Electronic Supplementary Material (ESI) for Chemical Communications.

Iron pentacarbonyl ligands on silver scorpionates

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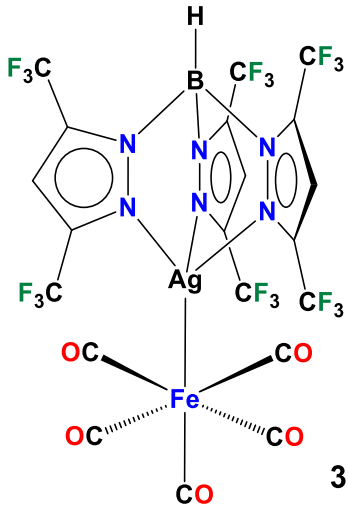
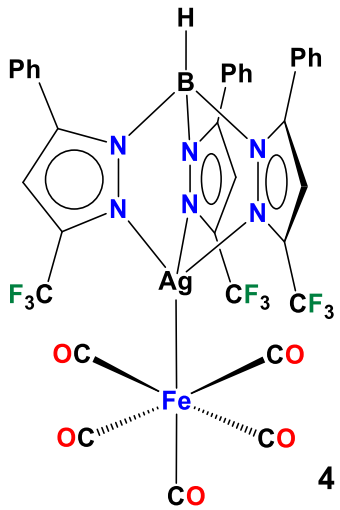
Supplementary Materials

Abbreviations and molecules



[HB(3,5-$(CF_3)_2$Pz)$_3$]Ag-Fe(CO)$_5$ (**3**)

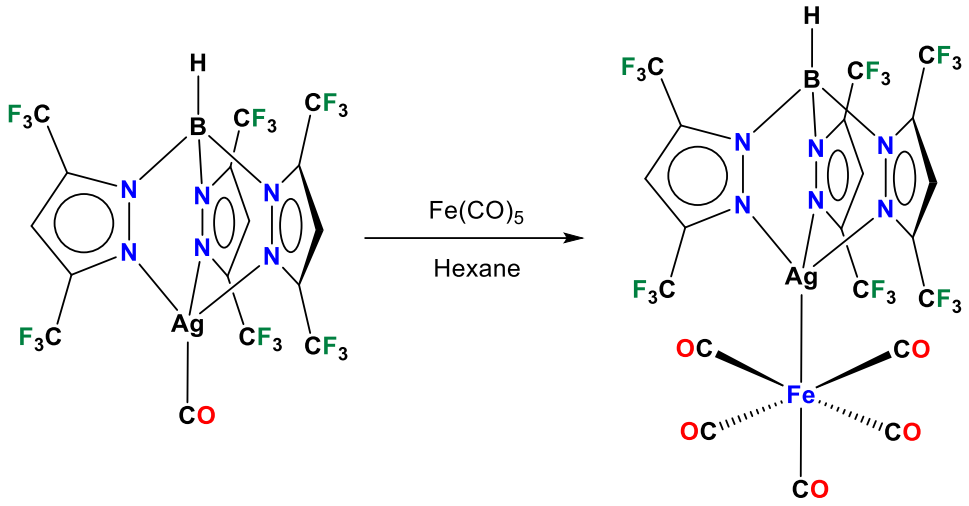


[HB(3-(CF_3),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (**4**)

General Information

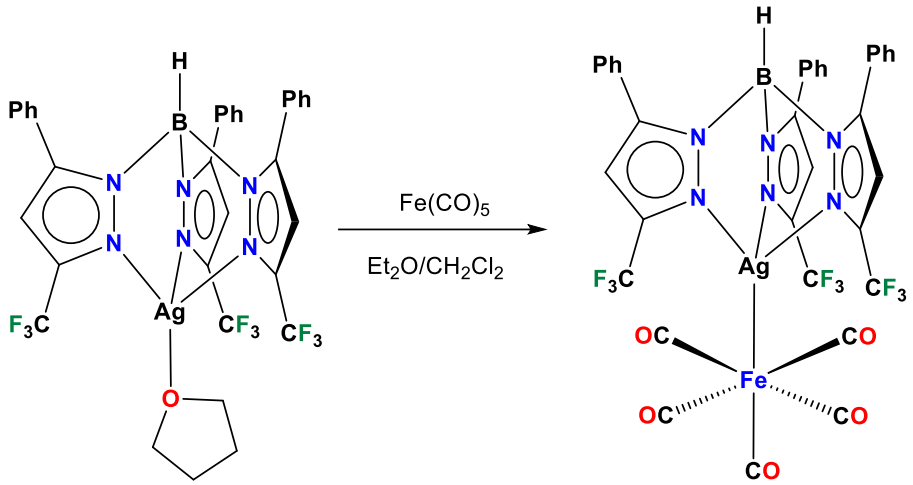
All manipulations were carried out under an atmosphere of purified nitrogen using standard Schlenk techniques or in a MBRAUN LABMaster glovebox equipped with a -10 °C refrigerator. Solvents were purchased from commercial sources, and purified by conventional methods prior to use. Glassware was oven-dried at 150 ºC overnight. The NMR spectra were recorded at the room temperature on a JEOL Eclipse 500 spectrometer (^{1}H: 500.16 MHz, ^{13}C: 125.77 MHz and 470.62 MHz) and a JEOL Eclipse 300 spectrometer (^{19}F: 282.78 MHz). Chemical shifts for ^{1}H and ^{13}C spectra are referenced to the solvent peak (^{1}H; CD_2Cl_2 δ 5.32, $CDCl_3$, δ 7.26 ^{13}C; CD_2Cl_2 δ 53.84, $CDCl_3$ δ 77.16, DMSO-*d*$_6$ δ 39.52). ^{1}H NMR coupling constants (J) are reported in Hertz (Hz) and multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet). ^{19}F NMR values were referenced to external $CFCl_3$. IR spectra were collected at room temperature on a Shimadzu IRPrestige-21 FTIR containing an ATR attachment at 2 cm^{-1} resolution. Elemental analyses were performed at Intertek USA, Whitehouse, NJ. Deuterated solvents were purchased from Acros Organics and Cambridge Isotope Laboratories, respectively. The $Fe(CO)_5$ was obtained from Sigma-Aldrich Company and distilled prior to use. Deuterated solvents were purchased from Acros Organics and Cambridge Isotope Laboratories, respectively. Heating was accomplished by either a heating mantle or a silicone oil bath. [HB(3,5-$(CF_3)_2Pz)_3$]Ag(CO)[1] and [HB(3-(CF_3),5-(Ph)$Pz)_3$]Na(THF)[2] were prepared according to literature procedures.

Synthesis and Characterization of Metal complexes



Synthesis of [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ (3)

To a colorless solution of [HB(3,5-$(CF_3)_2Pz)_3$]Ag(CO) (185 mg, 0.25 mmol) in anhydrous hexane (5 mL) at -20 °C was added dropwise a yellow solution of $Fe(CO)_5$ (98 mg, 0.5 mmol) in anhydrous hexane (0.5 mL) under N_2 atmosphere. The colorless solution was stirred for 10 min. The solution was kept in refrigerator under -20 °C overnight to obtain [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ as yellow single crystals (169 mg, 73 % yield). ^{1}H NMR (CD_2Cl_2, 500.16 MHz, 298 K) δ: 6.98 (s, Pz), 4.97 (br, 1H, B*H*). $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 125.77 MHz, 298 K) δ: 207.3 (br s, *C*O), 143.9 (q, J_{C-F} = 39.0 Hz, *C*CF_3), 140.8 (q, J_{C-F} = 40.5 Hz, *C*CF_3), 120.9 (q,$^1J_{CF}$ = 268.8 Hz, *C*F_3), 119.7 (q,$^1J_{CF}$ = 270 Hz, *C*F_3), 107.0 (s, *C*H-Pz). ^{19}F NMR (CD_2Cl_2, 470.62 MHz, 298 K) δ: -59.5 (s, CF_3), -61.7 (s, br, CF_3). IR (Selected bands) cm^{-1}: 2009 (CO), 2038 (CO), 2068 (CO), 2130 (CO). Anal. Calcd. for $C_{20}H_4AgBF_{18}FeN_6O_5$: C, 25.98; H, 0.44; N, 9.09. Found: C, 25.91; H, 0.36; N, 9.95.



Synthesis of [HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (4)

[HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag(THF) (165 mg, 0.2 mmol) (prepared by the reaction of [HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Na(THF) with AgOTf)[2] was dissolved in anhydrous Et$_2$O/CH$_2$Cl$_2$ (1:1, 10 mL) and the solvent was removed in order to remove the coordinated THF. The residue was dissolved in anhydrous CH$_2$Cl$_2$ (5 mL) at -20 °C a yellow solution of Fe(CO)$_5$ (78.5 mg, 0.4 mmol) in anhydrous CH$_2$Cl$_2$ (0.5 mL) was added under N$_2$ atmosphere. The yellow solution was stirred for 10 min. The solution was mixed with some hexane and kept in refrigerator under -20 °C overnight to obtain [HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ as yellow single crystals (90 mg, 47% yield). ^{1}H NMR (CD$_2$Cl$_2$, 500.16 MHz, 298 K) δ: 7.24-7.20 (m, 3H, Ph), 6.97-6.95 (m, 6H, Ph), 6.59 (s, 3H, Pz), 4.71 (br, 1H, B*H*). ^{13}C{^{1}H} NMR (CD$_2$Cl$_2$, 125.77 MHz, 298 K) δ: 208.5 (br s, *C*O), 152.2, 143.0 (q, $J_{C\text{-}F}$ = 37.2 Hz, *C*CF$_3$), 131.4, 130.0, 128.4, 128.1, 122.0 (q, $^1J_{CF}$ = 267.5 Hz, *C*F$_3$, 105.1 (s, *C*H-Pz). ^{19}F NMR (CD$_2$Cl$_2$, 282.78 MHz, 298 K) δ: -61.3 (s, CF$_3$). IR (Selected bands) cm^{-1}: 1996 (CO), 2032 (CO), 2043 (CO), 2058 (CO), 2123 (CO). Anal. Calcd. for C$_{35}$H$_{19}$AgFeBF$_9$N$_6$O$_5$ with 0.75 hexane: C, 46.80; H, 2.93; N, 8.29. Found: 46.75; H, 2.83; N, 8.21.

^{1}H, ^{13}C, ^{19}F NMR, and IR Spectra of Metal Complexes

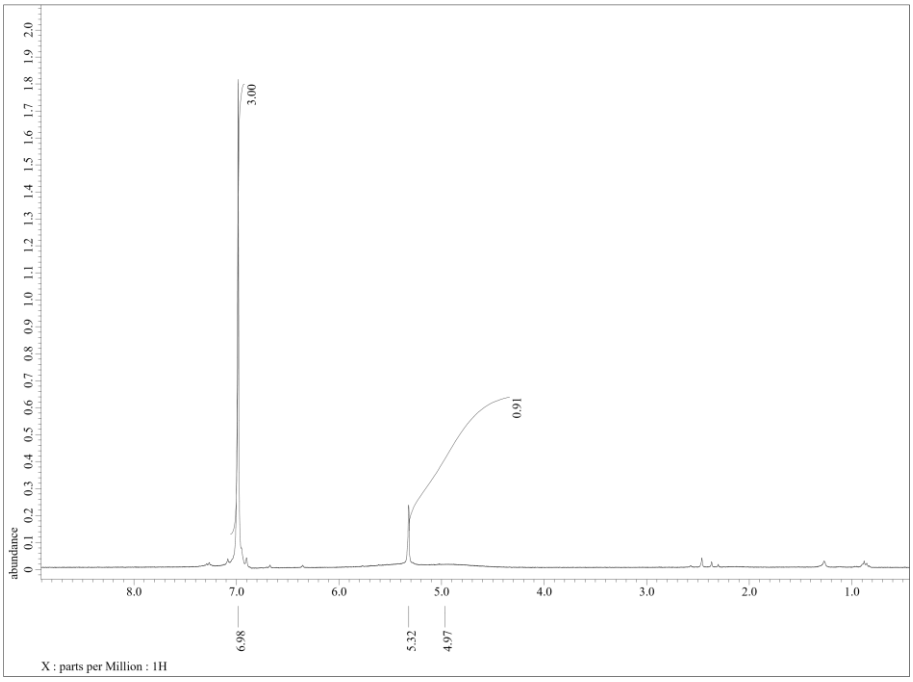


Figure S1: ^{1}H NMR Spectrum of **[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Ag-Fe(CO)$_5$ (3)** in CD_2Cl_2.

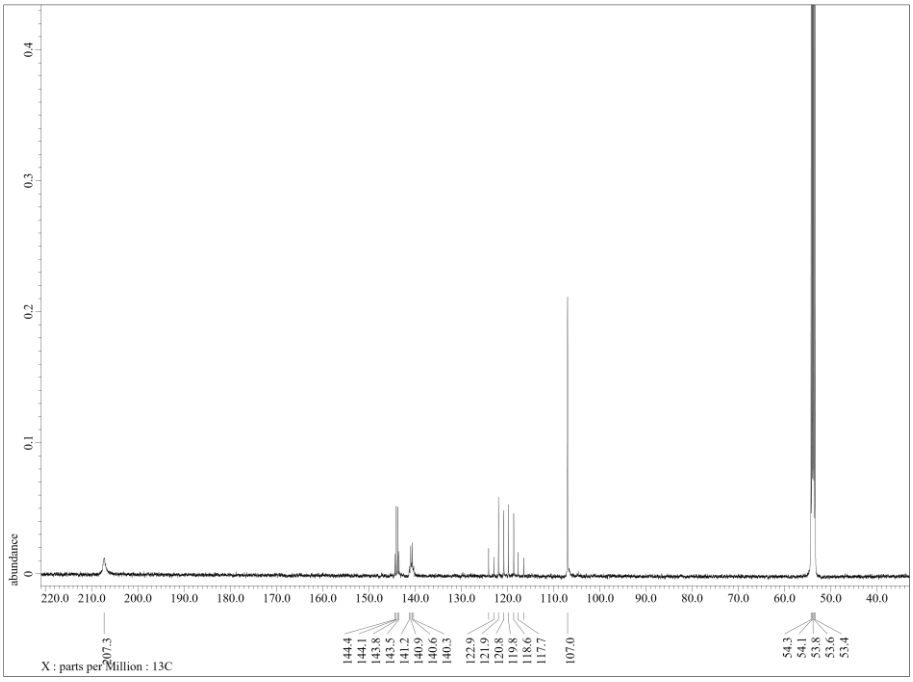


Figure S2: ^{13}C NMR Spectrum of **[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Ag-Fe(CO)$_5$ (3)** in CD_2Cl_2.

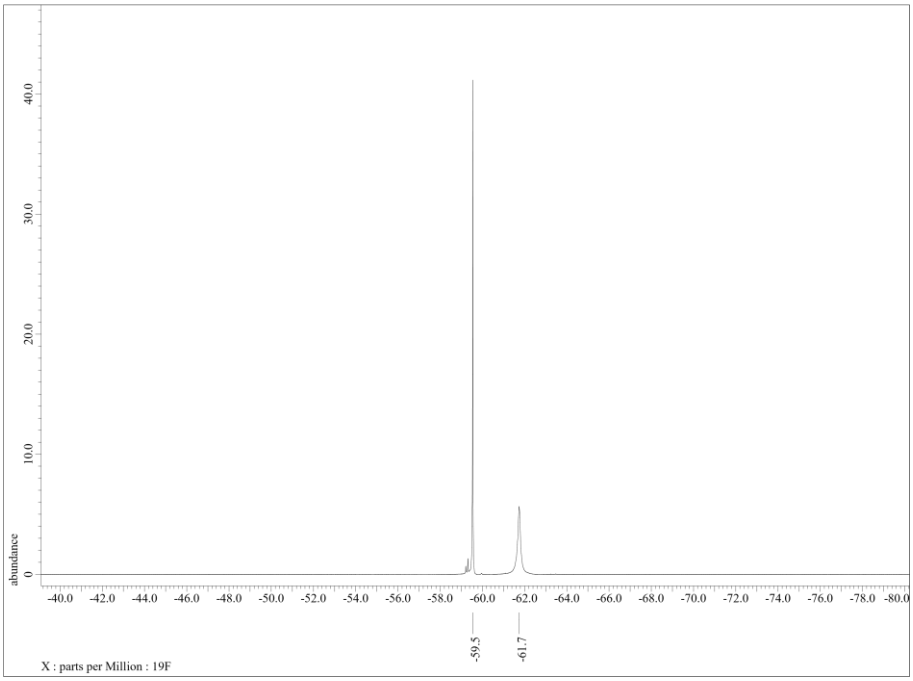


Figure S3: ^{19}F NMR Spectrum of **[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Ag-Fe(CO)$_5$ (3)** in CD_2Cl_2.

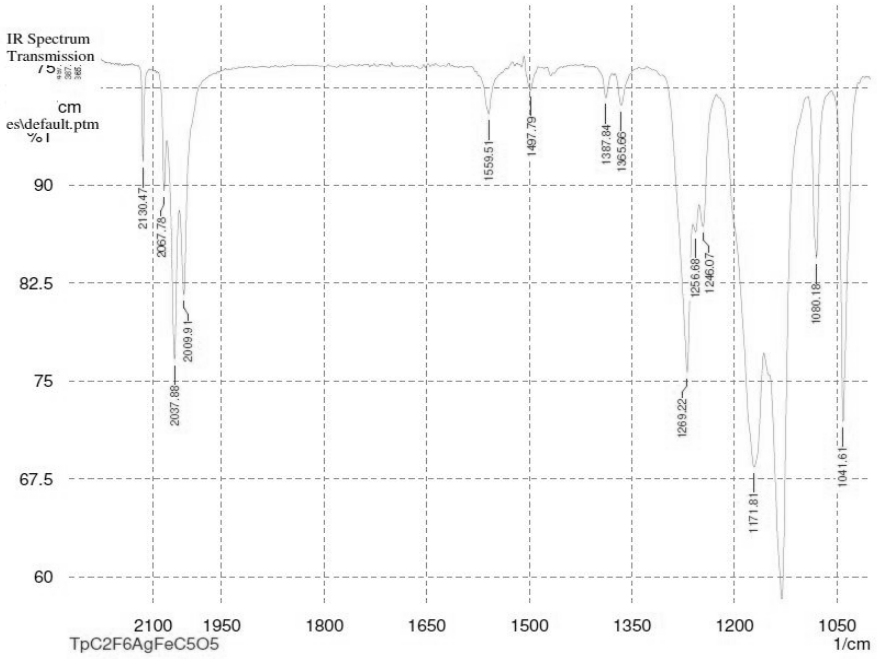


Figure S4: IR Spectrum of **[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Ag-Fe(CO)$_5$ (3).**

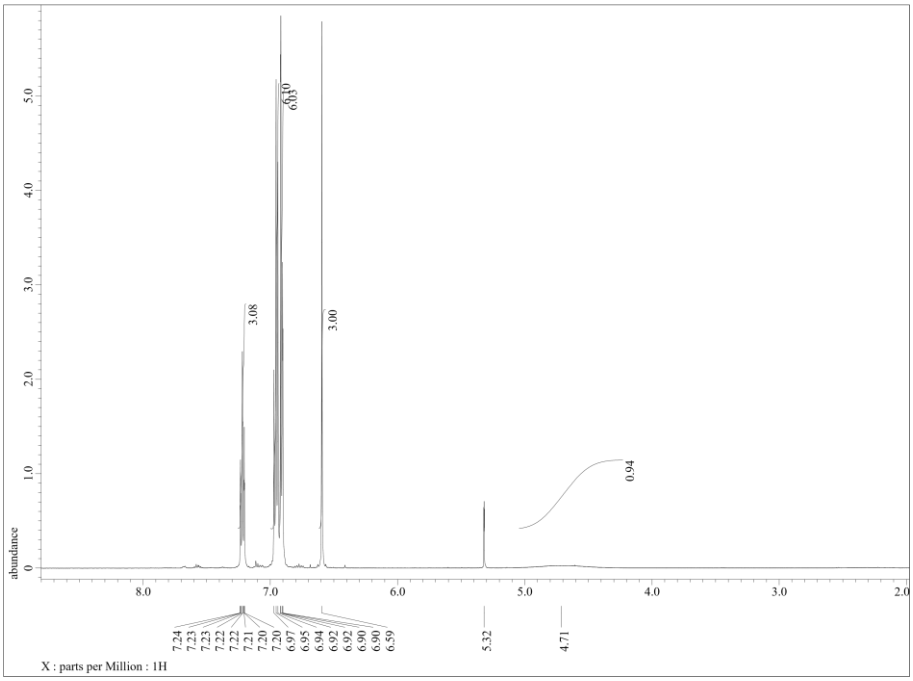


Figure S5: ^{1}H NMR Spectrum of **[[HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (4)** in CD_2Cl_2.

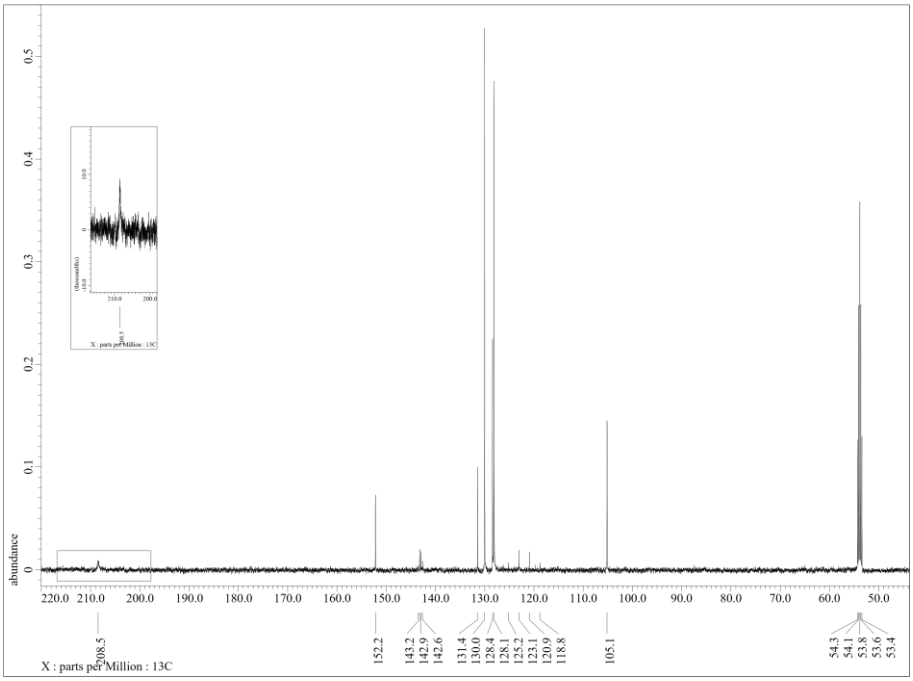


Figure S6: ^{13}C NMR Spectrum of **[HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (4)** in CD_2Cl_2.

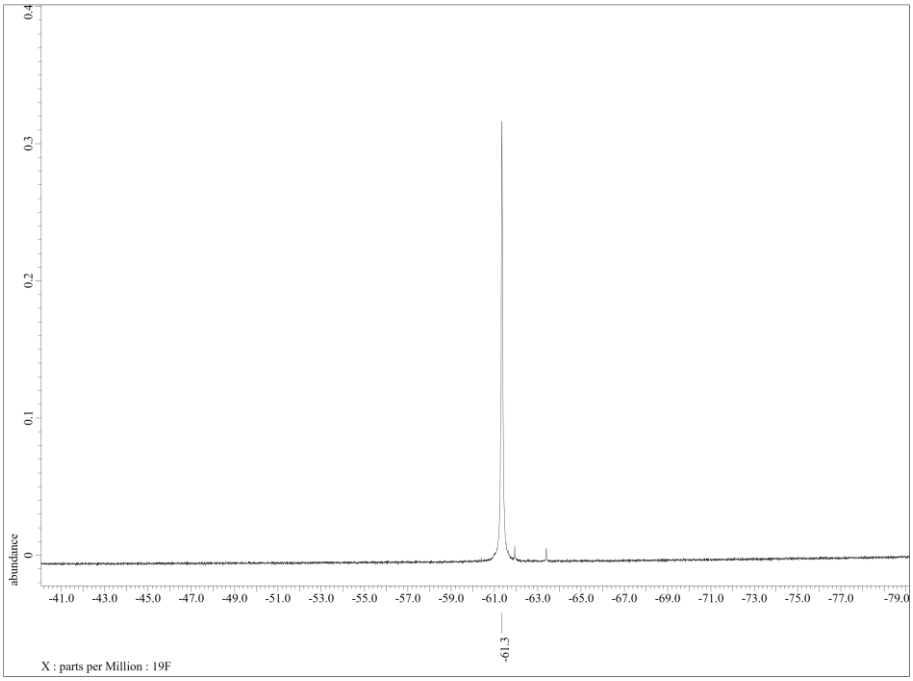


Figure S7: ^{19}F NMR Spectrum of **[HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (4)** in CD_2Cl_2.

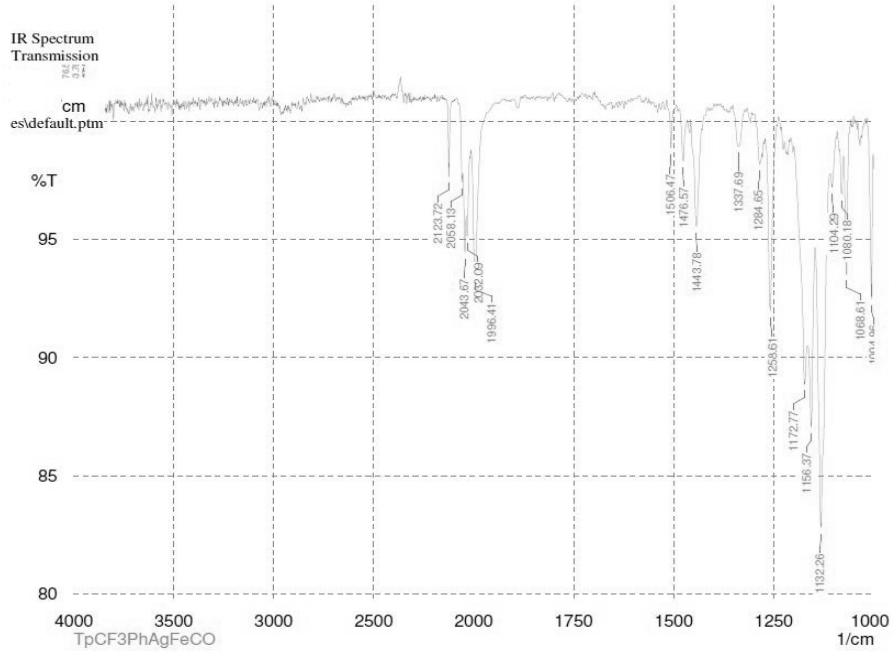


Figure S8: IR Spectrum of **[HB(3-(CF$_3$),5-(Ph)Pz)$_3$]Ag-Fe(CO)$_5$ (4)**.

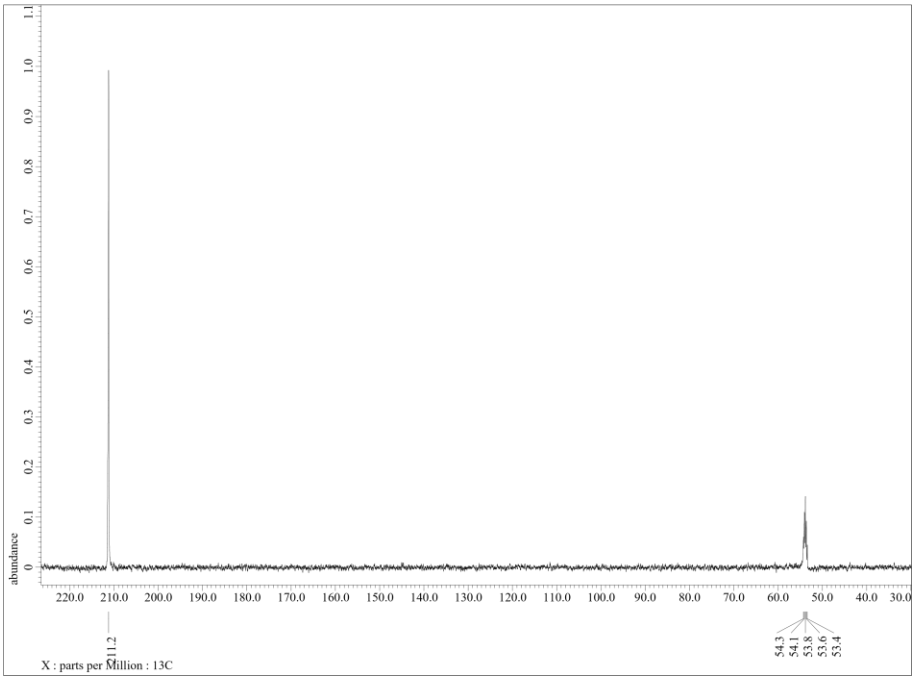


Figure S9: ^{13}C NMR Spectrum of **Fe(CO)$_5$** in CD_2Cl_2.

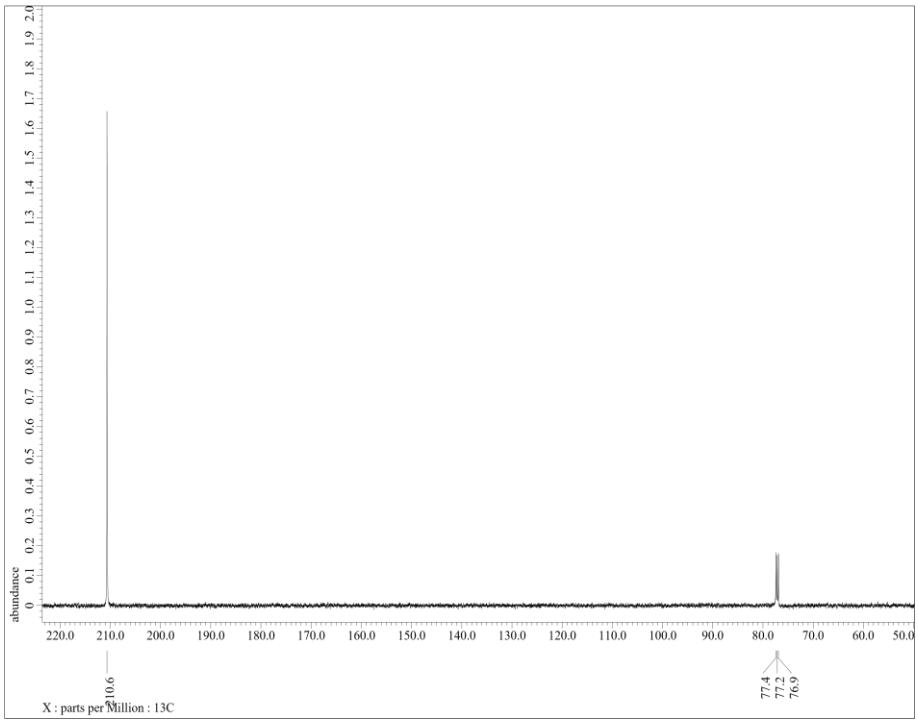


Figure S10: ^{13}C NMR Spectrum of **Fe(CO)$_5$** in $CDCl_3$.

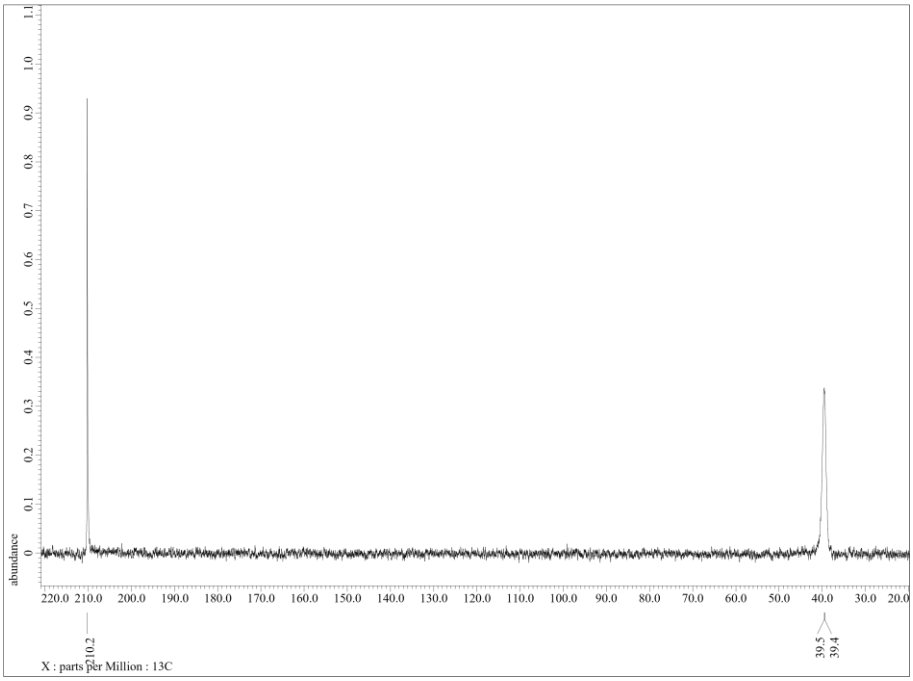


Figure S11: ^{13}C NMR Spectrum of **Fe(CO)$_5$** in DMSO-d_6.

X-ray Data Collection and Structure Determinations

A suitable crystal covered with a layer of hydrocarbon/Paratone-N oil was selected and mounted on a Cryo-loop, and immediately placed in the low temperature nitrogen stream. The X-ray intensity data were measured at 100(2) K (unless otherwise noted) on a Bruker D8 Quest with a Photon 100 CMOS detector equipped with an Oxford Cryosystems 700 series cooler, a Triumph monochromator, and a Mo Kα fine-focus sealed tube (λ = 0.71073 Å). Intensity data were processed using the Bruker Apex program suite. Absorption corrections were applied by using SADABS.[3] Initial atomic positions were located by SHELXT,[4] and the structures of the compounds were refined by the least-squares method using SHELXL[5] within Olex2 GUI.[6] All the non-hydrogen atoms were refined anisotropically. The H atoms were included in their calculated positions and refined as riding on the atoms to which they are joined. X-ray structural figures were generated using Olex2.[6] The CCDC 2126148 contain the supplementary crystallographic data for these molecules.

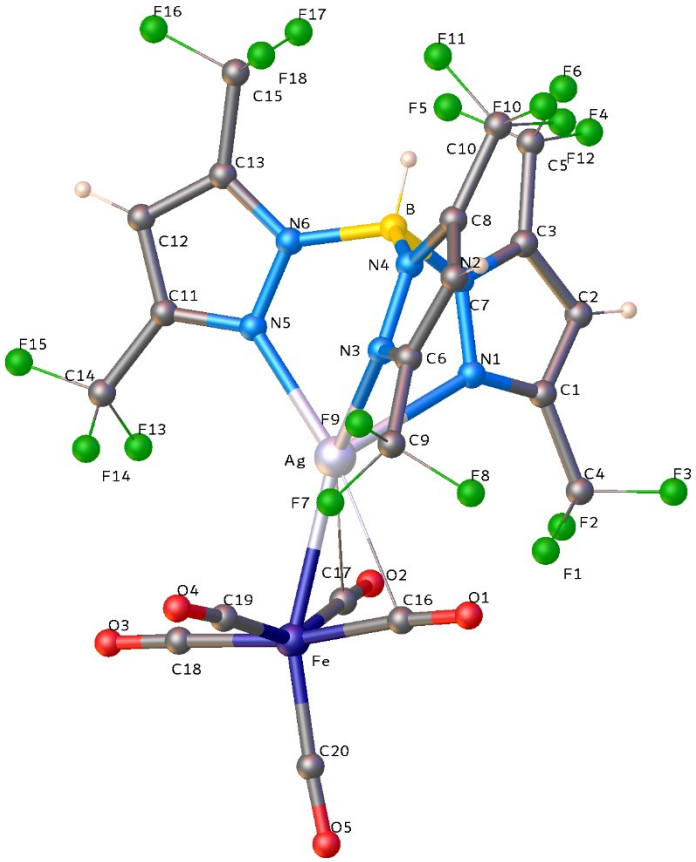


Figure S12. Atom labelling scheme of [HB(3,5-$(CF_3)_2Pz)_3$]Ag-Fe$(CO)_5$ (**3**)

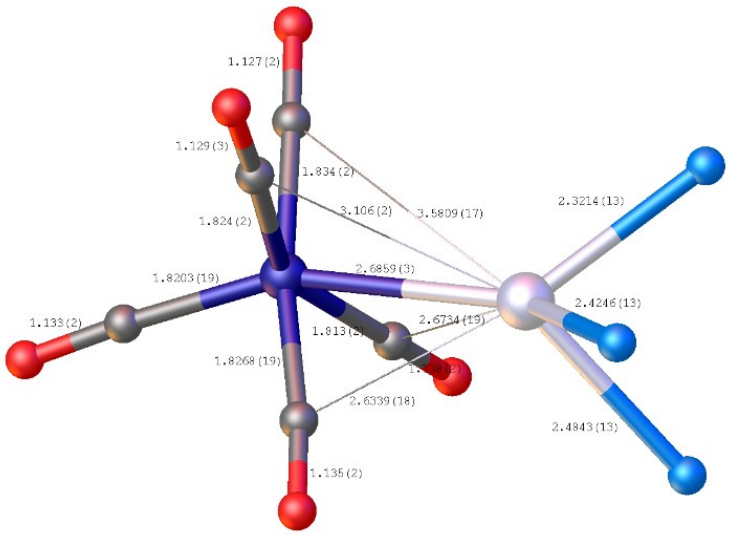


Figure S13. A view showing the coordination geometry at silver and iron in [HB(3,5-$(CF_3)_2Pz)_3$]Ag-Fe$(CO)_5$ (**3**), and selected bond distances

Table S1. Crystal data and structure refinement for $[HB(3,5\text{-}(CF_3)_2Pz)_3]Ag\text{-}Fe(CO)_5$ (**3**).

Identification code	rad526a_a
Empirical formula	$C_{20}H_4AgBF_{18}FeN_6O_5$
Formula weight	924.80
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.4955(4)
b/Å	25.9298(8)
c/Å	10.7081(3)
α/°	90
β/°	113.251(1)
γ/°	90
Volume/Å^3	2932.60(16)
Z	4
ρ_{calc}g/cm^3	2.0944
μ/mm^{-1}	1.322
F(000)	1783.6
Crystal size/mm^3	0.4 × 0.3 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.1 to 61.06
Index ranges	$-16 \le h \le 16$, $-36 \le k \le 37$, $-15 \le l \le 15$
Reflections collected	40436
Independent reflections	8966 [R_{int} = 0.0193, R_{sigma} = 0.0151]
Data/restraints/parameters	8966/0/469
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0277, wR_2 = 0.0680
Final R indexes [all data]	R_1 = 0.0297, wR_2 = 0.0692
Largest diff. peak/hole / e Å^{-3}	0.92/-0.95

Table S2. Bond Lengths for $[HB(3,5\text{-}(CF_3)_2Pz)_3]Ag\text{-}Fe(CO)_5$ (**3**)..

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag	Fe	2.6859(3)	O1	C16	1.135(2)
Ag	N1	2.4843(13)	O2	C17	1.138(2)
Ag	N3	2.4246(13)	O3	C18	1.127(2)
Ag	N5	2.3214(13)	O4	C19	1.129(3)
Ag	C16	2.6339(18)	O5	C20	1.133(2)
Ag	C17	2.6734(19)	N1	N2	1.3556(17)
Fe	C16	1.8268(19)	N1	C1	1.3325(19)

Table S2. Bond Lengths for [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ (**3**)..

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe	C17	1.813(2)	N2	C3	1.362(2)
Fe	C18	1.834(2)	N2	B	1.554(2)
Fe	C19	1.824(2)	N3	N4	1.3542(18)
Fe	C20	1.8203(19)	N3	C6	1.3344(19)
F1	C4	1.335(2)	N4	C8	1.3596(19)
F2	C4	1.3367(18)	N4	B	1.563(2)
F3	C4	1.3421(19)	N5	N6	1.3563(18)
F4	C5	1.335(2)	N5	C11	1.333(2)
F5	C5	1.332(3)	N6	C13	1.357(2)
F6	C5	1.326(3)	N6	B	1.548(2)
F7	C9	1.330(2)	C1	C2	1.389(2)
F8	C9	1.341(2)	C1	C4	1.490(2)
F9	C9	1.336(2)	C2	C3	1.374(2)
F10	C10	1.340(2)	C3	C5	1.492(3)
F11	C10	1.323(3)	C6	C7	1.396(2)
F12	C10	1.338(2)	C6	C9	1.487(2)
F13	C14	1.333(3)	C7	C8	1.372(2)
F14	C14	1.331(2)	C8	C10	1.493(2)
F15	C14	1.329(2)	C11	C12	1.390(2)
F16	C15	1.336(2)	C11	C14	1.489(3)
F17	C15	1.329(3)	C12	C13	1.375(3)
F18	C15	1.340(2)	C13	C15	1.493(2)

Table S3. Bond Angles for [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ (**3**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ag	Fe	128.16(3)	C1	C4	F2	112.72(14)
N3	Ag	Fe	135.10(3)	C1	C4	F3	110.42(14)
N3	Ag	N1	77.51(4)	F5	C5	F4	107.3(2)
N5	Ag	Fe	130.28(3)	F6	C5	F4	106.73(18)
N5	Ag	N1	83.29(5)	F6	C5	F5	107.36(19)
N5	Ag	N3	82.89(5)	C3	C5	F4	109.50(16)
C16	Ag	Fe	40.15(4)	C3	C5	F5	112.22(17)
C16	Ag	N1	105.09(5)	C3	C5	F6	113.43(19)
C16	Ag	N3	103.78(5)	C7	C6	N3	112.18(14)
C16	Ag	N5	170.14(5)	C9	C6	N3	122.22(14)
C17	Ag	Fe	39.54(4)	C9	C6	C7	125.58(14)
C17	Ag	N1	94.31(5)	C8	C7	C6	103.19(14)

Table S3. Bond Angles for [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ (**3**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C17	Ag	N3	159.42(5)	C7	C8	N4	109.42(14)
C17	Ag	N5	115.23(5)	C10	C8	N4	124.42(15)
C17	Ag	C16	59.72(6)	C10	C8	C7	126.08(15)
C16	Fe	Ag	68.39(6)	F8	C9	F7	106.51(15)
C17	Fe	Ag	69.86(6)	F9	C9	F7	107.13(15)
C17	Fe	C16	93.12(8)	F9	C9	F8	106.28(15)
C18	Fe	Ag	103.17(6)	C6	C9	F7	113.33(14)
C18	Fe	C16	170.88(8)	C6	C9	F8	111.80(15)
C18	Fe	C17	86.88(9)	C6	C9	F9	111.36(14)
C19	Fe	Ag	84.77(7)	F11	C10	F10	107.61(17)
C19	Fe	C16	90.51(9)	F12	C10	F10	106.39(18)
C19	Fe	C17	150.84(10)	F12	C10	F11	106.94(17)
C19	Fe	C18	85.13(10)	C8	C10	F10	109.54(16)
C20	Fe	Ag	158.78(6)	C8	C10	F11	114.27(17)
C20	Fe	C16	92.51(9)	C8	C10	F12	111.71(16)
C20	Fe	C17	103.42(10)	C12	C11	N5	111.86(15)
C20	Fe	C18	96.36(9)	C14	C11	N5	120.62(15)
C20	Fe	C19	105.31(11)	C14	C11	C12	127.52(16)
N2	N1	Ag	113.28(9)	C13	C12	C11	103.61(14)
C1	N1	Ag	137.94(10)	C12	C13	N6	109.23(15)
C1	N1	N2	105.79(12)	C15	C13	N6	124.63(16)
C3	N2	N1	109.30(13)	C15	C13	C12	126.04(16)
B	N2	N1	121.60(12)	F14	C14	F13	105.95(17)
B	N2	C3	128.52(13)	F15	C14	F13	108.23(19)
N4	N3	Ag	115.58(9)	F15	C14	F14	106.95(17)
C6	N3	Ag	136.53(11)	C11	C14	F13	112.46(16)
C6	N3	N4	105.79(12)	C11	C14	F14	112.40(16)
C8	N4	N3	109.42(13)	C11	C14	F15	110.55(17)
B	N4	N3	122.57(12)	F17	C15	F16	106.90(17)
B	N4	C8	128.00(13)	F18	C15	F16	107.37(17)
N6	N5	Ag	117.66(10)	F18	C15	F17	107.11(18)
C11	N5	Ag	133.85(11)	C13	C15	F16	108.89(17)
C11	N5	N6	106.08(13)	C13	C15	F17	114.07(16)
C13	N6	N5	109.23(13)	C13	C15	F18	112.16(16)
B	N6	N5	122.07(12)	Fe	C16	Ag	71.46(6)
B	N6	C13	128.65(14)	O1	C16	Ag	114.12(14)
C2	C1	N1	112.37(14)	O1	C16	Fe	174.33(16)
C4	C1	N1	122.07(14)	Fe	C17	Ag	70.60(6)
C4	C1	C2	125.52(14)	O2	C17	Ag	115.31(15)

Table S3. Bond Angles for [HB(3,5-$(CF_3)_2Pz)_3$]Ag-$Fe(CO)_5$ (**3**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	C2	C1	103.39(14)	O2	C17	Fe	173.44(17)
C2	C3	N2	109.15(15)	O3	C18	Fe	178.42(19)
C5	C3	N2	124.77(15)	O4	C19	Fe	175.3(2)
C5	C3	C2	126.05(15)	O5	C20	Fe	176.56(18)
F2	C4	F1	107.54(14)	N4	B	N2	109.33(12)
F3	C4	F1	106.83(14)	N6	B	N2	111.12(12)
F3	C4	F2	105.89(13)	N6	B	N4	110.17(12)
C1	C4	F1	113.03(13)				

Computational Details

Geometry optimizations of the complexes were performed without symmetry constraints using the Gaussian09[7] optimizer together with Turbomole 7.1[8] energies and gradients at the BP86[9]/def2-TZVPP[10] level of theory using the D3 dispersion correction suggested by Grimme et al.[11] and the resolution-of-identity (RI) approximation.[12] This level is denoted RI-BP86-D3/def2-TZVPP. Vibrational analysis was performed to ensure that the optimized geometry corresponds to an energy minimum. Natural charges were computed at the BP86-D3/def2-TZVPP with the help of the NBO6.0 program.[13]

The interaction ΔE_{int} between the selected fragments is analyzed with the help of the Energy Decomposition Analysis (EDA) method.[14] Within this approach, ΔE_{int} can be decomposed into the following physically meaningful terms:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$$

The term ΔE_{elstat} corresponds to the classical electrostatic interaction between the unperturbed charge distributions of the deformed reactants and is usually attractive. The Pauli repulsion ΔE_{Pauli} comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interaction ΔE_{orb} accounts for electron-pair bonding, charge transfer (interaction between occupied orbitals on one moiety with unoccupied orbitals on the other, including HOMO–LUMO interactions), and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). Finally, the ΔE_{disp} term takes into account the interactions which are due to dispersion forces. Moreover, the NOCV (Natural Orbital for Chemical Valence)[15] extension of the EDA method has been also used to further partition the ΔE_{orb} term. The EDA-NOCV approach provides pairwise energy

contributions for each pair of interacting orbitals to the total bond energy.

The program package AMS 2020.101[16] was used for the EDA-NOCV calculations at the same BP86-D3 level, in conjunction with a triple-ζ-quality basis set using uncontracted Slater-type orbitals (STOs) augmented by two sets of polarization functions with a frozen-core approximation for the core electrons.[17] Auxiliary sets of s, p, d, f, and g STOs were used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle.[18] Scalar relativistic effects were incorporated by applying the zeroth-order regular approximation (ZORA).[19] This level of theory is denoted ZORA-BP86-D3/TZ2P//RI-BP86-D3/def2-TZVPP.

Cartesian coordinates (in Å) and total energies (in a. u., ZPVE included) of all the stationary points described in the text (RI-BP86-D3/def2-TZVPP).

3: E= -4703.9690430

Ag	-1.116260000	-0.024930000	0.121808000
Fe	-3.763334000	0.047514000	-0.078575000
F	-1.824542000	-2.837548000	-1.616645000
F	-1.344789000	-2.796733000	-3.757542000
F	-0.500271000	-4.352206000	-2.478492000
F	4.001843000	-1.167383000	-3.994622000
F	3.737762000	0.644352000	-2.786839000
F	4.682685000	-1.127783000	-1.915785000
F	-1.761981000	-0.308956000	3.324196000
F	-1.282332000	-2.383147000	3.844845000
F	-0.531522000	-0.750641000	5.085620000
F	4.383503000	-2.393007000	3.050355000
F	4.780019000	-0.513710000	2.003819000
F	4.159500000	-2.281190000	0.871715000
F	-1.803101000	3.015758000	-1.832407000
F	-2.026587000	3.432836000	0.303754000
F	-1.118818000	4.932985000	-1.010838000
F	4.026440000	4.172097000	0.451404000
F	4.579128000	2.324783000	-0.581643000
F	3.994123000	2.260504000	1.525614000
O	-2.772361000	-2.461895000	1.196060000
O	-2.343820000	0.008025000	-2.691335000
O	-4.810135000	2.610166000	-1.113360000
O	-4.109776000	1.286809000	2.595091000
O	-6.206480000	-1.452672000	-0.765949000
N	0.480072000	-1.427316000	-1.142554000
N	1.703126000	-0.844727000	-1.198168000
N	0.496963000	-0.440904000	1.775970000
N	1.771009000	-0.553993000	1.322193000
N	0.342227000	1.700195000	-0.459410000
N	1.649673000	1.495805000	-0.179585000
C	0.365728000	-2.168853000	-2.254416000
C	1.513700000	-2.069477000	-3.055933000
H	1.718960000	-2.548229000	-4.004358000
C	2.341122000	-1.214084000	-2.347004000
C	-0.829145000	-3.032341000	-2.522644000
C	3.697553000	-0.715493000	-2.751238000
C	0.464841000	-1.044883000	2.974064000
C	1.719277000	-1.573151000	3.309835000
H	2.006765000	-2.110206000	4.203949000
C	2.521351000	-1.241469000	2.229864000
C	-0.781455000	-1.119731000	3.802216000
C	3.967758000	-1.597947000	2.031035000
C	0.162871000	3.029077000	-0.509829000
C	1.359737000	3.710793000	-0.256749000
H	1.534627000	4.777841000	-0.230450000
C	2.283521000	2.696144000	-0.048009000
C	-1.193960000	3.604428000	-0.767631000
C	3.729058000	2.852166000	0.330005000
C	-3.012460000	-1.454612000	0.686042000
C	-2.731489000	-0.008690000	-1.600010000
C	-4.372529000	1.626759000	-0.713683000
C	-3.949303000	0.780726000	1.575732000
C	-5.254222000	-0.862653000	-0.503357000
B	2.221471000	0.053444000	-0.039675000

H	3.410999000	0.103474000	-0.074264000

4: E= -4385.6002582

Ag	-1.652026000	-0.022699000	0.117063000
Fe	-4.287754000	0.075494000	-0.140310000
F	-2.399529000	-3.109439000	-1.067848000
F	-1.836530000	-3.336273000	-3.172190000
F	-1.181186000	-4.817510000	-1.707752000
F	-2.371858000	0.429368000	3.334162000
F	-1.848985000	-1.507719000	4.209218000
F	-1.188537000	0.334795000	5.180494000
F	-2.334970000	2.618867000	-2.468261000
F	-2.484265000	3.418498000	-0.438487000
F	-1.572468000	4.626920000	-2.026125000
O	-3.286793000	-2.125399000	1.617815000
O	-2.855181000	-0.454003000	-2.689900000
O	-5.347599000	2.353476000	-1.692453000
O	-4.682728000	1.834465000	2.214496000
O	-6.679326000	-1.611514000	-0.484038000
N	-0.101757000	-1.595071000	-0.908941000
N	1.185187000	-1.161134000	-0.924330000
N	-0.096315000	-0.150794000	1.843471000
N	1.205374000	-0.252615000	1.463571000
N	-0.202409000	1.569142000	-0.714998000
N	1.121858000	1.369531000	-0.504493000
C	-0.128848000	-2.711287000	-1.650329000
C	1.142883000	-3.017451000	-2.154999000
H	1.422454000	-3.842549000	-2.797987000
C	1.970160000	-2.002229000	-1.678872000
C	-1.386707000	-3.483736000	-1.894535000
C	-0.109017000	-0.265735000	3.180386000
C	1.185043000	-0.442946000	3.684165000
H	1.482977000	-0.582622000	4.715462000
C	2.010615000	-0.437426000	2.560387000
C	-1.379796000	-0.251934000	3.968288000
C	-0.326923000	2.806580000	-1.217213000
C	0.921981000	3.423272000	-1.348613000
H	1.135641000	4.423882000	-1.701339000
C	1.837512000	2.480833000	-0.874428000
C	-1.675177000	3.366288000	-1.537387000
C	-3.484902000	-1.226906000	0.915322000
C	-3.252499000	-0.271301000	-1.617363000
C	-4.906126000	1.478966000	-1.090837000
C	-4.503726000	1.128440000	1.324100000
C	-5.746802000	-0.948097000	-0.353383000
B	1.650844000	-0.003385000	-0.005499000
H	2.837547000	0.032780000	-0.028913000
C	3.297733000	2.609895000	-0.773288000
C	3.996207000	2.238881000	0.387841000
C	4.019917000	3.131192000	-1.861252000
C	5.384154000	2.348708000	0.445532000
C	5.407929000	3.259381000	-1.794160000
C	6.094960000	2.858146000	-0.644609000
H	3.451168000	1.864148000	1.251833000
H	3.486061000	3.414549000	-2.768774000
H	5.904916000	2.030371000	1.347984000
H	5.954692000	3.660603000	-2.647662000
H	7.180693000	2.943051000	-0.598928000
C	3.411744000	-1.827796000	-1.896154000
C	3.969740000	-0.575789000	-2.205787000

C	4.263919000	-2.941737000	-1.794620000
C	5.346259000	-0.433602000	-2.369130000
C	5.639942000	-2.801428000	-1.979167000
C	6.186522000	-1.544627000	-2.254957000
H	3.322316000	0.291775000	-2.319225000
H	3.840904000	-3.915427000	-1.545805000
H	5.757429000	0.552399000	-2.582219000
H	6.287715000	-3.674042000	-1.892475000
H	7.263221000	-1.432319000	-2.382433000
C	3.471316000	-0.585597000	2.507598000
C	4.269348000	0.133441000	3.414942000
C	4.097918000	-1.429435000	1.575148000
C	5.660132000	0.025534000	3.375389000
C	5.487421000	-1.520653000	1.524334000
C	6.273257000	-0.793475000	2.422650000
H	3.790899000	0.797511000	4.135378000
H	3.494837000	-2.016878000	0.885464000
H	6.265813000	0.592833000	4.082314000
H	5.951015000	-2.159727000	0.773697000
H	7.360149000	-0.864817000	2.381006000

5: E= -3388.2282227

Ag	-0.862677000	-0.107736000	0.200033000
Fe	-3.474665000	0.215331000	-0.087166000
O	-1.965812000	0.184806000	-2.662359000
O	-2.085363000	2.326922000	1.490650000
O	-4.817828000	-0.210154000	2.511723000
O	-4.317905000	-2.535506000	-0.791607000
O	-5.410199000	2.081149000	-1.286936000
N	0.599486000	1.570903000	-0.600506000
N	1.836087000	1.367632000	-0.050670000
N	0.530858000	-1.521321000	-0.839369000
N	1.807799000	-1.028319000	-0.890299000
N	0.532281000	-0.488527000	1.967801000
N	1.854670000	-0.597099000	1.602612000
C	0.450081000	2.895465000	-0.763389000
C	1.605674000	3.560162000	-0.308033000
H	1.792173000	4.627338000	-0.301094000
C	2.465497000	2.559681000	0.148309000
C	0.370494000	-2.342981000	-1.889678000
C	1.562394000	-2.382905000	-2.636064000
H	1.756499000	-2.957085000	-3.533858000
C	2.450819000	-1.526605000	-1.982021000
C	0.381322000	-1.157035000	3.125942000
C	1.619284000	-1.690672000	3.518009000
H	1.828232000	-2.271458000	4.410200000
C	2.533486000	-1.332951000	2.529448000
C	-2.375911000	0.182722000	-1.577862000
C	-2.372033000	1.398512000	0.848356000
C	-4.285149000	-0.043652000	1.504290000
C	-3.978759000	-1.465606000	-0.525943000
C	-4.652031000	1.353051000	-0.812842000
B	2.333676000	-0.074595000	0.218999000
H	3.531177000	-0.081441000	0.197522000
C	-0.917866000	-3.090722000	-2.080262000
H	-1.681061000	-2.547788000	-1.500993000
C	-0.814920000	-4.508778000	-1.488846000
C	-1.354329000	-3.124646000	-3.550373000
H	-1.439054000	-2.111533000	-3.963113000
H	-0.627673000	-3.680184000	-4.160695000

H	-2.326614000	-3.625931000	-3.652179000
H	-0.054210000	-5.094878000	-2.024244000
H	-1.776168000	-5.035220000	-1.572881000
H	-0.530443000	-4.469718000	-0.429292000
C	3.820174000	-1.065763000	-2.395044000
H	4.423343000	-0.933486000	-1.482606000
C	3.713241000	0.308348000	-3.088442000
C	4.523385000	-2.090099000	-3.292800000
H	4.598021000	-3.069639000	-2.802186000
H	3.980476000	-2.223368000	-4.239590000
H	5.537601000	-1.748344000	-3.539393000
H	3.134552000	0.217751000	-4.018600000
H	4.710628000	0.697551000	-3.337248000
H	3.205722000	1.039400000	-2.446094000
C	3.981503000	-1.754301000	2.470566000
H	4.125485000	-2.325688000	3.401742000
C	4.992225000	-0.594430000	2.504013000
C	4.257977000	-2.722034000	1.304176000
H	3.561318000	-3.570220000	1.323966000
H	4.144375000	-2.221443000	0.335509000
H	5.283319000	-3.113047000	1.368426000
H	4.999494000	-0.041892000	1.557158000
H	6.005869000	-0.985349000	2.670773000
H	4.759546000	0.111155000	3.312751000
C	-0.943182000	-1.326857000	3.823752000
H	-0.716557000	-1.845340000	4.769073000
C	-1.889056000	-2.233319000	3.014697000
C	-1.600878000	0.016490000	4.170401000
H	-0.942771000	0.628293000	4.801084000
H	-1.812434000	0.592426000	3.264399000
H	-2.549023000	-0.140378000	4.702856000
H	-2.138866000	-1.770829000	2.048618000
H	-2.827927000	-2.402426000	3.560159000
H	-1.423639000	-3.205426000	2.805940000
C	-0.784410000	3.451386000	-1.418441000
H	-1.599681000	2.732528000	-1.236767000
C	-0.588542000	3.543109000	-2.943066000
C	-1.198575000	4.799888000	-0.817344000
H	-1.356142000	4.718785000	0.265767000
H	-0.424866000	5.561139000	-0.993419000
H	-2.128330000	5.159447000	-1.278903000
H	0.227857000	4.238932000	-3.184127000
H	-1.503779000	3.904835000	-3.433332000
H	-0.334737000	2.560431000	-3.360758000
C	3.831628000	2.673077000	0.770518000
H	3.901124000	1.893763000	1.544752000
C	4.017770000	4.033906000	1.456489000
C	4.951133000	2.424499000	-0.257148000
H	4.865372000	1.429231000	-0.709140000
H	4.901324000	3.168051000	-1.065068000
H	5.937763000	2.500824000	0.221668000
H	4.004929000	4.851516000	0.721416000
H	4.986091000	4.069817000	1.973911000
H	3.224321000	4.224630000	2.190709000

3-Cu: E= -6197.6803769

Cu	0.996033000	-0.082768000	0.050452000
Fe	3.480240000	0.213600000	-0.111023000
F	1.840041000	3.405350000	1.212809000
F	2.054820000	3.706403000	-0.940299000

F	0.942940000	5.159758000	0.254292000
F	-3.984357000	3.988070000	-1.247672000
F	-3.902198000	1.956440000	-2.065129000
F	-4.491613000	2.277341000	0.017836000
F	1.927870000	-2.336518000	2.231096000
F	1.592659000	-1.398096000	4.183932000
F	0.717800000	-3.350127000	3.753709000
F	-4.176627000	-0.904360000	3.837605000
F	-4.586652000	-1.202360000	1.710048000
F	-4.026046000	0.781721000	2.443360000
F	2.026826000	-1.535997000	-3.397595000
F	2.099307000	-2.829474000	-1.633505000
F	1.216290000	-3.565526000	-3.500744000
F	-4.005479000	-2.852114000	-2.987744000
F	-4.342608000	-0.791927000	-2.330593000
F	-4.158228000	-2.393281000	-0.851202000
O	2.176994000	0.874179000	2.479639000
O	1.885697000	1.218747000	-2.401706000
O	4.900696000	-1.168795000	-2.302732000
O	4.817307000	-1.823939000	1.571060000
O	5.173351000	2.613536000	0.163794000
N	-0.237575000	1.766717000	0.016956000
N	-1.540547000	1.488551000	-0.245366000
N	-0.310081000	-0.900544000	1.479365000
N	-1.605250000	-0.525006000	1.302895000
N	-0.192207000	-1.034503000	-1.357169000
N	-1.531791000	-0.889218000	-1.187211000
C	-0.101358000	3.098740000	-0.124626000
C	-1.315126000	3.693090000	-0.494096000
H	-1.518727000	4.739546000	-0.675588000
C	-2.206610000	2.635524000	-0.561367000
C	1.189452000	3.834061000	0.102639000
C	-3.653992000	2.703423000	-0.958227000
C	-0.243659000	-1.502505000	2.678364000
C	-1.494526000	-1.498932000	3.309648000
H	-1.757971000	-1.906500000	4.276492000
C	-2.331214000	-0.867075000	2.404223000
C	1.008838000	-2.138458000	3.208360000
C	-3.788335000	-0.547722000	2.587038000
C	-0.021735000	-1.996155000	-2.280794000
C	-1.255368000	-2.483562000	-2.726870000
H	-1.442879000	-3.256671000	-3.459260000
C	-2.190434000	-1.758864000	-2.003981000
C	1.335766000	-2.476876000	-2.702501000
C	-3.682535000	-1.936027000	-2.039083000
C	2.444209000	0.592664000	1.382492000
C	2.322491000	0.795394000	-1.411652000
C	4.316059000	-0.638513000	-1.465516000
C	4.265546000	-1.037635000	0.937249000
C	4.511476000	1.678456000	0.055172000
B	-2.088192000	0.046321000	-0.069147000
H	-3.277275000	0.055018000	-0.109833000

3-Ru: E= -3535.0776302

Ag	-0.964971000	0.026440000	0.185423000
Ru	-3.678231000	0.036468000	-0.122848000
F	-1.700217000	-2.543783000	-2.073311000
F	-1.039608000	-2.438221000	-4.163329000
F	-0.308858000	-4.034051000	-2.861820000
F	4.141825000	-0.560424000	-4.110628000

F	3.849242000	1.062361000	-2.664611000
F	4.842252000	-0.789717000	-2.050707000
F	-1.566344000	-0.616899000	3.299417000
F	-1.120491000	-2.728687000	3.684880000
F	-0.316191000	-1.189277000	5.007901000
F	4.492900000	-2.912567000	2.642524000
F	4.951781000	-0.905254000	1.901792000
F	4.246682000	-2.443590000	0.513761000
F	-1.628047000	3.180690000	-1.442986000
F	-1.811781000	3.498887000	0.716080000
F	-0.879799000	5.034917000	-0.536361000
F	4.206347000	4.042011000	1.020286000
F	4.762605000	2.363626000	-0.266290000
F	4.159233000	1.993788000	1.804174000
O	-2.289917000	-2.592048000	0.841868000
O	-2.400710000	0.257290000	-2.943686000
O	-4.602471000	2.970694000	-0.526140000
O	-4.368201000	0.485993000	2.865122000
O	-6.229919000	-1.498107000	-0.940077000
N	0.650559000	-1.290859000	-1.298704000
N	1.865792000	-0.690067000	-1.278090000
N	0.685026000	-0.616397000	1.757116000
N	1.940610000	-0.730121000	1.262900000
N	0.511285000	1.742796000	-0.229366000
N	1.815040000	1.492341000	0.037111000
C	0.536978000	-1.856194000	-2.510872000
C	1.675058000	-1.620236000	-3.298632000
H	1.875013000	-1.945700000	-4.310979000
C	2.498122000	-0.870619000	-2.475038000
C	-0.629961000	-2.711769000	-2.895960000
C	3.839314000	-0.291016000	-2.814526000
C	0.639294000	-1.374521000	2.862668000
C	1.870509000	-2.005652000	3.095229000
H	2.145937000	-2.671917000	3.902037000
C	2.670737000	-1.570124000	2.050832000
C	-0.594080000	-1.475498000	3.707781000
C	4.096423000	-1.949282000	1.771433000
C	0.352555000	3.073589000	-0.147525000
C	1.555643000	3.707332000	0.185711000
H	1.744613000	4.763314000	0.323553000
C	2.462503000	2.662586000	0.298217000
C	-0.990741000	3.697682000	-0.356874000
C	3.906210000	2.754748000	0.705930000
C	-2.573115000	-1.537257000	0.449425000
C	-2.836723000	0.129389000	-1.888053000
C	-4.218624000	1.897690000	-0.387738000
C	-4.099695000	0.296779000	1.766075000
C	-5.287277000	-0.920124000	-0.626272000
B	2.386594000	0.042803000	-0.010295000
H	3.576274000	0.099296000	-0.043987000

3-Os: E= -3530.8948548

Ag	-0.727526000	0.016676000	0.213879000
Os	-3.458795000	0.031354000	-0.097774000
F	-1.445997000	-2.503872000	-2.145154000
F	-0.797155000	-2.336810000	-4.235081000
F	-0.026729000	-3.945073000	-2.972596000
F	4.320763000	-0.301666000	-4.172346000
F	4.033264000	1.230054000	-2.628979000
F	5.063636000	-0.639389000	-2.142455000

F	-1.294810000	-0.822892000	3.276426000
F	-0.812371000	-2.943241000	3.556326000
F	-0.023578000	-1.456215000	4.946876000
F	4.781004000	-3.018911000	2.451089000
F	5.220337000	-0.973707000	1.808872000
F	4.507278000	-2.443581000	0.352194000
F	-1.392681000	3.244483000	-1.295012000
F	-1.589519000	3.441382000	0.877556000
F	-0.662675000	5.050863000	-0.283134000
F	4.436769000	4.006866000	1.209016000
F	4.994874000	2.400957000	-0.166414000
F	4.402257000	1.919893000	1.884137000
O	-2.048840000	-2.660385000	0.739336000
O	-2.272190000	0.245105000	-2.982069000
O	-4.353898000	2.998857000	-0.463972000
O	-3.970051000	0.502466000	2.945560000
O	-6.118314000	-1.393886000	-0.783000000
N	0.894908000	-1.244090000	-1.341965000
N	2.097335000	-0.618455000	-1.313840000
N	0.950537000	-0.702687000	1.728175000
N	2.202509000	-0.779838000	1.218302000
N	0.748723000	1.755957000	-0.147589000
N	2.053754000	1.499838000	0.103716000
C	0.774088000	-1.757711000	-2.576357000
C	1.893412000	-1.461720000	-3.370813000
H	2.083570000	-1.737514000	-4.399593000
C	2.713708000	-0.731724000	-2.527134000
C	-0.375546000	-2.629245000	-2.976041000
C	4.039039000	-0.112321000	-2.857429000
C	0.919410000	-1.523900000	2.788359000
C	2.156380000	-2.159235000	2.974218000
H	2.442529000	-2.869415000	3.738701000
C	2.944487000	-1.659461000	1.949708000
C	-0.305426000	-1.684181000	3.636059000
C	4.368926000	-2.014625000	1.635132000
C	0.583002000	3.079984000	0.001598000
C	1.783549000	3.703021000	0.363999000
H	1.967477000	4.751796000	0.553781000
C	2.696178000	2.658794000	0.421798000
C	-0.763968000	3.704818000	-0.178742000
C	4.140713000	2.736536000	0.828444000
C	-2.372625000	-1.598905000	0.399702000
C	-2.689165000	0.115738000	-1.918658000
C	-3.989945000	1.915790000	-0.341510000
C	-3.773272000	0.300905000	1.832541000
C	-5.136635000	-0.851661000	-0.521463000
B	2.630251000	0.057509000	-0.019415000
H	3.819369000	0.120915000	-0.064152000

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