Supporting Information for:

Gauging Metal Lewis Basicity of Zerovalent Iron Complexes via Metal-Only Lewis Pairs

Holger Braunschweig,*[a] Rian D. Dewhurst,[a] Florian Hupp,[a] Christina Kaufmann,[a] Ashwini K. Phukan,[a,‡] Christoph Schneider,[a] Qing Ye[a]

[a]Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany
[‡]Department of Chemical Sciences, Tezpur University, Napaam 784028, Assam, India

Discussion of the synthesis of pentacoordinate $[Fe(CO)_4L]$ and $[Fe(CO)_3L_2]$ precursor complexes.

The complexes $[Fe(CO)_4L]$ (**1b**: L = PMe_3; **1c**: L = CN*t*Bu) and $[Fe(CO)_3L_2]$ (**1d**: L = PMe_3; **1e**: L = IMe = 1,3-dimethylimidazol-2-ylidene; **1f**: L = CN*t*Bu), intended for use as precursors in this study, have been previously reported in the literature.[1-4] However, for the synthesis of the carbene-containing complex **1e**, the literature description was modified slightly, through the use of three equivalents of the carbene ligand IMe per equivalent of iron pentacarbonyl. The ^{1}H NMR of **1e** exhibited two singlet signals (δ = 3.57 and 6.05) due to the high symmetry of the molecule. Single crystals suitable for X-ray diffraction analysis could be obtained by cooling **1e** in a toluene solution, to –30°C. The structure shows trigonal bipyramidal geometry with the IMe ligands at apical positions (Figure S1).

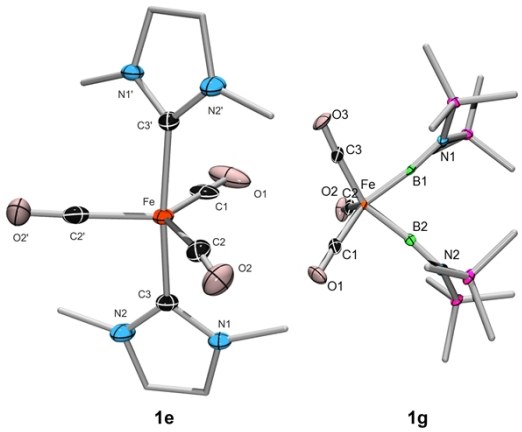

Fig S1. Molecular structures of **1e** and **1g** in the solid state. Thermal ellipsoids set to 50% probability level. Hydrogen atoms and ellipsoids of methyl groups are omitted for clarity. Selected bond lengths [Å] and angles [°] for **1e**: Fe-C3 1.9819(18), C3'-Fe-C3 168.00(12). For **1g**: Fe-B1 1.841(3), Fe1-B2 1.838(3), B1-B2 2.119(3); B1-Fe-B2 70.34(10), Fe-B1-N1 174.17(19), Fe-B2-N2 172.86(19).

In order to prepare the iron bis(borylene) complex $[(OC)_3Fe\{BN(SiMe_3)_2\}_2]$ (**1g**), the well-established intermetallic borylene transfer[5] protocol was applied. The reaction of $[Fe(CO)_5]$ with the borylene source $[(OC)_5Mo{=}BN(SiMe_3)_2]$ (2 eq.) led to near-quantitative formation of the expected product **1g** as was indicated by new ^{11}B and ^{1}H NMR resonances at δ 84 and 0.27 ppm, respectively. Single crystals suitable for X-ray diffraction analysis were obtained in a 65% yield upon fractional crystallization. The overall geometry of **1g** is analogous to the previously published iron bis(borylene) $[(OC)_3Fe(BDur)\{BN(SiMe_3)_2\}]$ (**A**),[6] adopting a strongly distorted trigonal bipyramidal geometry (Figure 3). However, the B-B interaction in **1g** is significantly weaker than that in $[(OC)_3Fe(BDur)\{BN(SiMe_3)_2\}]$, which is indicated by both the elongated B-B separation (**1g**: 2.119(3) Å; **A**: 1.982(3) Å), but also a more downfield ^{11}B NMR resonance for the aminoborylene nucleus (**1g**: 84; **A**: δ 78). These data are consistent with the borylene ligands in **1g** being more "borylene-like" than in the mixed derivative **A**.

General Information: All syntheses were performed under an inert atmosphere of dry argon using standard Schlenk techniques or in a glovebox (MBraun). Pentane, hexane, benzene, toluene, THF and CH_2Cl_2 were dried by distillation over potassium (benzene, toluene) or Na/K alloy (hexane, THF) or phosphorus pentoxide (CH_2Cl_2) under argon and stored over activated molecular sieves (4 Å). CD_3CN, C_6D_6 and CD_2Cl_2 were degassed by several *freeze-pump-thaw* cycles and stored over molecular sieves (4 Å). The NMR spectra were recorded on a Bruker AV 400 (^{1}H: 400 MHz, ^{13}C: 100 MHz, ^{11}B: 128 MHz, ^{31}P: 162) and/or a Bruker Avance 500 FT-NMR spectrometer (^{1}H: 500 MHz, ^{11}B: 160 MHz, ^{13}C{^{1}H}: 126 MHz). Chemical shifts are given in ppm and are referenced to external TMS (^{1}H, ^{13}C), [BF_3·OEt_2] (^{11}B{^{1}H}) or 85% H_3PO_4 (^{31}P{^{1}H}). Coupling constants are given in Hz. Elemental analysis were obtained from an Elementar Vario MICRO cube instrument. Infrared spectra were measured on a JASCO FT/IR-6200 spectrometer. The light source for photochemical experiments was a Hg/Xe arc lamp (400–550 W) equipped with IR filters, irradiating at 210–600 nm. PMe_3,[1] 1,3-dimethylimidazol-2-ylidene,[7] [$Fe(CO)_4(CN$*t*$Bu)$],[2] [$Fe(CO)_3(CN$*t*$Bu)_2$],[2] [$Fe(CO)_4(PMe_3)$],[3] [$Fe(CO)_3(PMe_3)_2$],[1] [$(OC)_5Mo{=}BN(SiMe_3)_2$][8] were prepared according to literature procedures. [$Fe(CO)_5$] was purchased from Aldrich and *tert*-butylisocyanide from Fluka, both were used without further purification.

Synthesis of [$(OC)_5Fe{\rightarrow}GaCl_3$] (2a): $GaCl_3$ (44.9 mg, 0.26 mmol) was added to a benzene solution (20 mL) of [$Fe(CO)_5$] (0.03 mL, 50.0 mg, 0.26 mmol). The mixture was shaken, causing an immediate precipitation of a white solid. The mixture was filtered and washed with benzene (3 × 5 mL) and pentane (3 × 5 mL). The residue was recrystallized from CH_2Cl_2/pentane to give **2a** (69 mg, 0.18 mmol, 72%) as a white solid. IR (CD_2Cl_2): 2086, 2022, 1986 (ν_{CO}) cm^{-1}. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 297 K): δ = 211.15 (*C*O). Elemental analysis (%) calcd. for $C_5Cl_3FeGaO_5$: C 16.14; Found: C 15.96.

Synthesis of *cis*-[$(Me_3P)(OC)_4Fe{\rightarrow}GaCl_3$] (2b): $GaCl_3$ (43.3 mg, 0.25 mmol) was added to a benzene solution (20 mL) of [$Fe(CO)_4(PMe_3)$] (50.0 mg, 0.21 mmol). The mixture was shaken, causing an immediate precipitation of a white solid. The mixture was filtered and washed with benzene (3 × 5 mL) and pentane (3 × 5 mL). The residue was recrystallized from CH_2Cl_2/pentane to give **2b** (76 mg, 0.18 mmol, 90%) as a white solid. IR (CH_2Cl_2): 2107, 2063, 2034, 1926 (ν_{CO}) cm^{-1}. ^{1}H NMR (400 MHz, CD_2Cl_2, 297 K): δ = 1.93 (d, $^2J_{HP}$ = 11.5 Hz, 9H, C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 297 K): δ = 20.07, (d, $^1J_{CP}$ = 35.5 Hz, 3C, *C*H$_3$), 201.63 (CO), 201.89 (*C*O). ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 297 K): δ = 9.75 (s). Elemental analysis (%) calcd. for $C_7H_9Cl_3FeGaO_4P$: C 20.02; H 2.16. Found: C 19.36, H 2.27.

Synthesis of *cis*-[(*t*$BuNC)(OC)_4Fe{\rightarrow}GaCl_3$] (2c): A procedure similar to that used for the preparation of **2b** was applied by using [$Fe(CO)_4(CN$*t*$Bu)$] (30.0 mg, 0.12 mmol) and 1.1 equiv of $GaCl_3$ (23.1 mg, 0.13 mmol) to yield **2c** (54 mg, 0.09 mmol, 78%) as a light yellow solid. IR (CH_2Cl_2): 2217 (ν_{CN}), 2127, 2071, 2019, 1994 cm^{-1}. ^{1}H NMR (400 MHz, CD_2Cl_2, 297 K): δ = 1.60 (s, 9H, *t*Bu). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 297 K): δ = 29.76 (*C*H$_3$), 62.80 (*C*(CH$_3$)$_3$), 200.90 (*C*O), 210.98 (*C*O). Elemental analysis (%) calcd. for $C_9H_9Cl_3FeGaO_4N$: C 25.31; H 2.12; N 3.28. Found: C 25.20; H 2.18; N 3.23.

Synthesis of *mer,trans*-[$(Me_3P)_2(OC)_3Fe\rightarrow GaCl_3$] (2d): A procedure similar to that used for the preparation of **2b** was applied by using [$Fe(CO)_3(PMe_3)_2$] (30.0 mg, 0.10 mmol) and 1.2 equiv of $GaCl_3$ (21.7 mg, 0.12 mmol) to provide **2d** (35 mg, 0.07 mmol, 72%) as a white solid. IR (CH_2Cl_2): 2051, 1990, 1930 (ν_{CO}) cm^{-1}. ^1H NMR (400 MHz, CD_2Cl_2, 297 K): δ = 1.86 (d, $^2J_{HP}$ = 9.41 Hz, 18H, C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2, 297 K): δ = 20.30-20.85 (m, 6C, *C*H_3), 206.22 (*C*O), 206.46 (*C*O), 206.70 (*C*O); $^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2, 297 K): δ = 11.84 (s). Elemental analysis (%) calcd. for $C_9H_{18}Cl_3FeGaO_3P_2$: C 23.09; H 3.88. Found: C: 23.33; H 3.79.

Synthesis of *mer,trans*-[$(Me_3P)_2(OC)_3Fe\rightarrow GaBr_3$] (3d): A procedure similar to that used for the preparation of **2b** was applied by using [$Fe(CO)_3(PMe_3)_2$] (20.0 mg, 0.07 mmol) and 1.1 equiv of $GaBr_3$ (23.3 mg, 0.08 mmol) to provide **3d** (31 mg, 0.05 mmol, 76%) as a white solid. IR (CH_2Cl_2): 2051, 1992 (ν_{CO}) cm^{-1}. ^1H NMR (400 MHz, CD_2Cl_2, 297 K): δ = 1.90 (d, $^2J_{H\text{-}P}$ = 9.04 Hz, 18H, C*H*$_3$), $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2, 297 K): δ = 20.14-2046 (m, 6C, *C*H_3), 207.40 (*C*O), 207.64 (*C*O), 207.88 (*C*O); $^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2, 297 K): δ = 12.23 (s). Elemental analysis (%) calcd. for $C_9H_{18}Br_3FeGaO_3P_2$: C 17.97; H 3.02. Found: C 18.44; H 3.07.

Synthesis of [$Fe(CO)_3(IMe)_2$] (1e): A solution of [$Fe(CO)_5$] (0.35 mL, 510 mg, 2.60 mmol) in 40 mL of thf was treated with 1,3-dimethylimidazol-2-ylidene (556 mg, 5.72 mmol). The reaction mixture was refluxed overnight and the orange solution was separated from the black solid by filtration. Volatiles were removed under vacuum and the resulting crude was recrystallized from toluene/pentane to yield **1e** (384 mg, 1.16 mmol, 44%) as an orange solid. IR (CH_3CN): 1812 (ν_{CO}) cm^{-1}. ^1H NMR (400 MHz, C_6D_6, 297 K): δ = 3.57 (s, 12H, CH_3), 6.05 (s, 4H, CH_{Imid}). $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6, 297 K): δ = 39.34, (*C*H_3), 122.02 (*C*H_{Imid}), 195.25 (Fe-$C_{Carbene}$), 223.08 (*C*O). Elemental analysis (%) calcd. for $C_{13}H_{16}FeN_4O_3$: C 47.01; H 4.86; N 16.87. Found: C 46.40; H 4.94; N 16.13.

Synthesis of *mer,cis*-[$(IMe)_2(OC)_3Fe\rightarrow GaCl_3$] (2e): A procedure similar to that used for the preparation of **2b** was applied by using [$Fe(CO)_3(IMe)_2$] (30.0 mg, 0.09 mmol) and 1.1 equiv of $GaCl_3$ (17.5 mg, 0.10 mmol) to provide **2e** (36 mg, 0.07 mmol, 78%) as a light orange solid. IR (CH_3CN): 2048, 1970, 1918 (ν_{CO}) cm^{-1}. ^1H NMR (400 MHz, CD_3CN, 297 K): δ = 3.47 (s, 6H, C*H*$_3$), 3.52 (s, 6H, C*H*$_3$), 7.14 (s, 2H, *C*H_{Imid}), 7.18 (s, 2H, C*H*$_{Imid}$). $^{13}C\{^1H\}$ NMR (100 MHz, CD_3CN, 297 K): δ = 37.66 (*C*H_3), 38.64 (*C*H_3), 124.57 (*C*H_{Imid}), 125.14 (*C*H_{Imid}), 173.00 (Fe-$C_{Carbene}$), 176.59 (Fe-$C_{Carbene}$), 210.00 (*C*O), 210.86 (*C*O). Elemental analysis (%) calcd. for $C_{13}H_{16}Cl_3FeGaO_3N_4$: C 30.72; H 3.17; N 11.02. Found: C 31.16; H 3.43; N 11.02.

Synthesis of *fac,cis*-[$(t$BuNC$)_2(OC)_3Fe\rightarrow GaCl_3$] (2f): A procedure similar to that used for the preparation of **2b** was applied by using [$Fe(CO)_3(CNt$Bu$)_2$] (50.0 mg, 0.16 mmol) and 1.1 equiv of $GaCl_3$ (31.6 mg, 0.18 mmol) to yield **2f** (54 mg, 0.11 mmol, 69%) as a light yellow solid. IR (CH_2Cl_2): 2213, 2200 (ν_{CN}), 2088, 2044, (ν_{CO}) cm^{-1}. ^1H NMR (500 MHz, CD_2Cl_2, 297 K): δ = 1.54 (s, 1H, *t*Bu) 1.57 (s, 0.4H, *t*Bu). $^{13}C\{^1H\}$ NMR (126 MHz, CD_2Cl_2, 297 K): δ =

29.88 (CH_3), 20.90 (CH_3), 61.23 ($C(CH_3)_3$), 61.35 ($C(CH_3)_3$), 199.23 (CO), 204.33 (CO). Elemental analysis (%) calcd. for $C_{13}H_{18}Cl_3FeGaO_3N_2$: C 32.38; H 3.76; N 5.51. Found: C 32.76, H 3.90, N 5.92.

Synthesis of $[(OC)_3Fe\{BN(SiMe_3)_2\}_2]$ (1g): A hexane solution (16 mL) of $[Fe(CO)_5]$ (0.08 mL, 120 mg, 0.61 mmol) and $[(OC)_5Mo\{BN(SiMe_3)_2\}]$ (500 mg, 1.22 mmol) was stirred overnight at 40 °C. The resulting light yellow solution was concentrated to ca. 8 mL, and stored at –30 °C overnight, yielding colorless crystals of $[Mo(CO)_6]$. The light-yellow mother liquor was transferred to another flask by cannula, concentrated to ca. 4 mL and stored at –70 °C for 4 d, yielding **1g** (190 mg, 0.39 mmol, 65%) as light-yellow needles. IR (solid): 1917, 1886 (ν_{CO}) cm^{-1}. ^1H NMR (500 MHz, C_6D_6, 297 K): 0.27 (s, 36H, $SiMe_3$). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6, 297 K): δ = 217.69 (s, *C*O), 2.88 (s, *C*H_3). ^{11}B NMR (160 MHz, C_6D_6, 297 K): δ = 84 (bs). Elemental analysis (%) calcd. for $C_{15}H_{36}B_2FeN_2O_3Si_4$: C 37.36, H 7.52, N 5.81; found, C 36.94, H 7.10, N 5.44.

Synthesis of *mer,trans*-$[\{(Me_3Si)_2NB\}_2(OC)_3Fe\rightarrow GaCl_3]$ (2g): Benzene solutions (0.5 mL respectively) of **1h** (10 mg, 0.02 mmol) and $GaCl_3$ (3.6 mg, 0.02 mmol) were mixed at ambient temperature. The resulting colorless solution was layered with 0.2 mL hexane, and slowly concentrated under vacuum until **2g** began to crystallize. The obtained colorless crystals of **2g** were washed with pentane (3 × 1 mL) and dried under vacuum (8 mg, 0.012 mmol, 61%). IR (solid): 2073, 2025, 1986 (ν_{CO}) cm^{-1}. ^1H NMR (500 MHz, C_6D_6, 297 K): 0.28 (s, 36H, $SiMe_3$). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6, 297 K): δ = 201.00, 206.60 (s, *C*O), 2.77 (s, *C*H_3). ^{11}B NMR (160 MHz, C_6D_6, 297 K): δ = 86 (bs). Elemental analysis (%) calcd. for $C_{15}H_{36}B_2Cl_3FeGaN_2O_3Si_4$: C 27.37, H 5.51, N 4.26; found, C 26.52, H 5.56, N 4.20.

Transfer reaction of $GaCl_3$ from $[(OC)_5Fe\rightarrow GaCl_3]$ (2a) to $[(OC)_3Fe(PMe_3)_2]$ (1b): In a J. Young NMR tube **2a** (5 mg, 0.01 mmol) and **1b** (4 mg, 0.01 mmol) were dissolved in CH_2Cl_2. The $^{31}P\{^1H\}$ NMR spectra of this solution showed the signals for **2b** and no signal of the precursor **1b**, indicating complete transfer of the $GaCl_3$.

Transfer reaction of $GaCl_3$ from $[(Me_3P)(OC)_4Fe\rightarrow GaCl_3]$ (2b) to $[(OC)_3Fe(PMe_3)_2]$ (1d): In a J. Young NMR tube **2b** (10 mg, 0.02 mmol) and **1d** (7 mg, 0.02 mmol) were dissolved in CH_2Cl_2. The $^{31}P\{^1H\}$ NMR spectra of this solution showed signals for **1b** and **2d** and no signals of the two precursors, indicating complete transfer of the $GaCl_3$.

Transfer reaction of $GaCl_3$ from $[(Me_3P)_2(OC)_3Fe\text{-}GaCl_3]$ (2d) to $[Pt(PCy_3)_2]$ (4): In a J. Young NMR tube **2d** (10 mg, 0.02 mmol) and $[Pt(PCy_3)_2]$ (**4**) (16 mg, 0.02 mmol) were dissolved in C_6H_5F. An immediate color change from colorless to yellow takes place. The $^{31}P\{^1H\}$ NMR spectra of this solution showed signals for **1e** and $[(Cy_3P)_2Pt\rightarrow GaCl_3]$ (**5**) and no signals for the two precursors, indicating complete transfer of the $GaCl_3$.

Crystallographic Details

The crystal data of **1e** were collected on a Bruker D8-QUEST diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **1e**: $C_{13}H_{16}FeN_4O_3$, $M_r = 332.15$, yellow block, $0.18\times0.06\times0.04$ mm^3, tetragonal space group $P4_32_12$, $a = 7.9922(6)$ Å, $b = 7.9922(6)$ Å, $c = 23.1283(17)$ Å, $\alpha = 90.00°$, $\beta = 90.00°$, $\gamma = 90.00°$, $V = 1477.33(19)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.493$ g·cm^{-3}, $\mu = 1.036$ mm^{-1}, $F(000) = 688$, $T = 100(2)$ K, $R_1 = 0.0396$, $wR^2 = 0.0740$, 1582 independent reflections [$2\theta\leq53.6°$] and 99 parameters. CCDC 1004633.

The crystal data of **1g** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **1g**: $C_{15}H_{36}B_2FeN_2O_3Si_4$, $M_r = 482.29$, colourless plate, $0.20\times0.10\times0.05$ mm^3, monoclinic space group $P2_1/n$, $a = 8.8462(3)$ Å, $b = 17.0403(6)$ Å, $c = 35.7439(12)$ Å, $\beta = 90.2270(10)°$, $V = 5388.1(3)$ Å^3, $Z = 8$, $\rho_{calcd} = 1.189$ g·cm^{-3}, $\mu = 0.754$ mm^{-1}, $F(000) = 2048$, $T = 100(2)$ K, $R_1 = 0.0521$, $wR^2 = 0.0852$, 10964 independent reflections [$2\theta\leq52.744°$] and 511 parameters. CCDC 1004634.

The crystal data of **2a** were collected on a Bruker D8-QUEST diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2a**: $C_5Cl_3FeGaO5$, $M_r = 482.29$, colourless plate, $0.214\times0.147\times0.065$ mm^3, monoclinic space group Cc, $a = 9.0504(17)$ Å, $b = 10.731(2)$ Å, $c = 11.634(4)$ Å, $\beta = 92.431(15)°$, $V = 1128.9(5)$ Å^3, $Z = 4$, 2.189 g·cm^{-3}, $\mu = 4.374$ mm^{-1}, $F(000) = 712$, $T = 100(2)$ K, $R_1 = 0.0137$, $wR^2 = 0.0275$, 2256 independent reflections [$2\theta\leq53.46°$] and 136 parameters. CCDC 1004635.

The crystal data of **2b** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and graphite monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2b**: $C_7H_9Cl_3FeGaO_4P$, $M_r = 420.03$, colourless block, $0.15\times0.10\times0.08$ mm^3, orthorhombic space group $Pna2_1$, $a = 12.3102(5)$ Å, $b = 8.7578(4)$ Å, $c = 13.2384(5)$ Å, $V = 1427.24(10)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.955$ g·cm^{-3}, $\mu = 3.573$ mm^{-1},

$F(000) = 824$, $T = 100(2)$ K, $R_1 = 0.0137$, $wR^2 = 0.0307$, 2907 independent reflections [$2\theta \leq 52.74°$] and 157 parameters. CCDC 1004636.

The crystal data of **2c** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2c**: $C_9H_9Cl_3FeGaNO_4$, $M_r = 427.09$, colourless block, $0.217\times0.078\times0.077$ mm^3, monoclinic space group $P2_1/n$, $a = 7.2763(3)$ Å, $b = 22.2271(9)$ Å, $c = 9.6226(4)$ Å, $\beta = 90.5320(10)°$, $V = 1556.21(11)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.823$ g·cm^{-3}, $\mu = 3.183$ mm^{-1}, $F(000) = 840$, $T = 100(2)$ K, $R_1 = 0.0227$, $wR^2 = 0.0472$, 3178 independent reflections [$2\theta \leq 52.74°$] and 175 parameters. CCDC 1004637.

The crystal data of **2d** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and graphite monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2d**: $C_9H_{18}Cl_3FeGaO_3P_2$, $M_r = 468.09$, colourless plate, $0.32\times0.09\times0.02$ mm^3, monoclinic space group $P2_1/c$, $a = 17.8670(16)$ Å, $b = 13.5823(12)$ Å, $c = 15.9356(14)$ Å, $\beta = 109.018(3)°$, $V = 3656.1(6)$ Å^3, $Z = 8$, $\rho_{calcd} = 1.701$ g·cm^{-3}, $\mu = 2.879$ mm^{-1}, $F(000) = 1872$, $T = 100(2)$ K, $R_1 = 0.0521$, $wR^2 = 0.0954$, 7463 independent reflections [$2\theta \leq 52.74°$] and 355 parameters. CCDC 1004638.

The crystal data of **2e** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and graphite monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2e**: $C_{14}H_{18}Cl_5FeGaN_4O_3$, $M_r = 593.14$, colourless needle, $0.26\times0.09\times0.04$ mm^3, monoclinic space group $P2_1/c$, $a = 8.6242(5)$ Å, $b = 14.4623(8)$ Å, $c = 17.4482(10)$ Å, $\beta = 98.852(2)°$, $V = 2150.3(2)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.832$ g·cm^{-3}, $\mu = 2.572$ mm^{-1}, $F(000) = 1184$, $T = 100(2)$ K, $R_1 = 0.0332$, $wR^2 = 0.0611$, 4394 independent reflections [$2\theta \leq 52.74°$] and 257 parameters. CCDC 1004639.

The crystal data of **2f** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2f**: $C_{13}H_{18}Cl_3FeGaN_2O_3$, $M_r = 482.21$, colourless plate, $0.133\times0.10\times0.02$ mm^3, orthorhombic space group *Pnma*,

a = 11.8260(8) Å, b = 18.0027(12) Å, c = 9.6374(6) Å, V = 2051.8(2) Å^3, Z = 4, ρ_{calcd} = 1.561 g·cm^{-3}, μ = 2.422 mm^{-1}, F(000) = 968, T = 100(2) K, R_1 = 0.0285, wR^2 = 0.0473, 2165 independent reflections [2θ≤52.74°] and 115 parameters. CCDC 1004640.

The crystal data of **2g** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **2g**: $C_{15}H_{36}B_2Cl_3FeGaN_2O_3Si_4$, M_r = 658.36, colourless needle, 0.28×0.06×0.05 mm^3, orthorhombic space group $Pna2_1$, a = 28.6201(15) Å, b = 15.3682(8) Å, c = 7.0307(4) Å, V = 3092.4(3) Å^3, Z = 4, ρ_{calcd} = 1.414 g·cm^{-3}, μ = 1.773 mm^{-1}, F(000) = 1352, T = 100(2) K, R_1 = 0.0517, wR^2 = 0.0965, 6247 independent reflections [2θ≤52.74°] and 292 parameters. CCDC 1004641.

The crystal data of **3d** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **3d**: $C_9H_{18}Br_3FeGaO_3P_2$, M_r = 601.47, colourless block, 0.28×0.22×0.15 mm^3, orthorhombic space group $Pbca$, a = 17.8212(17) Å, b = 16.5290(17) Å, c = 26.155(3) Å, V = 7704.4(13) Å^3, Z = 16, ρ_{calcd} = 2.074 g·cm^{-3}, μ = 8.540 mm^{-1}, F(000) = 4608, T = 100(2) K, R_1 = 0.0675, wR^2 = 0.0993, 8256 independent reflections [2θ≤53.7°] and 355 parameters. CCDC 1004642.

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Table S1: DFT calculated Bond Dissociation Energies (BDE in kcal.mol^{-1}) of the Fe→Ga Dative Bond Calculated at the PBE(DFT-D3-BJDAMP)/DZP,TZ2P level of theory. The calculated and experimental (*within parenthesis in italics*) M→Ga (M=Fe, Pt) bond lengths are also given for a quick comparison.

Molecule	**E_{Pauli}**	**E_{Elast}**	**E_{Orb}**	**E_{Int}**	**E_{Prep}**	**BDE**	***d*(Fe-Ga) (Å)**
2a	92.52	–65.21	–51.0	–43.75	15.96	**–27.80**	**2.638**
2b	130.37	–99.96	–75.61	–72.81	31.48	**–41.33**	**2.510**
2c	131.27	–99.78	–75.85	–72.06	26.43	**–45.63**	**2.522**
2d	121.25	–91.96	–69.41	–68.49	25.39	**–43.10**	**2.530** *(2.497)*
2e	166.16	–134.28	–98.92	–101.66	41.14	**–60.2**	**2.444** *(2.461)*
2f	151.26	–122.0	–92.56	–88.92	32.6	**–56.32**	**2.440** *(2.442)*
2g	144.64	–114.42	–86.0	–90.0	34.0	**–56.0**	**2.465** *(2.464)*
2h	173.67	–138.0	–98.86	–109.31	45.1	**–64.2**	**2.459** *(2.445)*
5	153.71	–120.52	–95.83	–114.0	35.16	**–78.84**	**2.391** *(2.402)*
7	131.53	–99.10	–73.26	–72.34	27.14	**–45.20**	**2.524**

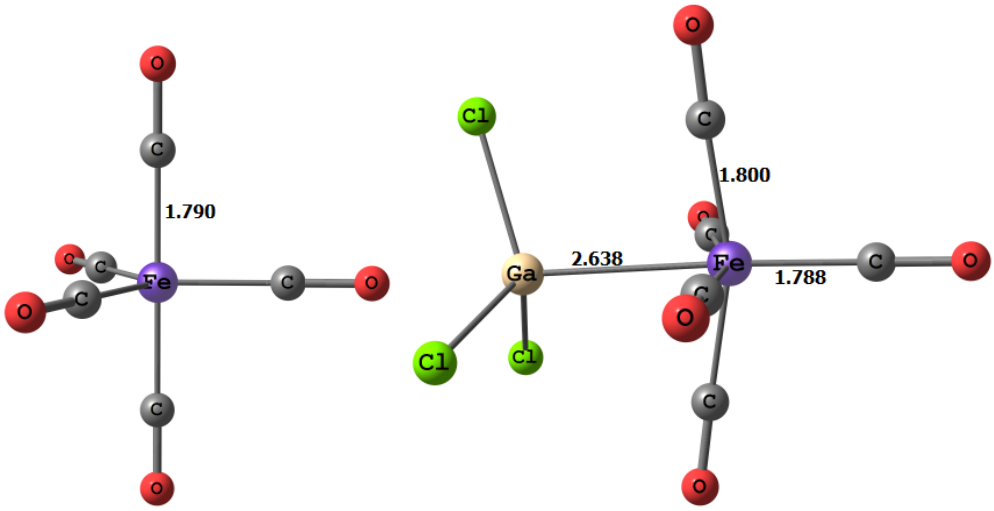

Figure S2. Calculated minimum-energy structures of **1a** and **2a**.

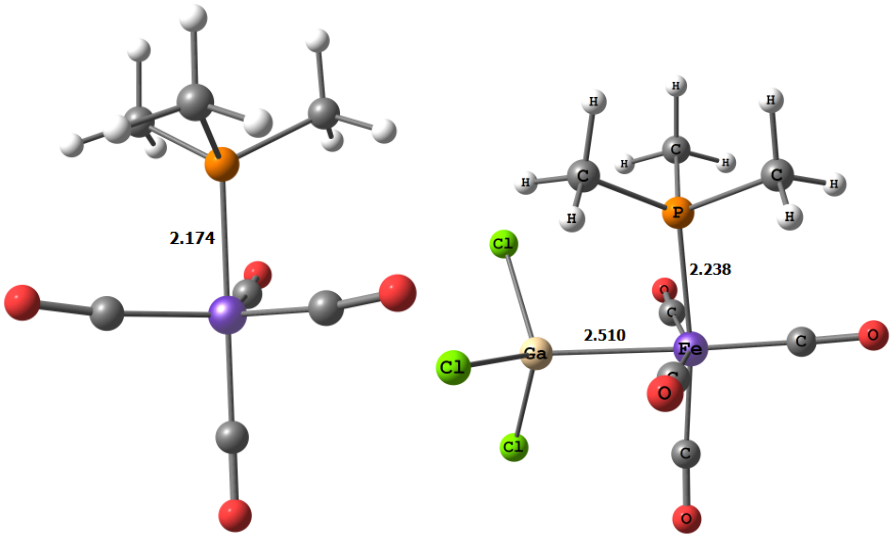

Figure S3. Calculated minimum-energy structures of **1b** and **2b**.

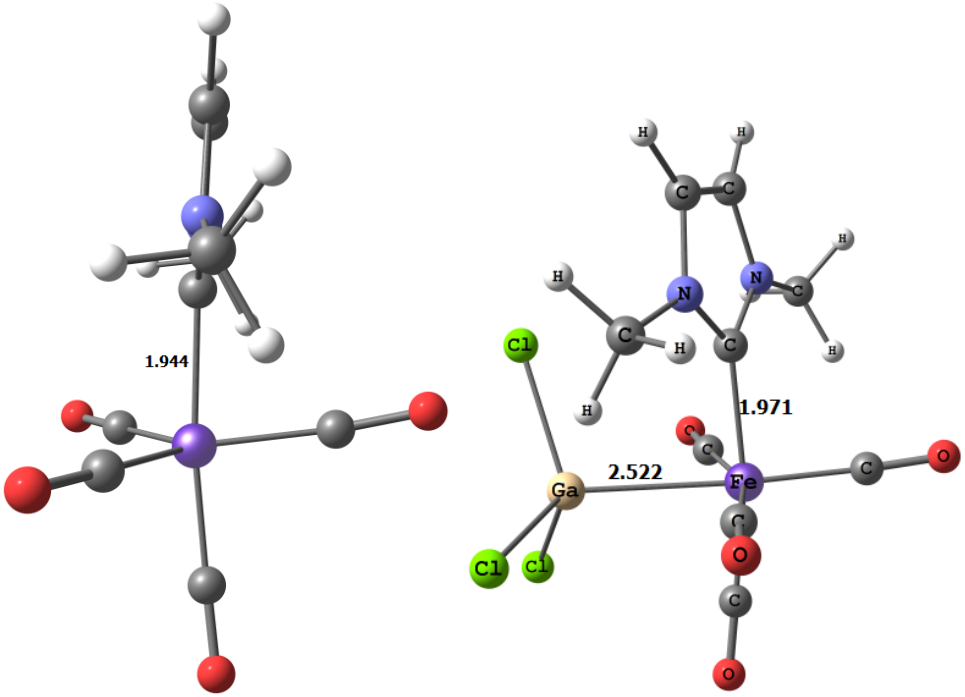

Figure S4. Calculated minimum-energy structures of **1c** and **2c**.

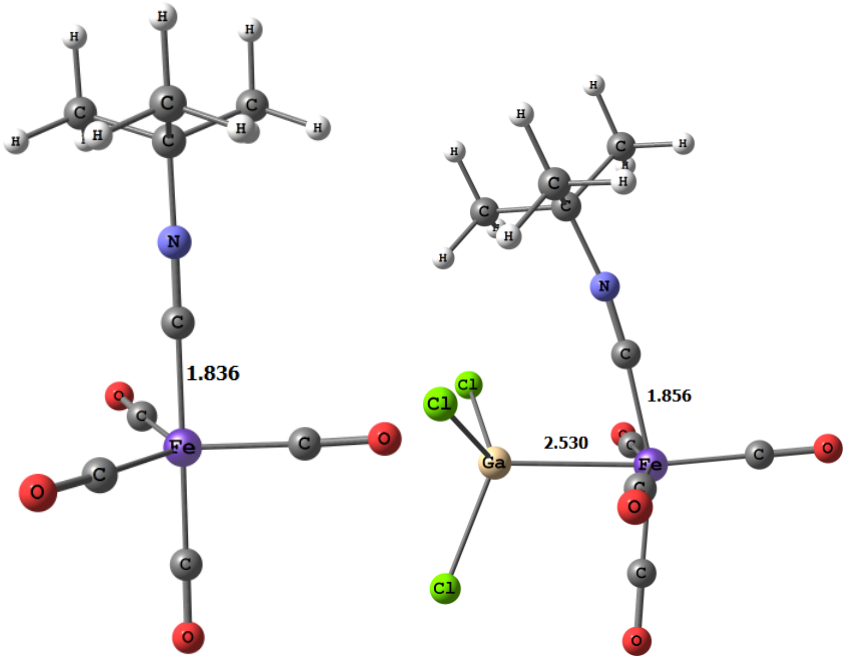

Figure S5. Calculated minimum-energy structures of **1d** and **2d**.

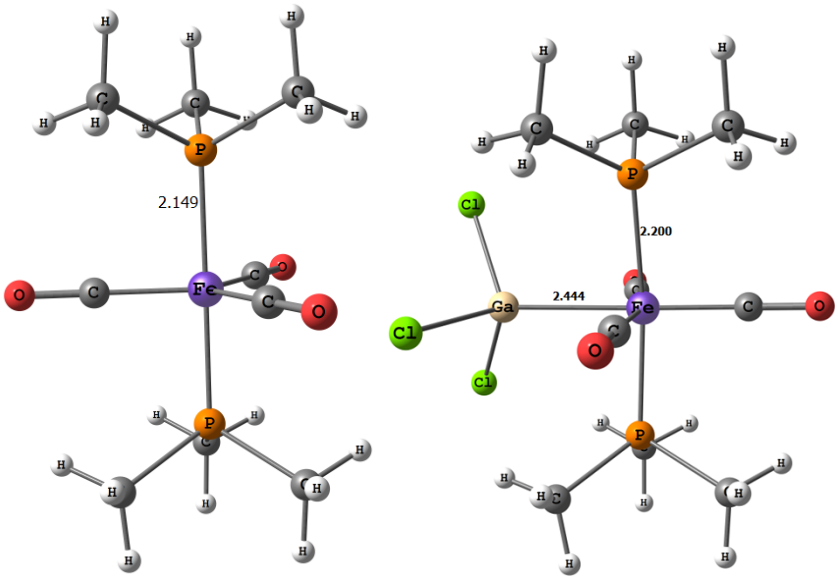

Figure S6. Calculated minimum-energy structures of **1e** and **2e**.

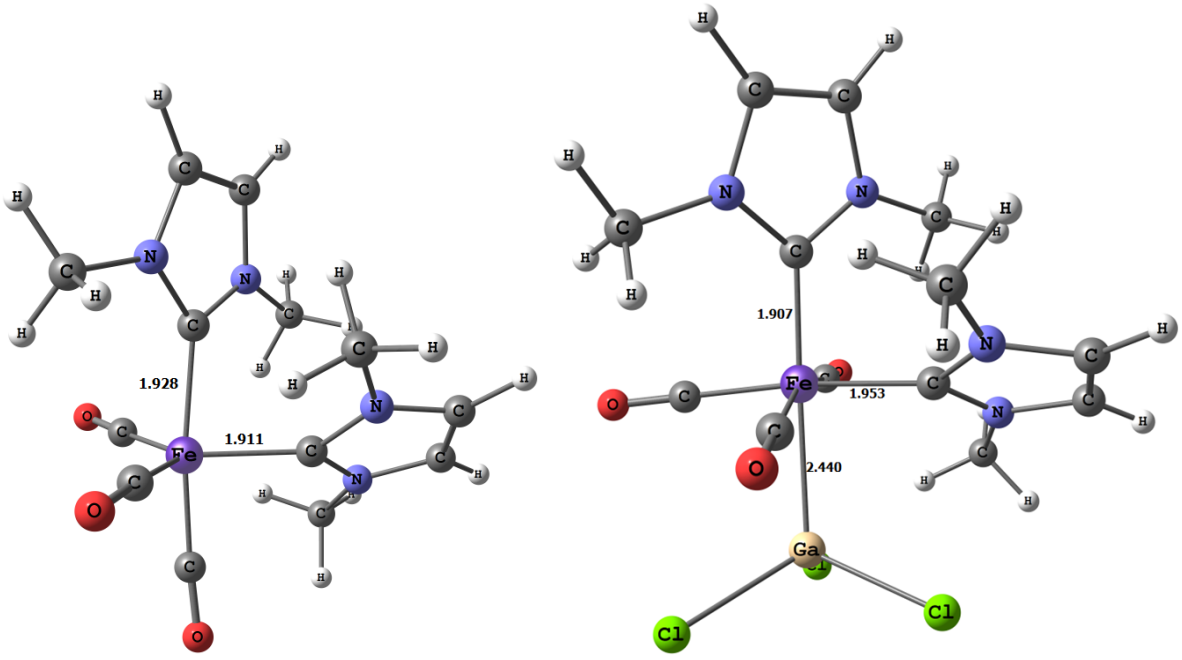

Figure S7. Calculated minimum-energy structures of **1f** and **2f**.

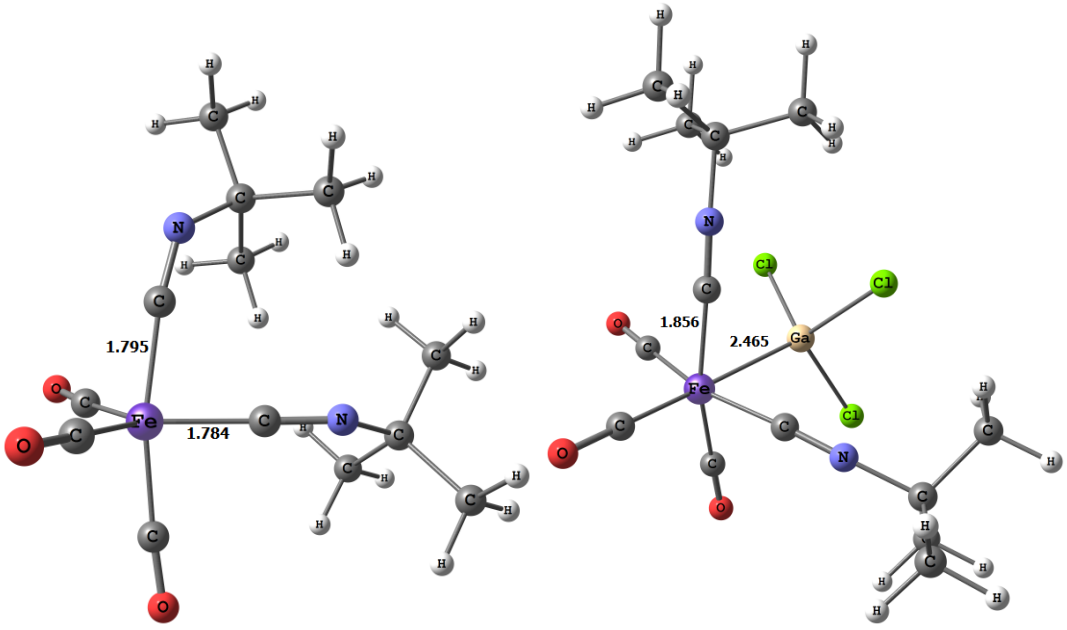

Figure S8. Calculated minimum-energy structures of **1g** and **2g**.

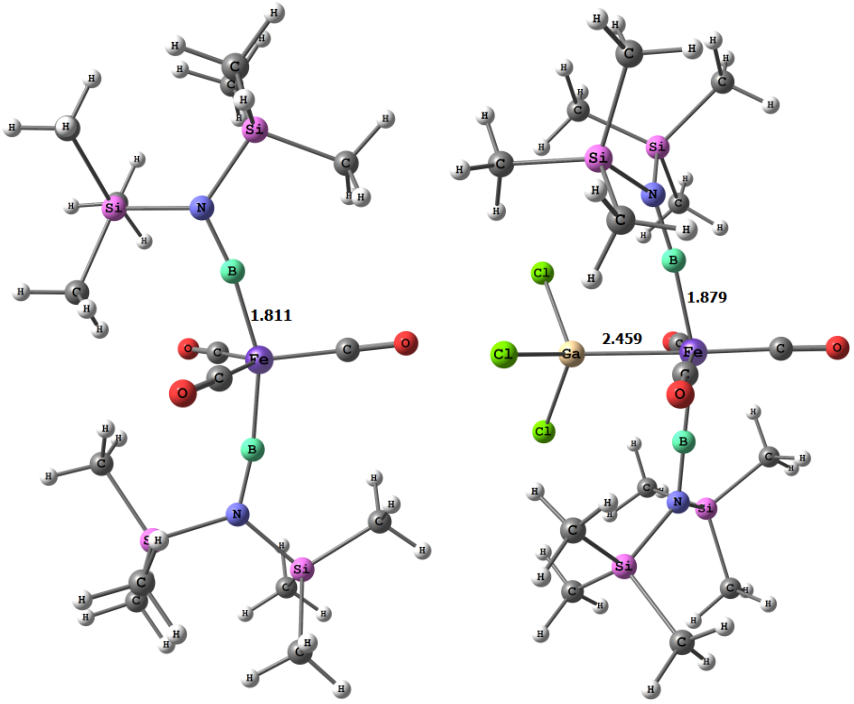

Figure S9. Calculated minimum-energy structures of **1h** and **2h**.

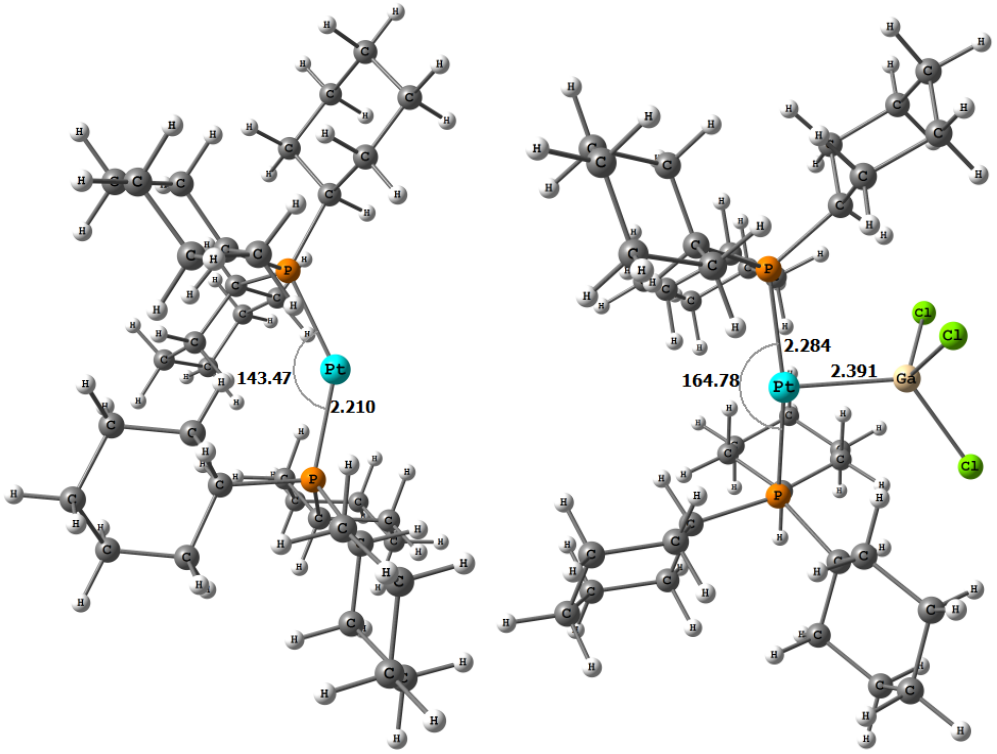

Figure S10. Calculated minimum-energy structures of **4** and **5**.

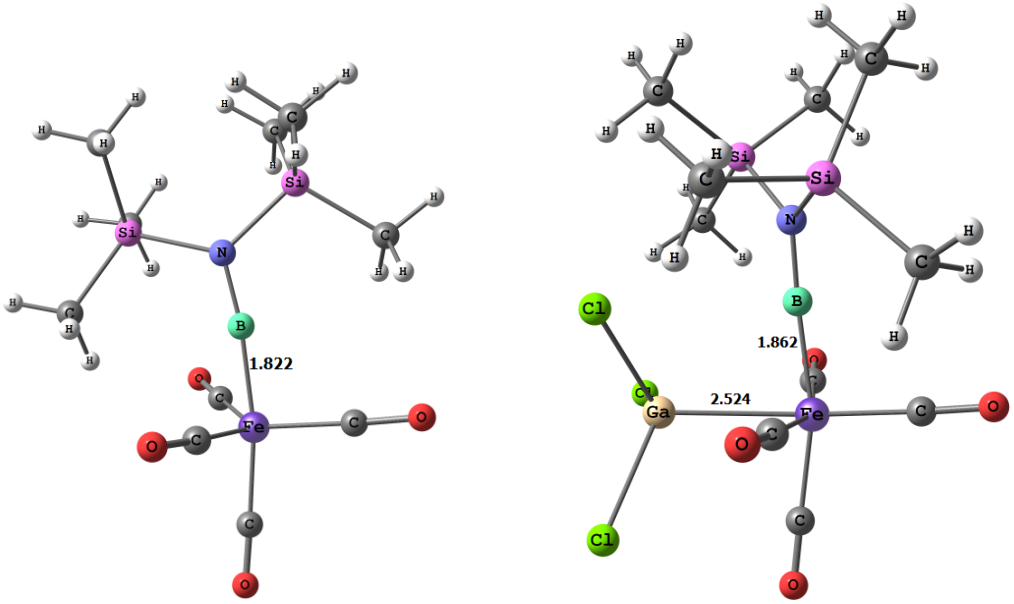

Figure S11. Calculated minimum-energy structures of **6** and **7**.

Optimized Coordinates of the Calculated MOLP Complexes

Compound 2a

26	-1.285783000	-0.000195000	0.020852000
6	-0.896428000	-1.279473000	1.228808000
8	-0.678425000	-2.110074000	1.960210000
6	-0.882155000	1.283798000	1.219254000
8	-0.652716000	2.115131000	1.946034000
6	-1.154634000	-1.249317000	-1.267620000
8	-1.122309000	-2.019979000	-2.090549000
6	-1.148104000	1.237293000	-1.278634000
8	-1.110994000	1.999146000	-2.109421000
6	-3.064463000	0.007421000	0.205059000
8	-4.188243000	0.011985000	0.323176000
31	1.351725000	-0.001377000	-0.036284000
17	1.885707000	-0.028142000	2.066279000
17	1.895192000	1.846710000	-1.013525000
17	1.905457000	-1.813874000	-1.071412000

Compound 2b

31	1.469169000	-0.265792000	0.047875000
17	2.989087000	1.158072000	-0.572670000
17	1.875037000	-1.106200000	2.019246000
17	1.446459000	-1.931676000	-1.405222000
26	-0.760046000	0.886692000	-0.013737000
15	-1.712016000	-1.138356000	-0.032176000
8	-3.363375000	2.146090000	-0.230285000
6	-2.334874000	1.669685000	-0.149185000
8	-0.255976000	0.498312000	-2.856510000
6	-0.408734000	0.664867000	-1.745395000
8	0.751157000	3.376325000	0.190607000
6	0.201341000	2.393053000	0.097925000
8	-0.822760000	0.393796000	2.847433000
6	-0.727687000	0.622330000	1.739306000
6	-3.361243000	-1.031366000	0.683340000
1	-3.991327000	-0.375478000	0.086596000
1	-3.283402000	-0.624175000	1.691309000
1	-3.808285000	-2.023646000	0.729555000
6	-1.964433000	-1.832938000	-1.663644000
1	-0.989247000	-2.023371000	-2.108713000
1	-2.519205000	-1.130001000	-2.282439000
1	-2.518501000	-2.766403000	-1.570332000
6	-0.956540000	-2.449983000	0.928341000
1	-1.655379000	-3.286685000	0.958185000
1	-0.741475000	-2.101902000	1.935950000
1	-0.025375000	-2.760415000	0.460963000

Compound 2c

26	-0.333315000	1.131393000	0.319601000
8	-2.464691000	3.068257000	0.684237000
6	-1.612582000	2.326682000	0.562460000
8	0.039197000	0.447518000	3.127670000

6	-0.091879000	0.665971000	2.022821000
6	-3.325812000	-1.509948000	-0.844858000
1	-4.097799000	-1.725168000	-1.556111000
7	-2.638086000	-0.321508000	-0.859051000
6	-2.813915000	-2.231145000	0.165488000
1	-3.039979000	-3.216142000	0.520354000
6	-1.679228000	-0.291508000	0.095046000
8	-0.094359000	1.130953000	-2.589338000
6	-0.163839000	1.123230000	-1.456279000
7	-1.827420000	-1.470323000	0.736141000
6	-2.928786000	0.674249000	-1.856382000
1	-2.580133000	1.644356000	-1.532563000
1	-4.004980000	0.718575000	-1.989158000
1	-2.443524000	0.410157000	-2.791603000
6	-1.007887000	-2.016435000	1.786524000
1	0.025655000	-1.720451000	1.669073000
1	-1.036887000	-3.096879000	1.697523000
1	-1.374088000	-1.702517000	2.759242000
6	1.080249000	2.211453000	0.443293000
8	1.986854000	2.882934000	0.529043000
31	1.407585000	-0.610523000	-0.222145000
17	2.907720000	0.291243000	-1.519605000
17	0.318454000	-2.232658000	-1.228907000
17	2.388581000	-1.323509000	1.603751000

Compound 2d

31	-0.747541000	-1.192769000	0.034176000
17	-2.773900000	-1.931849000	-0.171018000
17	0.514201000	-1.875602000	-1.630237000
17	0.202446000	-1.814441000	1.898899000
26	-0.724670000	1.337009000	-0.007514000
8	-3.636824000	1.194315000	-0.133569000
7	2.160644000	0.511141000	0.068568000
6	-2.509181000	1.241305000	-0.084674000
8	-0.859301000	1.039687000	2.899219000
6	-0.802368000	1.125775000	1.774211000
8	-0.390649000	4.233969000	-0.043150000
6	-0.518442000	3.109377000	-0.029973000
8	-0.595375000	0.902848000	-2.897059000
6	-0.645019000	1.048142000	-1.777586000
6	1.073678000	0.882522000	0.061430000
6	3.427422000	-0.141957000	-0.015725000
6	4.442952000	0.736407000	0.672413000
1	4.491339000	1.710680000	0.188834000
1	5.416957000	0.256652000	0.607504000
1	4.178563000	0.864935000	1.720578000
6	3.735941000	-0.307590000	-1.485702000
1	2.967999000	-0.919685000	-1.952877000
1	4.701520000	-0.801031000	-1.577972000
1	3.780053000	0.663524000	-1.976159000
6	3.301482000	-1.484161000	0.664198000
1	3.021397000	-1.359888000	1.707323000
1	4.267870000	-1.982540000	0.601052000

1	2.544173000	-2.086969000	0.169181000

Compound 2e

31	0.000766000	-1.488165000	0.054007000
17	0.001177000	-2.140171000	2.148318000
17	-1.708387000	-2.460800000	-0.973705000
17	1.711033000	-2.458559000	-0.973991000
15	-2.195535000	0.869693000	0.019668000
26	-0.000557000	0.950808000	-0.106774000
8	-0.002067000	3.804771000	-0.522123000
6	-0.001540000	2.673456000	-0.361396000
8	-0.000511000	0.992061000	2.788125000
15	2.194484000	0.871783000	0.020203000
6	-0.000599000	0.934299000	1.648899000
8	0.000752000	0.133547000	-2.895048000
6	-0.000210000	0.436290000	-1.796670000
6	2.852315000	2.458513000	0.566891000
1	3.935716000	2.399576000	0.670561000
1	2.408928000	2.708543000	1.530669000
1	2.595087000	3.237483000	-0.148306000
6	2.902560000	-0.253951000	1.229285000
1	2.762492000	-1.282333000	0.905321000
1	2.400350000	-0.116396000	2.185700000
1	3.967094000	-0.041445000	1.331711000
6	3.043916000	0.561784000	-1.526668000
1	2.764619000	1.335774000	-2.240524000
1	2.734658000	-0.412566000	-1.900541000
1	4.121977000	0.571920000	-1.367052000
6	-2.854698000	2.455817000	0.566454000
1	-2.597661000	3.235081000	-0.148514000
1	-2.411900000	2.705998000	1.530464000
1	-3.938105000	2.396117000	0.669604000
6	-2.902854000	-0.257150000	1.228150000
1	-2.401172000	-0.119290000	2.184785000
1	-2.761482000	-1.285287000	0.903935000
1	-3.967677000	-0.045948000	1.330245000
6	-3.044281000	0.559551000	-1.527558000
1	-4.122406000	0.568747000	-1.368313000
1	-2.734096000	-0.414381000	-1.901727000
1	-2.765373000	1.334056000	-2.241014000

Compound 2f

31	-2.081352000	-0.261940000	-0.080004000
17	-2.888927000	-2.017442000	-1.121189000
17	-2.349067000	1.564121000	-1.315883000
17	-3.201180000	-0.006368000	1.807585000
6	-0.074416000	-2.207009000	0.670158000
8	-0.328530000	-3.288638000	0.918952000
7	1.334547000	1.806943000	-1.213014000
26	0.315981000	-0.533694000	0.283357000
6	0.082947000	-0.817639000	-1.444642000
8	-0.027143000	-0.974110000	-2.570792000
7	0.045113000	2.466919000	0.342213000

6	0.043407000	-0.091111000	1.969780000
8	-0.071779000	0.192221000	3.068917000
7	2.960776000	-1.667227000	-0.236557000
6	1.282645000	3.177643000	-1.304387000
1	1.804635000	3.715746000	-2.070446000
6	0.553870000	1.342005000	-0.206378000
7	3.130462000	0.197352000	0.769404000
6	2.214113000	-0.703782000	0.350816000
6	-0.920449000	2.569085000	1.404641000
1	-1.487164000	1.655083000	1.506915000
1	-1.626403000	3.349260000	1.139535000
1	-0.424627000	2.793321000	2.346474000
6	2.135491000	1.043284000	-2.133054000
1	2.381927000	0.082303000	-1.704342000
1	3.055653000	1.589817000	-2.318622000
1	1.589068000	0.892364000	-3.060374000
6	0.469979000	3.591317000	-0.316030000
1	0.128556000	4.568496000	-0.038130000
6	4.407228000	-0.180250000	0.427913000
1	5.263785000	0.410098000	0.685493000
6	4.300156000	-1.363405000	-0.207443000
1	5.042604000	-2.016781000	-0.620030000
6	2.844589000	1.433968000	1.451335000
1	2.714779000	2.247130000	0.739155000
1	3.671279000	1.651911000	2.121092000
1	1.941602000	1.317577000	2.034509000
6	2.422900000	-2.849731000	-0.857150000
1	3.238868000	-3.392162000	-1.322429000
1	1.697728000	-2.577617000	-1.616749000
1	1.945223000	-3.479239000	-0.114311000

Compound 2g

31	-1.042280000	-0.836664000	0.000476000
17	-2.188065000	-1.297074000	1.810266000
17	0.720564000	-2.171381000	-0.005774000
17	-2.196775000	-1.290692000	-1.805673000
26	-0.243146000	1.495512000	0.002759000
8	1.085674000	4.090089000	0.001275000
7	1.227126000	0.192997000	2.269141000
6	0.756879000	0.704539000	1.351188000
8	-2.210319000	1.965223000	-2.093296000
6	0.576172000	3.076682000	0.002770000
6	-1.457656000	1.784484000	-1.266196000
6	1.567050000	-0.544072000	3.443045000
6	0.310260000	-0.627521000	4.279363000
1	-0.029801000	0.369452000	4.555415000
1	0.534779000	-1.195517000	5.180972000
1	-0.474142000	-1.128870000	3.716013000
6	2.661826000	0.208100000	4.159580000
1	3.547071000	0.275843000	3.529485000
1	2.912977000	-0.327674000	5.072495000
1	2.323287000	1.210658000	4.415690000
6	2.021383000	-1.924054000	3.033694000

1	1.204997000	-2.465151000	2.564126000
1	2.346633000	-2.449363000	3.930560000
1	2.847766000	-1.861722000	2.328422000
7	1.222875000	0.199635000	-2.269872000
6	0.755152000	0.707978000	-1.348850000
8	-2.211387000	1.960005000	2.099159000
6	-1.457977000	1.781855000	1.272214000
6	1.557421000	-0.532092000	-3.448578000
6	0.296589000	-0.611196000	-4.279261000
1	-0.044823000	0.387216000	-4.548428000
1	0.516751000	-1.174446000	-5.184905000
1	-0.485132000	-1.115452000	-3.714797000
6	2.648857000	0.223650000	-4.166371000
1	3.536934000	0.288554000	-3.539972000
1	2.895901000	-0.307732000	-5.082950000
1	2.309014000	1.227371000	-4.416141000
6	2.013685000	-1.913998000	-3.047868000
1	1.199857000	-2.456824000	-2.575864000
1	2.333481000	-2.435550000	-3.948858000
1	2.844268000	-1.854994000	-2.347216000

Compound 2h

31	-0.074607000	-1.118953000	-0.776904000
17	1.767573000	-1.344222000	-1.975723000
17	-0.534139000	-3.017015000	0.218900000
17	-1.587845000	-0.808190000	-2.366500000
26	0.027927000	0.798198000	0.759052000
14	-3.884951000	-1.157669000	1.025652000
7	-3.129137000	0.358955000	0.394567000
5	-1.832890000	0.599811000	0.587780000
14	-4.033678000	1.350000000	-0.808245000
7	3.170952000	0.374858000	0.456962000
5	1.858540000	0.502728000	0.632173000
14	3.951075000	1.720344000	-0.454468000
14	4.018976000	-1.191142000	0.729239000
8	0.136317000	-1.082200000	2.962949000
6	0.056404000	-0.352712000	2.091803000
8	0.167477000	3.247532000	2.286016000
6	0.089173000	2.270539000	1.703968000
8	0.347253000	2.068881000	-1.826215000
6	0.177996000	1.564092000	-0.817625000
6	-2.862264000	-1.678816000	2.468617000
1	-1.933970000	-2.126717000	2.116626000
1	-3.397757000	-2.437912000	3.044077000
1	-2.631071000	-0.845791000	3.133599000
6	-3.920446000	-2.442401000	-0.297773000
1	-4.825674000	-2.383454000	-0.899956000
1	-3.869790000	-3.429429000	0.166912000
1	-3.055092000	-2.342026000	-0.951701000
6	-5.599154000	-0.676016000	1.544058000
1	-5.583739000	0.138935000	2.267274000
1	-6.082406000	-1.537794000	2.010543000
1	-6.211179000	-0.376481000	0.695185000

6	-4.916169000	0.179667000	-1.931542000
1	-4.218876000	-0.552407000	-2.334152000
1	-5.350800000	0.739551000	-2.762652000
1	-5.723171000	-0.343154000	-1.421497000
6	-5.221223000	2.402822000	0.145820000
1	-5.951274000	1.806090000	0.689275000
1	-5.761798000	3.062453000	-0.536936000
1	-4.684912000	3.026399000	0.862596000
6	-2.790565000	2.397265000	-1.682518000
1	-2.197378000	2.977513000	-0.972409000
1	-3.292598000	3.100665000	-2.350357000
1	-2.119652000	1.776060000	-2.273513000
6	2.999656000	3.248914000	-0.015137000
1	2.049513000	3.288800000	-0.546396000
1	3.569265000	4.138666000	-0.293531000
1	2.797326000	3.296940000	1.055992000
6	5.700555000	1.815314000	0.141830000
1	5.735977000	2.004280000	1.214224000
1	6.213682000	2.634602000	-0.366409000
1	6.251087000	0.899766000	-0.064937000
6	3.818963000	1.317447000	-2.246757000
1	4.302632000	0.370011000	-2.478836000
1	4.273411000	2.103152000	-2.854255000
1	2.768568000	1.221250000	-2.522583000
6	5.172976000	-0.891941000	2.148169000
1	5.961514000	-0.185546000	1.894128000
1	5.644016000	-1.833328000	2.440505000
1	4.629086000	-0.507128000	3.011839000
6	4.975131000	-1.625151000	-0.792532000
1	4.301680000	-1.814408000	-1.625779000
1	5.541968000	-2.538631000	-0.595139000
1	5.685112000	-0.850417000	-1.075589000
6	2.752355000	-2.453625000	1.170427000
1	2.082403000	-2.109486000	1.958573000
1	3.251621000	-3.352897000	1.540426000
1	2.148036000	-2.736805000	0.311225000

Compound 5

78	0.079901000	0.183782000	-0.177536000
15	-2.185061000	0.410808000	0.011006000
15	2.305510000	0.280840000	0.138931000
6	3.414973000	-0.702040000	-0.878971000
1	3.347414000	-1.692903000	-0.422590000
6	2.714324000	2.037444000	-0.032946000
1	1.904814000	2.544786000	0.508011000
6	-3.362834000	-0.936673000	-0.277772000
1	-2.779518000	-1.839534000	-0.083535000
6	-3.842264000	-1.011381000	-1.711820000
1	-4.527682000	-0.184905000	-1.910244000
1	-3.001699000	-0.940626000	-2.393012000
6	2.111423000	-1.481689000	2.186883000
1	1.050740000	-1.482198000	1.923668000
1	2.587582000	-2.241558000	1.572636000

6	-4.563457000	-2.322669000	-1.916027000
1	-4.894528000	-2.411032000	-2.951546000
1	-3.853011000	-3.131979000	-1.727653000
6	4.866033000	-0.283184000	-0.880144000
1	5.233325000	-0.155295000	0.138688000
1	4.967618000	0.673170000	-1.396894000
6	3.999668000	4.452795000	-0.952718000
1	4.848391000	4.044713000	-1.512009000
1	4.061905000	5.539955000	-1.015611000
6	2.881873000	-0.839622000	-2.292232000
1	1.834411000	-1.138362000	-2.270044000
1	2.932933000	0.126772000	-2.798200000
6	2.658627000	-0.102379000	1.872771000
1	3.739107000	-0.074712000	2.045610000
6	2.612978000	2.458305000	-1.483686000
1	3.432176000	1.999164000	-2.040253000
1	1.679479000	2.088156000	-1.914089000
6	3.705377000	-1.857022000	-3.045058000
1	3.572574000	-2.825913000	-2.558155000
1	3.338612000	-1.951302000	-4.067534000
6	4.022045000	2.493177000	0.576223000
1	4.851673000	2.059666000	0.021613000
1	4.109475000	2.155269000	1.608169000
6	-2.682288000	1.876510000	-0.924042000
1	-2.011669000	2.652147000	-0.535279000
6	-2.435169000	0.910612000	1.738683000
1	-3.503712000	1.039351000	1.926826000
6	2.716372000	3.961946000	-1.588402000
1	2.664712000	4.273509000	-2.632244000
1	1.863669000	4.410965000	-1.068807000
6	-1.833495000	2.591563000	3.475729000
1	-1.298608000	3.524177000	3.661242000
1	-2.887232000	2.765635000	3.716916000
6	-5.289063000	-2.271016000	0.466080000
1	-4.608559000	-3.088617000	0.724591000
1	-6.143155000	-2.324529000	1.142790000
6	1.960583000	0.931277000	2.736801000
1	2.331522000	1.935179000	2.536392000
1	0.902245000	0.912431000	2.458875000
6	4.106925000	4.000922000	0.488501000
1	3.285564000	4.439084000	1.065254000
1	5.040482000	4.353530000	0.928495000
6	5.680893000	-1.321932000	-1.620724000
1	6.735315000	-1.042019000	-1.622129000
1	5.591648000	-2.278809000	-1.097730000
6	-4.101984000	2.322090000	-0.667629000
1	-4.280514000	2.416024000	0.404434000
1	-4.787112000	1.562747000	-1.047651000
6	1.507029000	-0.769234000	4.478761000
1	0.451349000	-0.760837000	4.193742000
1	1.562010000	-1.005411000	5.542301000
6	2.102037000	0.591886000	4.201748000
1	3.164941000	0.580319000	4.464477000

1	1.629133000	1.358779000	4.815687000
6	-5.737011000	-2.435445000	-0.969154000
1	-6.463163000	-1.649922000	-1.206392000
1	-6.240995000	-3.394469000	-1.098199000
6	-1.729932000	2.221668000	2.012966000
1	-0.675313000	2.109832000	1.732633000
1	-2.152004000	3.017610000	1.399980000
6	5.170872000	-1.481036000	-3.036505000
1	5.757682000	-2.233097000	-3.565875000
1	5.303100000	-0.531191000	-3.566732000
6	-4.546324000	-0.966725000	0.666608000
1	-5.205540000	-0.119306000	0.458418000
1	-4.224362000	-0.893241000	1.702551000
6	2.218065000	-1.817640000	3.653756000
1	1.781847000	-2.802219000	3.823673000
1	3.270665000	-1.862629000	3.951086000
6	-1.299025000	1.487583000	4.359783000
1	-1.380814000	1.766665000	5.411330000
1	-0.241945000	1.346256000	4.138896000
6	-2.370348000	1.762154000	-2.401806000
1	-3.015731000	1.017148000	-2.860805000
1	-1.340407000	1.421200000	-2.528739000
6	-1.889404000	-0.182100000	2.634564000
1	-0.835369000	-0.324968000	2.378219000
1	-2.368238000	-1.133098000	2.420222000
6	-4.360584000	3.637137000	-1.369690000
1	-5.394601000	3.949456000	-1.218727000
1	-3.717967000	4.404507000	-0.925305000
6	-4.047728000	3.532127000	-2.847003000
1	-4.715669000	2.791105000	-3.299148000
1	-4.237462000	4.486022000	-3.340914000
6	-2.615585000	3.094449000	-3.070634000
1	-1.939331000	3.843869000	-2.645666000
1	-2.400848000	3.025526000	-4.137617000
6	-2.024908000	0.191025000	4.088522000
1	-3.085248000	0.308424000	4.336052000
1	-1.633009000	-0.609411000	4.716989000
31	-0.025796000	-2.190133000	-0.445751000
17	-1.137657000	-3.070765000	1.243805000
17	-1.046153000	-2.459847000	-2.368844000
17	1.766265000	-3.453346000	-0.593540000

Compound 7

31	-1.746429000	-0.905970000	-0.480595000
26	-1.001305000	1.209482000	0.677830000
17	-0.101114000	-1.614183000	-1.771266000
17	-2.331510000	-2.427472000	0.951686000
7	1.932092000	0.060052000	0.251096000
5	0.690487000	0.460018000	0.471265000
17	-3.392931000	-0.308551000	-1.777113000
14	2.888807000	1.094223000	-0.882584000
14	2.503797000	-1.584851000	0.737412000
8	-1.040373000	-0.372549000	3.117448000

6	-1.058224000	0.240838000	2.162886000
8	0.093873000	3.670997000	1.748138000
6	-0.362161000	2.711242000	1.347719000
8	-0.631362000	1.827556000	-2.141866000
6	-0.820777000	1.588184000	-1.047950000
6	2.268090000	2.825611000	-0.667549000
1	1.284789000	2.971766000	-1.110759000
1	2.951129000	3.518203000	-1.165221000
1	2.221097000	3.104130000	0.385289000
6	4.649812000	0.969676000	-0.335090000
1	4.752445000	1.313568000	0.693974000
1	5.271756000	1.606079000	-0.968070000
1	5.035221000	-0.045332000	-0.400310000
6	2.577631000	0.453402000	-2.580179000
1	2.949702000	-0.562007000	-2.702484000
1	3.056634000	1.092053000	-3.325214000
1	1.504452000	0.434701000	-2.772526000
6	3.757927000	-1.280919000	2.064831000
1	4.639603000	-0.762586000	1.693105000
1	4.078865000	-2.230821000	2.497777000
1	3.318736000	-0.682384000	2.864451000
6	3.244552000	-2.371394000	-0.759589000
1	2.481070000	-2.491099000	-1.527308000
1	3.620737000	-3.362029000	-0.493894000
1	4.075078000	-1.798297000	-1.166850000
6	1.059879000	-2.520252000	1.387616000
1	0.517288000	-1.976931000	2.160759000
1	1.408478000	-3.454093000	1.836413000
1	0.357920000	-2.772181000	0.595449000
6	-2.774259000	1.560691000	0.707479000
8	-3.881468000	1.780692000	0.748977000