61983000	2.52523100	1.58737200
H	4.60203100	1.59095100	2.17379300
H	5.51493800	2.49181200	0.94363600
H	4.74427900	3.36536600	2.29283300
C	-0.98650700	-2.93447000	1.58303700
H	-2.03654900	-2.84018300	1.31064700
C	-0.05812600	-3.88433900	1.06572800
H	-0.26845200	-4.64296800	0.31323700
C	1.20643400	-3.64212000	1.67456400
H	2.12622700	-4.18873100	1.47107800
C	1.06176000	-2.55034700	2.57927600
H	1.84876500	-2.11670500	3.19436000
C	-0.29105500	-2.11196800	2.51250600
H	-0.71721300	-1.27549200	3.06347800
N	-2.77495400	0.53077400	1.80101300
C	-3.56885500	-0.47282400	2.11536200
C	-4.33795000	-1.24922400	1.24467000
C	-4.48751400	-1.00864600	-0.12641100
N	-3.89614000	-0.06950400	-0.83052900
C	-2.16568600	1.32052500	2.84987300
H	-2.52194300	2.36182100	2.79131400
H	-1.06876400	1.33449500	2.73649500
H	-2.41335300	0.91716500	3.84489500
H	-3.64038100	-0.71644400	3.18660400
H	-4.91933100	-2.06198800	1.67823800
H	-5.18391700	-1.66334000	-0.67210300
C	-4.17609800	0.06940900	-2.24225500
H	-4.95542400	-0.63811600	-2.56658000
H	-4.51505600	1.09380400	-2.46449100
H	-3.26581900	-0.12432200	-2.83512400

VI.4.45 Int4^{M} – As/Ge

0 1

Ga	-3.24282100	-0.88117300	0.00007000
Fe	1.18420600	1.77097700	0.00002200
Cl	-4.61244700	-2.60252600	-0.00006100
Ge	2.43259700	-1.08132100	-0.00010000
N	2.67777000	-3.07086700	-0.00020500
N	-3.77574100	0.31010100	1.45837700
N	4.33756600	-1.66459000	-0.00026300
N	-3.77586600	0.31040400	-1.45794400
C	0.18503200	3.54804800	0.00029500
C	1.01879900	3.46296900	1.15226100
C	1.01838700	3.46310800	-1.15198200
C	2.36828000	3.32931300	0.70826100
C	2.36802300	3.32940600	-0.70848300
C	3.98508000	-2.93414100	-0.00029900
C	-4.19168400	2.20803600	0.00043200
H	-4.45144000	3.26591900	0.00055300
C	-4.08077600	1.57126700	1.24161900
C	-4.08088600	1.57152400	-1.24089700
H	-4.28253800	2.18452300	-2.13283100
H	-4.28234100	2.18408300	2.13369900
H	4.69996600	-3.77470000	-0.00043700
H	3.24254500	3.22142800	-1.34730600
H	0.68384600	3.48899600	-2.18843600
H	-0.90136000	3.63281600	0.00049400
H	0.68463000	3.48873100	2.18883800
H	3.24303300	3.22126100	1.34675600
As	-0.86753200	-1.40675900	-0.00005900
As	-0.31467400	0.52021600	-1.45542500
As	-0.31459000	0.52009100	1.45544600
As	2.00328100	0.25218300	1.88869200
As	2.00317100	0.25229800	-1.88879200
C	5.65959100	-1.11843100	-0.00059500
H	5.82738600	-0.49025700	0.88949300
H	6.41587300	-1.92078500	-0.00070100
H	5.82700400	-0.49038100	-0.89084500
C	1.90442700	-4.27453900	0.00004200
H	1.25229900	-4.32064500	-0.88644500
H	2.55924400	-5.16179200	-0.00116800
H	1.25421500	-4.32165200	0.88789700
C	-3.75123700	-0.21615100	-2.80322000
H	-4.05642900	0.54647600	-3.53733600
H	-2.73447400	-0.55791900	-3.06335700
H	-4.43105900	-1.07946900	-2.88402500
C	-3.75096700	-0.21672800	2.80354300
H	-2.73417300	-0.55853800	3.06350300

H	-4.05608900	0.54574700	3.53784600
H	-4.43077200	-1.08006900	2.88424400

VI.4.46 Int5^{M} – As/Ge

0 1

Ga	-3.36917400	0.32832300	0.13570600
Fe	0.97828700	-0.79696800	0.87334100
Cl	-2.90781800	0.04306700	2.28866300
As	0.00516500	1.23824300	0.07589600
As	1.89365300	0.37542600	-1.08117200
As	1.54245900	-1.95656900	-1.18955700
As	-0.72407400	-1.87011100	-0.47211900
As	-1.56608900	0.20665900	-1.48406900
Ge	4.15795500	1.30936500	-1.11219600
N	-4.88376200	-0.84894600	-0.24676900
N	-4.35576600	2.01629100	0.03531400
N	4.93720200	0.10095200	0.14000300
N	4.06191700	1.98730500	0.66926300
C	0.23322100	-1.66334000	2.60104000
C	1.42944000	-2.32111800	2.19811000
C	2.47649200	-1.35514300	2.17250100
C	1.92925800	-0.10318200	2.57770600
C	0.54173900	-0.29547600	2.83459300
C	4.73737700	0.95129600	1.12831900
C	-6.08557900	-0.37421100	-0.49576000
C	-6.47313900	0.96937400	-0.53092700
H	-7.51521500	1.18387600	-0.76448200
C	-5.63760200	2.05718800	-0.25826200
H	-6.87099700	-1.12004000	-0.69372500
H	-6.09967400	3.05626300	-0.28783200
H	5.09454700	0.82657100	2.16495200
H	-0.17791600	0.46044900	3.14214800
H	2.46072300	0.84108400	2.66906300
H	3.50965200	-1.55471500	1.89856200
H	1.52503300	-3.37294100	1.93301300
H	-0.75639300	-2.10501400	2.69724700
C	3.56352900	3.11281900	1.39964100
H	2.46053900	3.13242200	1.37614400
H	3.88632400	3.06764700	2.45255200
H	3.93015200	4.05838000	0.97000200
C	5.62520100	-1.15329800	0.17649800
H	6.01270100	-1.35686000	1.18798800
H	4.94469700	-1.97453500	-0.10421300
H	6.47629800	-1.16191500	-0.52299000
C	-4.65943700	-2.27699200	-0.19647100
H	-3.87188100	-2.57286800	-0.90897100
H	-4.31751400	-2.57352600	0.80868900
H	-5.57915900	-2.83475100	-0.43531900
C	-3.63549700	3.23084400	0.34291000
H	-3.26809900	3.20387700	1.38218100
H	-2.75589900	3.33599100	-0.31412500
H	-4.27455900	4.11978400	0.21800500

VI.4.47 Int6^{M} – As/Ge

0 1

Ga	2.67265200	0.06913300	-0.01689500
Fe	-1.56819100	-1.10112700	0.87990200
Cl	1.99874800	1.68079500	1.40992400
Ge	-0.37012000	3.02770500	-0.50526400
N	-1.15468400	3.30024900	1.34583000
N	3.65111900	-1.17418000	1.12515800
N	-2.40428200	3.35611400	-0.43708300
N	4.23477800	0.84911300	-0.90446000
C	-1.04242900	-1.91254600	2.70392100
C	-0.94145800	-0.49348600	2.72340700
C	-2.38947600	-2.26367600	2.39843400
C	-2.23820200	0.03564400	2.43383900
C	-3.12612600	-1.05830200	2.23029900
C	-2.35876600	3.53503900	0.86282200
C	5.83380000	-0.59057500	0.21603500
H	6.89424300	-0.82958600	0.28463500
C	4.96255000	-1.28964400	1.05509400
C	5.45665600	0.42216400	-0.67190000
H	6.26401600	0.91889000	-1.23187300
H	5.41937000	-2.01590200	1.74451100
H	-3.21964500	3.85548800	1.47786200
H	-4.17952400	-0.98618900	1.96421700

H	-2.78121900	-3.27377100	2.29376100
H	-0.22894600	-2.61450900	2.87909900
H	-0.03363600	0.08525300	2.89109300
H	-2.49410000	1.09037600	2.36083600
As	1.05131100	-0.65271000	-1.68788900
As	0.10094300	-2.46799900	-0.28725800
As	-0.66809600	0.53711300	-0.50504500
As	-2.78057100	-0.32042200	-1.16455800
As	-2.17028700	-2.59116500	-0.97703700
C	-3.54993100	3.50595200	-1.28117500
H	-3.77076100	2.56448100	-1.81109300
H	-4.44179600	3.77885200	-0.69157800
H	-3.38969400	4.29155300	-2.03816600
C	-0.73270600	3.46245400	2.70417000
H	0.02397700	4.25863800	2.79903300
H	-1.58842000	3.72481200	3.34956600
H	-0.28060000	2.53494400	3.08671400
C	4.00340800	1.94668500	-1.81669800
H	4.94072000	2.27931500	-2.29055600
H	3.29813900	1.64533400	-2.60914300
H	3.55662000	2.80129600	-1.28190600
C	2.91720800	-1.91946900	2.12565000
H	2.13709600	-2.53811000	1.65167400
H	3.58790600	-2.57604100	2.70217900
H	2.41757900	-1.22848800	2.82466400

VI.4.48 Int7^{M} – As/Ge

0 1

Ga	2.72785800	-0.57811000	0.08975900
Fe	-2.25494600	-1.14004800	0.47127900
Cl	2.27747000	-0.08638800	2.21810700
As	1.17958300	0.32005600	-1.54901500
As	-1.42764900	0.80825700	1.61115400
As	-0.56332900	-1.42149100	-1.23182600
Ge	0.20568100	1.66426200	0.14407800
As	-2.59664100	-0.36157300	-1.84636300
As	-3.14786100	1.08367400	-0.03717300
N	3.13498700	-2.48717600	0.09217500
N	1.33447400	3.14285200	0.87530600
N	4.54821500	0.04813800	-0.27250700
N	-0.21068700	3.45717700	-0.62393500
C	-3.71964500	-1.69223600	1.84973500
C	4.33914600	-2.93692300	-0.19164800
C	5.53544300	-0.78797000	-0.52006100
C	-3.92578900	-2.34473700	0.60347100
C	-2.77131000	-3.12434800	0.31480400
C	5.47245800	-2.18324000	-0.51519100
H	6.38678300	-2.72837400	-0.74588000
C	0.69406700	4.02964000	0.13262800
C	-1.84103800	-2.94628500	1.38322400
C	-2.42947800	-2.06320900	2.32795400
H	0.89628800	5.11392500	0.15041400
H	6.51284200	-0.33625600	-0.74987900
H	4.46606100	-4.02983000	-0.16157900
H	-4.41508600	-1.01294500	2.34019100
H	-4.80151300	-2.24093700	-0.03530300
H	-2.62015200	-3.73643000	-0.57363800
H	-0.85512500	-3.39937600	1.46240000
H	-1.96870700	-1.72621400	3.25503300
C	2.09411400	-3.41311500	0.48871200
H	1.71555200	-3.14425000	1.48834600
H	1.24540500	-3.36661900	-0.21402900
H	2.47446600	-4.44632900	0.52098700
C	4.79149900	1.47216800	-0.25906400
H	4.01582900	1.99802500	-0.83980400
H	4.75647300	1.86493700	0.77109100
H	5.77544200	1.71675100	-0.69051000
C	-1.00612000	4.04081000	-1.66065600
H	-2.06044200	3.75116900	-1.53275100
H	-0.93643100	5.14074500	-1.63634600
H	-0.68219700	3.69118800	-2.65496300
C	2.16380800	3.42997500	2.01107600
H	2.72528800	4.36718700	1.85809900
H	1.57206100	3.52489500	2.93772800
H	2.87611700	2.60904100	2.16542700

VI.4.49 Int8^{M} – As/Ge

0 1

Fe	2.65657700	-0.41271100	0.64723800
As	2.41639800	1.74743500	-0.53809100
As	3.15097100	-0.12802700	-1.77271200
As	2.08648300	-2.10293900	-1.02749600
As	0.33899300	-1.41319300	0.41796200
As	-1.09507000	-0.28869200	-1.30453100
Ge	0.11634600	1.42177800	-0.22986600
Ga	-3.15414300	-0.15743800	-0.02062000
Cl	-3.99711100	1.84179700	0.48175700
N	-0.48946800	1.95161300	1.56562600
C	-1.07409500	3.05721900	1.11948200
N	-0.92210200	3.19982100	-0.16852700
C	-0.16584500	1.66680600	2.93115900
H	-0.20438600	0.58413200	3.10744900
H	0.84611400	2.01311800	3.20290700
H	-0.88906300	2.15150300	3.60818000
H	-1.62819800	3.75316700	1.76872200
C	-1.65739700	4.09177200	-1.01340900
H	-2.55463600	3.59692400	-1.42228900
H	-1.02525800	4.42576400	-1.84906600
H	-1.99114900	4.98309300	-0.45597800
C	2.63737700	-0.61149700	2.71049600
H	1.75135900	-0.61659400	3.34164900
C	3.22865000	-1.75520000	2.10092900
H	2.87858400	-2.78273300	2.18900300
C	4.35859500	-1.31285900	1.35129000
H	5.00708900	-1.94146600	0.74293600
C	4.46464700	0.09412400	1.49854300
H	5.21143800	0.73141000	1.02758000
C	3.39408700	0.53071400	2.33662700
H	3.19877800	1.55896200	2.63480300
N	-4.54361000	-1.00329200	-1.11955600
C	-5.23237400	-2.04142400	-0.69928500
C	-5.11956200	-2.67360500	0.54327900
C	-4.27799300	-2.26269800	1.57909800
N	-3.41776500	-1.26391800	1.56505200
C	-4.81739700	-0.42306900	-2.41490600
H	-3.90378500	-0.40834300	-3.03259900
H	-5.16026100	0.61850800	-2.30035300
H	-5.59248100	-0.99102800	-2.95383100
H	-5.98012800	-2.44816300	-1.39756600
H	-5.76397000	-3.53125700	0.73149000
H	-4.34394400	-2.82841900	2.52088200
C	-2.66451700	-0.95114600	2.75856600
H	-2.78619800	0.11353600	3.01372200
H	-3.00449300	-1.55609000	3.61413600
H	-1.59119100	-1.14802400	2.59637000

VI.4.50 Int9^{M} – As/Ge

0 1

Ga	-3.02528000	0.07439800	-0.12172700
Fe	2.24612200	-1.14074500	0.18026500
Cl	-2.84385400	-0.66640800	-2.18435600
As	0.07341900	1.65858100	-1.21350000
As	1.04657000	-0.58252200	-1.97106100
As	0.21829700	-2.26352600	-0.56251500
As	0.16627800	-1.00036700	1.46218900
As	-1.04482600	1.06998800	0.87093600
Ge	1.97583800	1.07847100	0.11371400
N	-4.45716200	1.41715200	-0.17250400
N	-3.99877900	-1.25825000	0.92566900
N	2.38281500	2.35213400	1.60181800
N	3.52316100	2.31529100	-0.25250300
C	3.45189900	-1.75786600	1.74698400
C	3.08669700	-2.86274800	0.93226000
C	3.55531500	-2.61008000	-0.39456400
C	4.21082300	-1.35196300	-0.39896400
C	4.13504000	-0.81616800	0.92515000
C	3.36347500	2.89861200	0.91672900
C	-5.59981500	1.24577800	0.45288500
C	-5.97993300	0.13158100	1.20931100
H	-6.96804000	0.14856400	1.66744900
C	-5.21365800	-1.02509000	1.37906400
H	-6.33514600	2.06086100	0.36385000
H	-5.67937300	-1.84319400	1.94996100

H	3.97345400	3.74534200	1.27611400
H	4.56398100	0.12837200	1.25796700
H	4.66527300	-0.87113800	-1.26353400
H	3.41307200	-3.26123900	-1.25555100
H	2.53734700	-3.74486000	1.25714200
H	3.21893100	-1.63625300	2.80347500
C	4.43738900	2.68216700	-1.28904200
H	3.90031500	3.00037600	-2.19799300
H	5.08745100	3.51400000	-0.96954500
H	5.08396400	1.83337400	-1.56600000
C	1.90987000	2.70688800	2.90484100
H	2.48122100	3.55664700	3.31482900
H	0.84448400	2.98535500	2.86684000
H	2.00442500	1.85853900	3.60237800
C	-4.22452900	2.60031500	-0.96832400
H	-3.32231400	3.12963600	-0.61777500
H	-4.05444100	2.32180400	-2.02130500
H	-5.07936000	3.29403600	-0.91829200
C	-3.38482300	-2.55096200	1.14669500
H	-3.09554400	-3.00295600	0.18406000
H	-2.46702300	-2.45018400	1.74900800
H	-4.07756100	-3.23434800	1.66366200

VII. References

[S1] J. Schoening, A. Gehlhaar, C. Wölper and S. Schulz, *Chem. Eur. J.*, 2022, **28**, e202201031;

[S2] N. J. Hardman, B. E. Eichler and P. P. Power, *Chem. Commun*., 2022, 1991-1992.

[S3] S. Nagendran, S. S. Sen, H. W. Roesky, D. Koley, H. Grubmüller, A. Pal. and R. Herbst-Irmer, *Organometallics*, 2008, **27**, 5459-5436.

[S4] O. J. Scherer and T. Brück, *Angew. Chem. Int. Ed*, 1987, **26**, 59-59.

[S5] O. J. Scherer, C. Blath and G. Wolmershäuser, *J. Organomet. Chem*, 1990, **387**, C21-C24.

[S6] P. H. M. Budzelaar, *I*vory Software Corp.: Centennial, CO, 2006.

[S7]. G. Sheldrick, *Acta Cryst. A* 2008, **64**, 112-122.

[S8] G. Sheldrick, *Acta Cryst. C* 2015, **A71**, 3-8.

[S9] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst*. 2009, **42**, 339-341.

[S10] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson *et al*., Gaussian 16, Revision B.01, 2016.