Supplementary Information for

Group 3 Metal Stilbene Complexes: Synthesis, Reactivity, and Electronic Structure Studies

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Contents:

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1. Experimental details

General considerations: All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or an MBraun inert-gas glove box unless otherwise specified. Solvents, toluene, hexanes, diethyl ether (Et_2O), and tetrahydrofuran (THF) were purified using a two-column solid-state purification system by the method of Grubbs[1] and transferred to the glove box without exposure to air. *n*-Pentane was distilled over calcium hydride under a dinitrogen atmosphere. Methanol was distilled over calcium oxide under a dinitrogen atmosphere. All solvents were stored on activated molecular sieves and/or sodium for at least a day prior to use. NMR solvents, benzene-d_6 (C_6D_6), THF-d_8 (C_4D_8O) and toluene-d_8 (C_7D_8), were obtained from Cambridge Isotope Laboratories, degassed or brought directly into a glove box in a sealed ampoule, and stored over activated molecular sieves for one week prior to use. (*E*)-stilbene, biphenyl, naphthalene, and anthracene were bought from Sigma-Aldrich and used as received. $(NN^{TBS})YI(THF)_2$,[2] $(NN^{TBS})LaI(THF)$,[2] $[(NN^{TBS})Y(THF)]_2(\mu\text{-}C_{10}H_8)$ (**Y_2-naph**),[3] and $[(NN^{TBS})Y]_2(\mu\text{-}C_6H_5Ph)[K(OEt_2)]_2$ (**Y_2K_2-biph**)[2] were prepared following literature protocols. Nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV300, Bruker DRX500, Bruker AV500 (work supported by the NSF grant CHE-1048804), or Bruker AV600 spectrometers at 25 °C in C_6D_6 or C_7D_8 unless otherwise specified. Chemical shifts are reported with respect to internal solvent (C_6D_6 at 7.16 ppm or C_7D_8 at 2.09 ppm). CHN analyses were performed in house on a CE-440 Elemental Analyzer manufactured by Exeter Analytical, INC.

Synthesis of Y_2-stilbene: $(NN^{TBS})YI(THF)_2$ (0.6000 g, 0.748 mmol) and 0.5 equiv (*E*)-stilbene (0.0680 g, 0.377 mmol) were weighed in a scintillation vial. THF (10 mL) was added to make a yellow solution which was cooled down to -78 °C with a dry ice / isoproponal bath. 1.25 equiv KC_8 (0.1280 g, 0.947 mmol) was added to the solution. The reaction mixture was allowed to warm up to 0 °C with a ice bath and stirred for 1 h. The resulting red solution was filtered through Celite and dried under reduced pressure. The remaining solid was washed with ca. 50 mL of Et_2O and an orange solid was collected on a medium frit after filtration. Yield: 0.4107 g, 79.2%. **Y_2-stilbene** obtained by this method contains ca. 15% (wt%) potassium iodide as determined by elemental analysis of the sample. Due to low solubility of **Y_2-stilbene** in saturated hydrocarbons and aromatic solvents and an equilibrium in THF (**Y_2-stilbene** + KI ↔ **Y-stilbene-K** + YI), it is difficult to remove the residue KI. In most cases, the residue KI did not interfere the succeeding reactivity study and could be removed upon the work-up. Therefore, **Y_2-stilbene** was used in this form. Analytical pure **Y_2-stilbene** could be obtained by the following protocol: extraction with a large amount of toluene (ca. 1 mg/mL solubility for **Y_2-stilbene** in toluene at 25 °C), removal of toluene under reduced pressure, and wash of the remaining solid with Et_2O. The resulting vermeil solid was collected on a medium frit. Single crystals of **Y_2-stilbene** were grown from a concentrated toluene solution layered with hexanes stored in a -35 °C freezer. The solubility of **Y_2-stilbene** in aromatic solvents increased upon heating so NMR spectroscopic data was collected at 50 °C. ^{1}H NMR (500 MHz, C_6D_6, 50 °C) δ, ppm: broad peak around 7.00 overlapping with residual peak of C_6D_6 (*ortho*- and *meta*-C*H* of (*E*)-stilbene), 6.37 (t, 2H, *para*-C*H* of (*E*)-stilbene), 4.04 (s, 2H, PhC*H*C*H*Ph) 3.96, 3.93, 3.27, and 3.26 (br s, 4H each, C*H* of Cp rings), 3.58 (br s, 8H, CH_2O of THF), 1.37 (br s, 8H, CH_2CH_2O of THF), 1.08 (s, 36H, $(CH_3)_3C$), and 0.31 (br s, 24H, $SiCH_3$). ^{13}C NMR (126 MHz, C_6D_6, 50 °C) δ, ppm: 139.9 (*ipso-C* of (*E*)-stilbene), 115.3 (*para-C* of (*E*)-stilbene), 107.0 (*C*N of Cp rings), 70.1, 67.7 and 66.8 (*C*H of Cp rings), 66.8 (CH_2O of THF), 58.9 (Ph*C*H*C*HPh), 28.0 ($(CH_3)_3C$), 25.4 (CH_2CH_2O of THF), 20.6 ($(CH_3)_3C$), and -0.9 and -1.1 ($SiCH_3$). Peaks of *ortho*- and *meta-C* of (*E*)-stilbene were missing likely due to their intrinsic broadness or were masked by deuterated solvent peaks. Anal. (%): Calcd. for $C_{66}H_{104}N_4O_2Fe_2Y_2Si_4$, M_w = 1387.430: C, 57.14; H, 7.56; N, 4.04. Found: C, 57.03; H, 7.54; N, 3.74.

Synthesis of La_2-stilbene: (NN^{TBS})LaI(THF) (0.2000 g, 0.256 mmol) and 0.5 equiv (*E*)-stilbene (0.0261 g, 0.145 mmol) were weighed in a scintillation vial. THF (6 mL) was added to make a yellow solution which was cooled down to -78 °C with a dry ice / isoproponal bath. 1.25 equiv KC_8 (0.0447 g, 0.331 mmol) was added to the solution. The reaction mixture was allowed to warm up to 0 °C with a ice bath and stirred for 1 h. The resulting brown solution was filtered through Celite and dried under reduced pressure. The solubility of **La_2-stilbene** in aromatic solvents is higher than that of **Y_2-stilbene**. The residual KI could be removed by extraction of **La_2-stilbene** with ca. 30 mL of toluene. Toluene was then removed under reduced pressure. The remaining brown solid was washed with ca. 20 mL of Et_2O and a brown solid was collected on a medium frit after filtration. Yield: 0.0927 g, 48.6%. Single crystals of **La_2-stilbene** were grown from a toluene solution layered with hexanes stored in a -35 °C freezer. Due to the lability of coordinating solvent molecules, **La_2-stilbene** contained both Et_2O and THF with a total amount of one solvent molecule per lanthanum. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.28 and 6.90 (t, 2H each, *meta*-C*H* of (*E*)-stilbene), 7.13 and 6.31 (m, 2H each, *ortho*-C*H* of (*E*)-stilbene), 6.25 (t, 2H, *para*-C*H* of (*E*)-stilbene), 3.77 (s, 2H, PhC*H*C*H*Ph), 4.02 (br, 8H, C*H* of Cp rings), 3.27 and 3.14 (br s, 4H each, C*H* of Cp rings), 3.49 (br s, CH_2O of THF), 3.17 (br s, CH_2O of Et_2O), 1.33 (br s, CH_2CH_2O of THF), 1.11 (s, 36H, (CH_3)$_3$C), 0.98 (t, CH_3CH_2O of Et_2O), and 0.32 (br s, 24H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 50 °C) δ, ppm: 140.6 (*ipso*-*C* of (*E*)-stilbene), 134.1, 130.8, 123.0, 107.1 (*ortho*- and *meta*-*C* of (*E*)-stilbene), 113.3 (*para*-*C* of (*E*)-stilbene), 106.6 (*C*N of Cp rings), 70.9, 67.0 and 66.2 (*C*H of Cp rings), 69.7 (*C*H_2O of THF), 66.2 (*C*H_2O of Et_2O), 65.2 (Ph*C*H*C*HPh), 27.7 ((*C*H_3)$_3$C), 25.3 (*C*H_2CH_2O of THF), 20.6 ((CH_3)$_3$*C*), 14.6 (*C*H_3CH_2O of Et_2O), and -1.7 and -2.0 (Si*C*H_3). Anal. (%): Calcd. for $C_{66}H_{108}N_4O_2Fe_2La_2Si_4$, M_w = 1491.462: C, 53.15; H, 7.30; N, 3.76. Found: C, 52.22; H, 6.94; N, 3.72.

Synthesis of Y-stilbene-K: (NN^{TBS})YI(THF)$_2$ (0.3000 g, 0.374 mmol) and 0.5 equiv (*E*)-stilbene (0.0342 g, 0.190 mmol) were weighed in a scintillation vial. THF (10 mL) was added to make a yellow solution which was cooled down to -78 °C with a dry ice / isoproponal bath. 2.5 equiv KC_8 (0.1350 g, 0.999 mmol) was added to the solution. The reaction mixture was allowed to warm up to 25 °C and stirred for 15 min. The resulting red solution was filtered through Celite and dried under reduced pressure. The remaining solid was extracted with Et_2O. All volatiles were removed under reduced pressure to yield a dark green solid. The solid was washed with hexanes and collected on a medium frit to yield a brown solid with a formula of [(NN^{TBS})Y(THF)][K(THF)](μ-stilbene) as determined by ^{1}H NMR spectroscopy. Yield: 0.1650 g, 53.5%. Attempts to grow single crystals of **Y-stilbene-K** were not successful due to loss of solvent upon crystal mounting process. 1 equiv 18-crown-6 was added to a THF solution of **Y-stilbene-K** to afford the crown ether version **Y-stilbene-K-crown** to increase crystallinity. Single crystals of **Y-stilbene-K-crown** were grown from a concentrated hexanes solution with a formula of [(NN^{TBS})Y(THF)][K(18-crown-6)](μ-stilbene). ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.00, 6.82, 6.49, 6.08, and 5.50 (br s, 2H each, C*H* of phenyl rings of (*E*)-stilbene), 3.74 (br s, overlapped by THF peaks, 2H, PhC*H*C*H*Ph), 4.13, 3.99, 3.41, and 3.26 (br s, 2H each, C*H* of Cp rings), 3.74 (br s, 4H, CH_2O of THF), 1.40 (br s, 4H, CH_2CH_2O of THF), 1.20 (s, 36H, (CH_3)$_3$C), and 0.54 and 0.46 (br s, 12H total, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 50 °C) δ, ppm: 132.6, 122.9, 107.6, 105.7, 71.0, 67.0, 65.9, 28.3 ((*C*H_3)$_3$C), 25.4 (*C*H_2CH_2O of THF), 20.9 ((CH_3)$_3$*C*), and -0.6 and -0.9 (Si*C*H_3). Anal. (%): Calcd. for $C_{40}H_{58}N_2OFeKYSi_2$, M_w = 822.938: C, 58.38; H, 7.10; N, 3.40. Found: C, 58.54; H, 7.08; N, 3.38.

Synthesis of Y_2-anth: (NN^{TBS})YI(THF)$_2$ (0.2030 g, 0.253 mmol) and 0.5 equiv anthracene (0.0230 g, 0.129 mmol) were weighed in a scintillation vial. THF (6 mL) was added to make a yellow solution,

which was cooled down to -78 °C with a dry ice / isoproponal bath. 1.25 equiv KC_8 (0.0477 g, 0.353 mmol) was added to the solution. The reaction mixture was allowed to warm up to 0 °C with an ice bath and stirred for 1 h. The resulting red solution was filtered through Celite and dried under reduced pressure. The remaining solid was extracted with ca. 50 mL toluene until the filtration was colorless. Toluene was removed under reduced pressure to yield a violet solid. The solid was washed with ca. 30 mL of Et_2O and was collected on a medium frit after filtration. Yield: 0.1091 g, 62.3%. Single crystals of **Y_2-anth** were grown from a Et_2O solution in a -35 °C freezer. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 5.94 and 5.69 (t, 4H each, C*H*-C*H* of anthracene), 3.92 (s, 2H, C*H*-C of anthracene), 4.22, 3.89, 3.85, and 3.76 (br s, 4H each, C*H* of Cp rings), 3.94 (br s, 8H, CH_2O of THF), 1.44 (br s, 8H, CH_2CH_2O of THF), 1.04 (s, 36H, (CH_3)$_3$C), and 0.22 and 0.17 (br s, 12H each, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 50 °C) δ, ppm: 143.7, 121.3, 114.0, and 82.4 (*C* and *C*H of anthracene), 108.3 (*C*N of Cp rings), 71.4, 69.3 and 65.6 (*C*H of Cp rings), 68.6 (*C*H_2O of THF), 27.9 ((*C*H_3)$_3$C), 25.7 (*C*H_2CH_2O of THF), 20.6 ((CH$_3$)$_3$*C*), and -1.1 and -2.8 (Si*C*H_3). Anal. (%): Calcd. for $C_{66}H_{102}N_4O_2Fe_2Y_2Si_4$, M_w = 1385.414: C, 57.22; H, 7.42; N, 4.04. Found: C, 56.64; H, 7.21; N, 3.97.

Reaction of Y_2-stilbene and KC_8: Y_2-stilbene (0.0335 g, 0.024 mmol) was dissolved in THF (3 mL) and cooled down to -78 °C with a dry ice / isoproponal bath. 2.5 equiv KC_8 (0.0107 g, 0.079 mmol) was added and the mixture was allowed to warm up to ambient temperature and stirred for 10 min. The color of the solution immediately changed from red to dark greenish-brown upon addition of KC_8. The volatiles were removed under reduced pressure. The crude product was identified as **Y-stilbene-K** by ^{1}H NMR spectroscopy.

Reaction of Y_2K_2-biph and (*E*)-stilbene: Y_2K_2-biph (0.0250 g, 0.017 mmol) was dissolved in cold THF (3 mL) and cooled down to -78 °C with a dry ice / isoproponal bath. (*E*)-stilbene (0.0062 g, 0.034 mmol) was dissolved in THF (1 mL) and added dropwise to **Y_2K_2-biph** solution. The mixture was allowed to stir at 0 °C for 30 min. The volatiles were removed under reduced vacuum. The crude product was identified as **Y-stilbene-K** by ^{1}H NMR spectroscopy and biphenyl was identified as a byproduct.

Reaction of Y_2-naph and (*E*)-stilbene: Y_2-naph (0.0065 g, 0.005 mmol) and excess (*E*)-stilbene (0.0026 g, 0.014 mmol) were dispersed in ca. 0.5 mL C_6D_6 in a J-Young tube. The reaction was monitored by routine ^{1}H NMR spectroscopy. The formation of **Y_2-stilbene** and naphthalene could be observed after 5 h at 25 °C albeit the conversion was slow. Heating the J-Young tube in a 50 °C bath for additional 30 h led to the complete conversion of **Y_2-naph** to **Y_2-stilbene**.

Reaction of Y_2-stilbene and anthracene: Y_2-stilbene (0.0079 g, 0.006 mmol) and excess anthracene (0.0024 g, 0.013 mmol) were dispersed in ca. 0.5 mL C_6D_6 in a J-Young tube. The reaction was monitored by routine ^{1}H NMR spectroscopy. The formation of **Y_2-anth** and (*E*)-stilbene could be observed after 40 min at 25 °C albeit the conversion was slow. Heating the J-Young tube in a 70 °C bath for additional 70 min led to the complete conversion of **Y_2-stilbene** to **Y_2-anth**.

Thermodecomposition of Y_2-stilbene: Y_2-stilbene (0.0125 g, 0.009 mmol) was dispersed in ca. 0.5 mL C_6D_6 in a J-Young tube. After 24 h at 25 °C, no decomposition was observed. The J-Young tube was then left in a 50 °C bath. After 18 h at 50 °C, no decomposition was observed. Decomposition was observed after prolong heating at 70 °C. After 77 h at 70 °C, all **Y_2-stilbene** was transformed. Bibenzyl

was identified as a decomposition product but we were not able to identify the yttrium decomposition products.

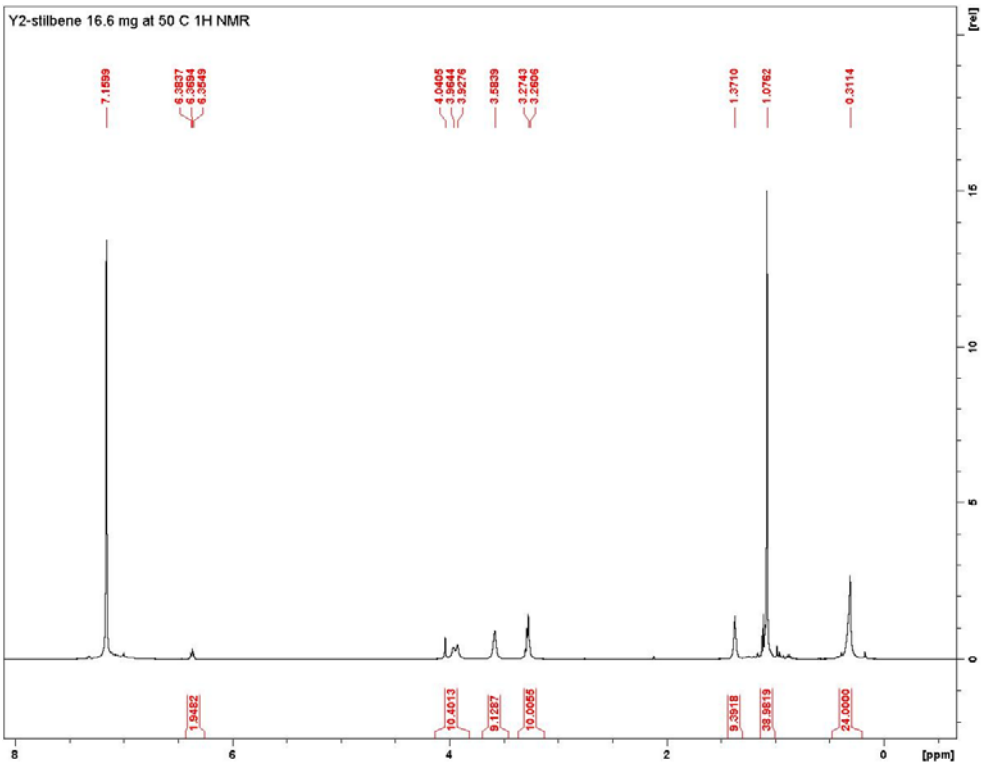
Reaction of Y_2-stilbene and phenylacetylene: Y_2-stilbene (0.1600 g, 0.115 mmol) was dispersed in toluene (6 mL) and was cooled down to -78 °C with a dry ice / isoproponal bath. 2 equiv phenylacetylene (0.0279 g, 0.273 mmol) was added as a toluene solution (1 mL) dropwise. The color of solution gradually changed from orange to yellow. The reaction mixture was filtered through Celite and volatiles were removed under reduced pressure to yield a yellow solid. A single yttrium product was identified in the crude reaction mixture with concomitant formation of $C_{14}H_{14}$ isomers (the majority was bibenzyl) by ^{1}H NMR spectroscopy. Single crystals of the product were grown from a concentrated toluene solution layered with *n*-pentane with the formula of $[(NN^{TBS})Y(THF)][(NN^{TBS})Y](\mu\text{-}CCPh)_2$. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.73 (d, 2H, *ortho*-C*H* of phenyl ring), 7.03 (t, 2H, *meta*-C*H* of phenyl ring), 6.98 (t, 1H, *para*-C*H* of phenyl ring), 3.93 (br s, 2H, C*H* of Cp rings), 3.78 (br s, 6H, C*H* of Cp rings), 1.15 (s, 18H, $(CH_3)_3C$), and 0.64 (s, 12H, $SiCH_3$). ^{13}C NMR (126 MHz, C_6D_6, 50 °C) δ, ppm: 139.0 (t, *C*CPh), 132.8, 129.7, 128.7, and 123.3 (*C* and *C*H of phenyl ring), 106.0 (*C*N of Cp rings), 72.0 (C*C*Ph), 67.2 and 66.7 (*C*H of Cp rings), 28.1 ($(CH_3)_3C$), 20.5 ($(CH_3)_3C$), and -0.6 ($SiCH_3$). Anal. (%): Calcd. for $C_{64}H_{94}N_4OFe_2Y_2Si_4$, M_w = 1337.329, with two hexanes molecule (2*C_6H_{14}, M_w = 2*86.178): C, 60.47; H, 8.15; N, 3.71. Found: C, 60.27; H, 7.84; N, 4.02.

Note: The ^{1}H NMR spectra of both an NMR scale reaction and the crude product of a larger scale reaction showed a singlet at 2.74 ppm (in C_6D_6), which is the characteristic peak for the benzylic proton of bibenzyl. In both spectra, some minor peaks in the benzylic range (2.9 ppm) and in the olefinic range (6.3 ppm) were also present and were attributed to other $C_{14}H_{14}$ isomers (likely, some protonation took place at the phenyl ring and caused dearomatization of the phenyl ring). We were unable to determine the identity of those minor by-products. A similar phenomenon was observed when reacting **Sc_2-naph** with phenylacetylene: mixtures of $C_{10}H_{10}$ isomers were present.

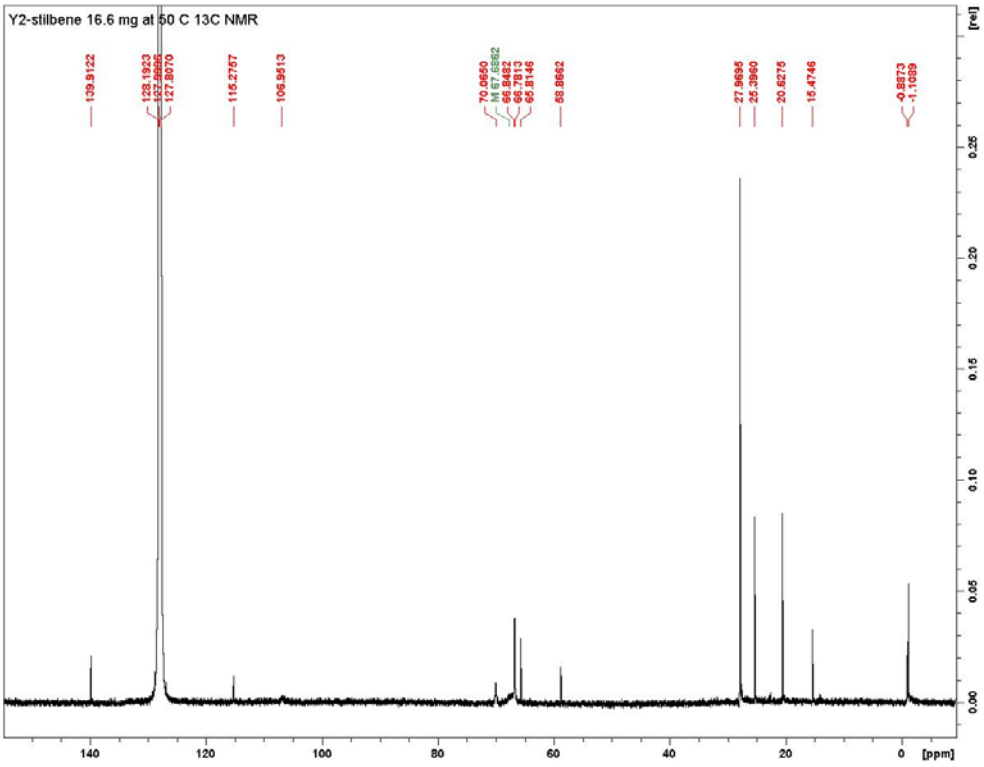
Reaction of Y_2-stilbene and 2,2′-bipyridine: Y_2-stilbene (0.1550 g, 0.112 mmol) was dispersed in toluene (6 mL) and 2 equiv 2,2′-bipyridine (bipy, 0.0350 g, 0.224 mmol) was added as a toluene solution (1 mL) dropwise. The color of the solution changed immediately from orange to dark. A single yttrium product was identified in the crude reaction mixture with concomitant formation of (*E*)-stilbene by ^{1}H NMR spectroscopy. The reaction mixture was filtered through Celite and volatiles were removed under reduced pressure to yield a dark solid. The solid was extracted with hexanes. Dark green crystals were grown after storing the hexanes solution in a -35 °C freezer for 1 d. Yield: 0.0926 g, 60.3%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 4.63, 4.01, 3.79, 3.37, 3.30, 2.89, 1.26, 1.23, and 0.89; all peaks were broad due to the paramagnetism caused by the bipy radical anion and could not be assigned. However, the formation of $(NN^{TBS})Y(bipy)$ was confirmed by comparison to the analogous $(NN^{TBS})Sc(bipy)$ complex.[4] Anal. (%): Calcd. for $C_{36}H_{54}N_4OFeYSi_2$, M_w = 759.778, with one hexanes molecule (C_6H_{14}, M_w = 86.178): C, 59.63; H, 8.10; N, 6.62. Found: C, 59.42; H, 7.78; N, 7.09.

2. NMR spectra

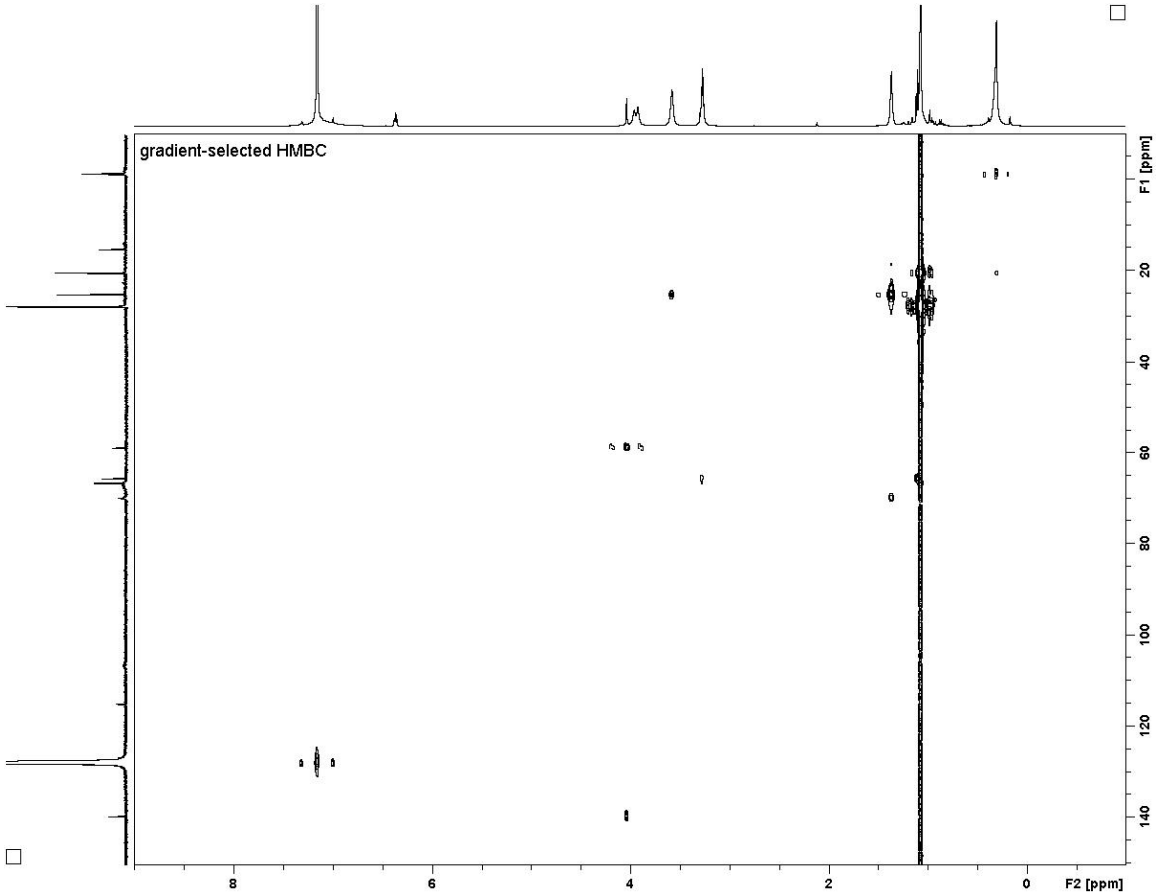
^{1}H NMR spectrum of **Y_2-stilbene** (500 MHz, C_6D_6, 50 °C)



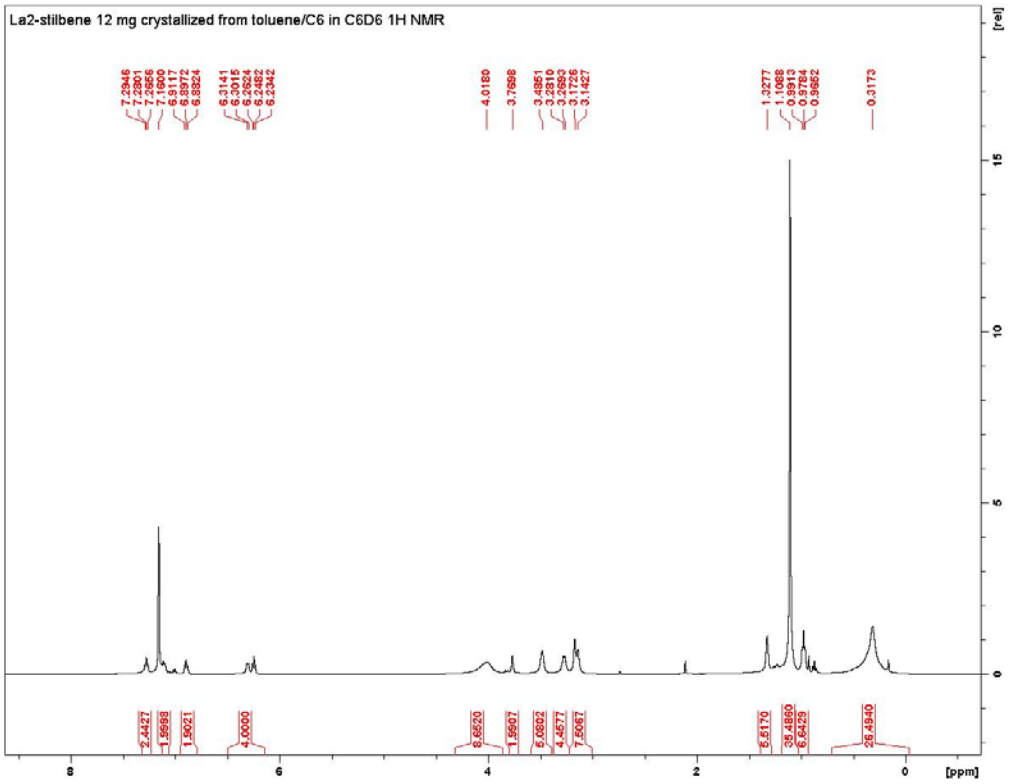
^{13}C NMR spectrum of **Y_2-stilbene** (126 MHz, C_6D_6, 50 °C)



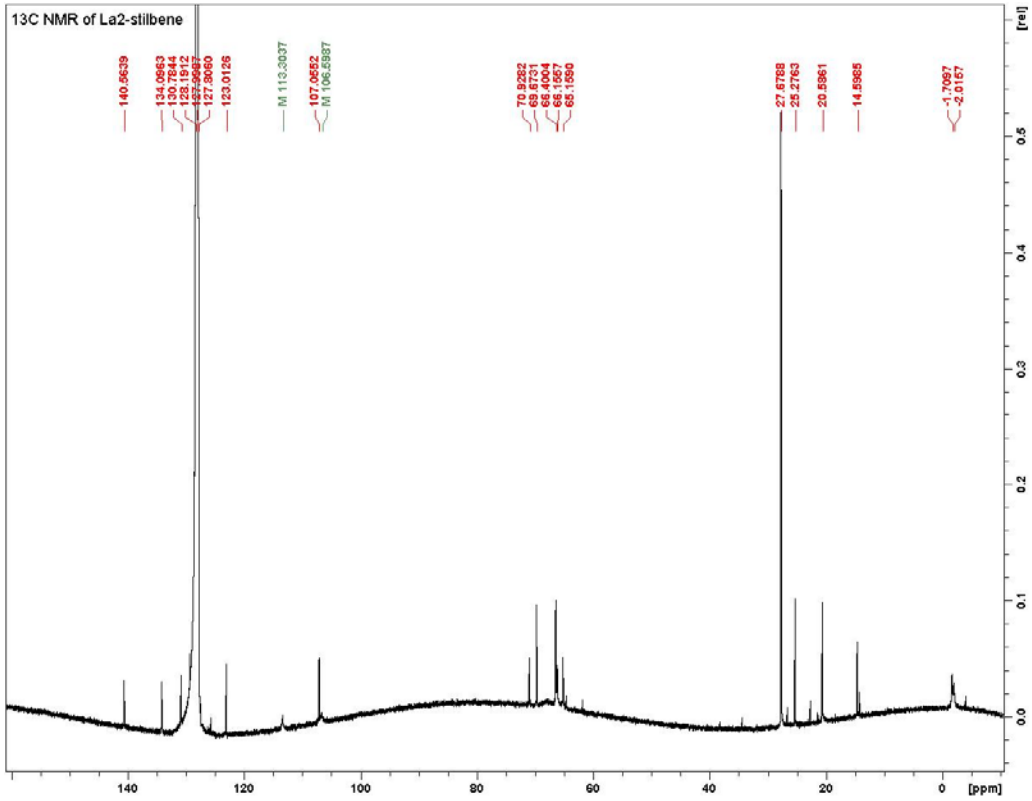
HMBC NMR spectrum of **Y_2-stilbene** (500 MHz, C_6D_6, 50 °C)



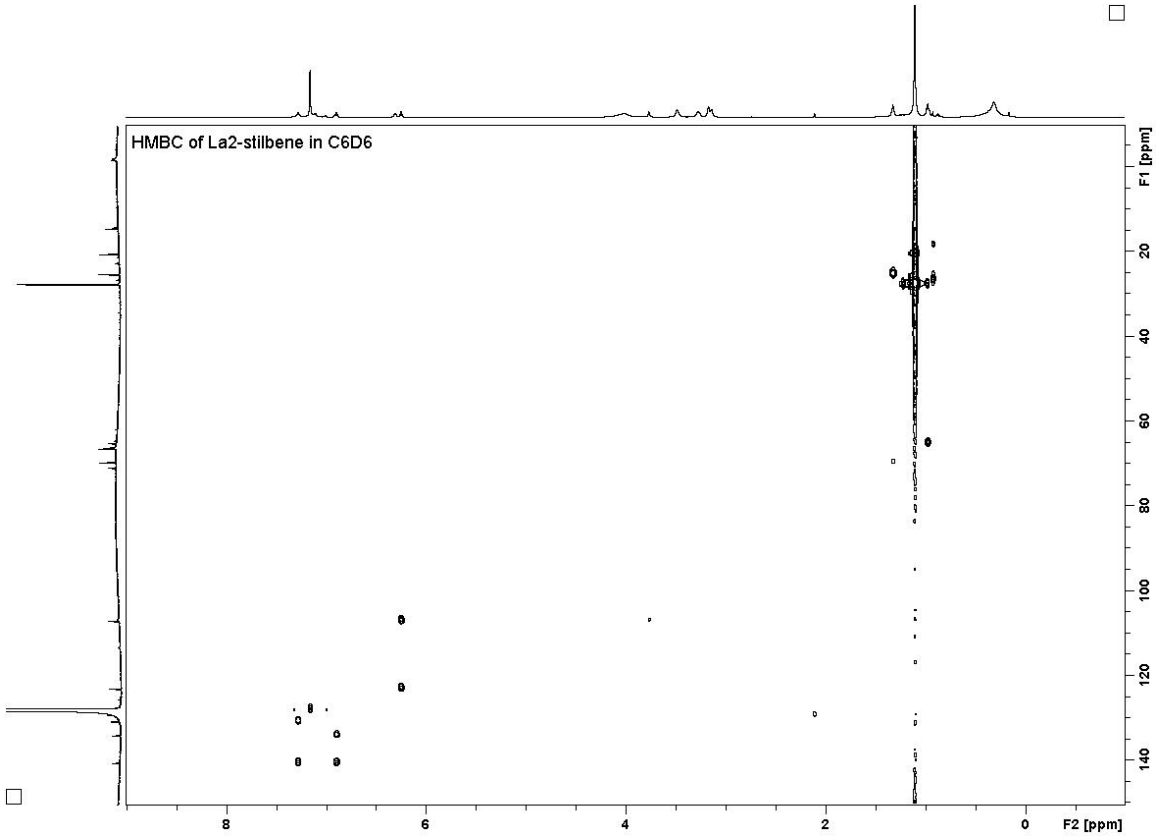
^{1}H NMR spectrum of **La$_2$-stilbene** (500 MHz, C_6D_6, 25 °C)



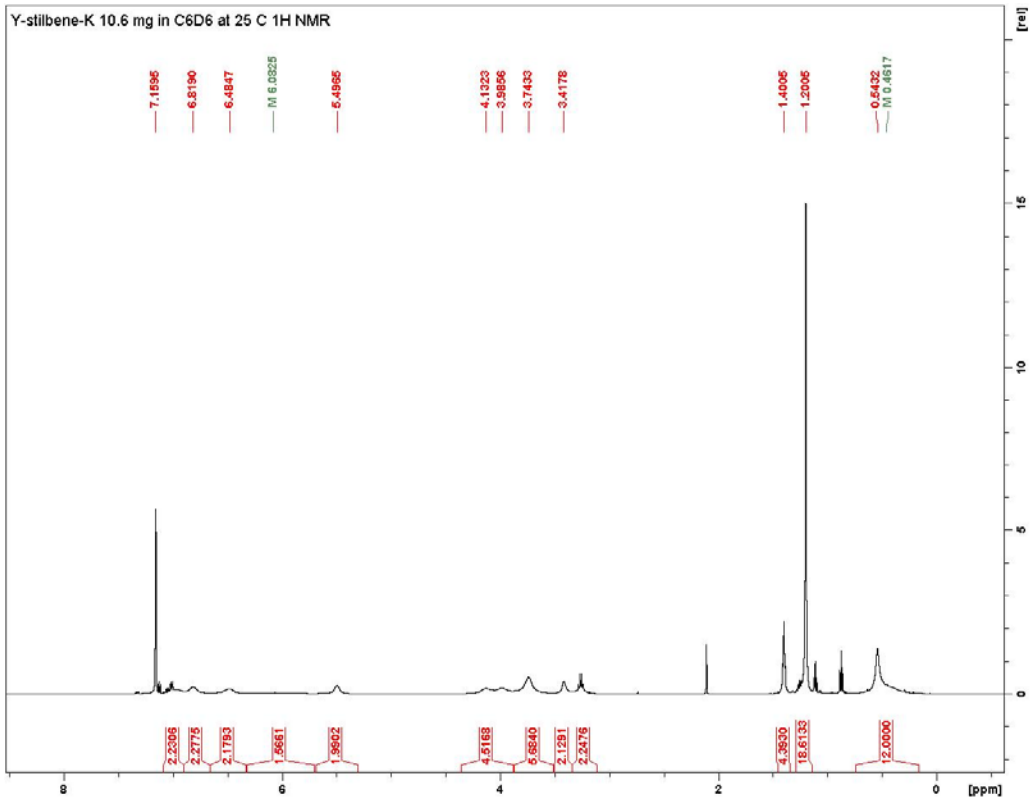
^{13}C NMR spectrum of **La$_2$-stilbene** (126 MHz, C_6D_6, 25 °C)



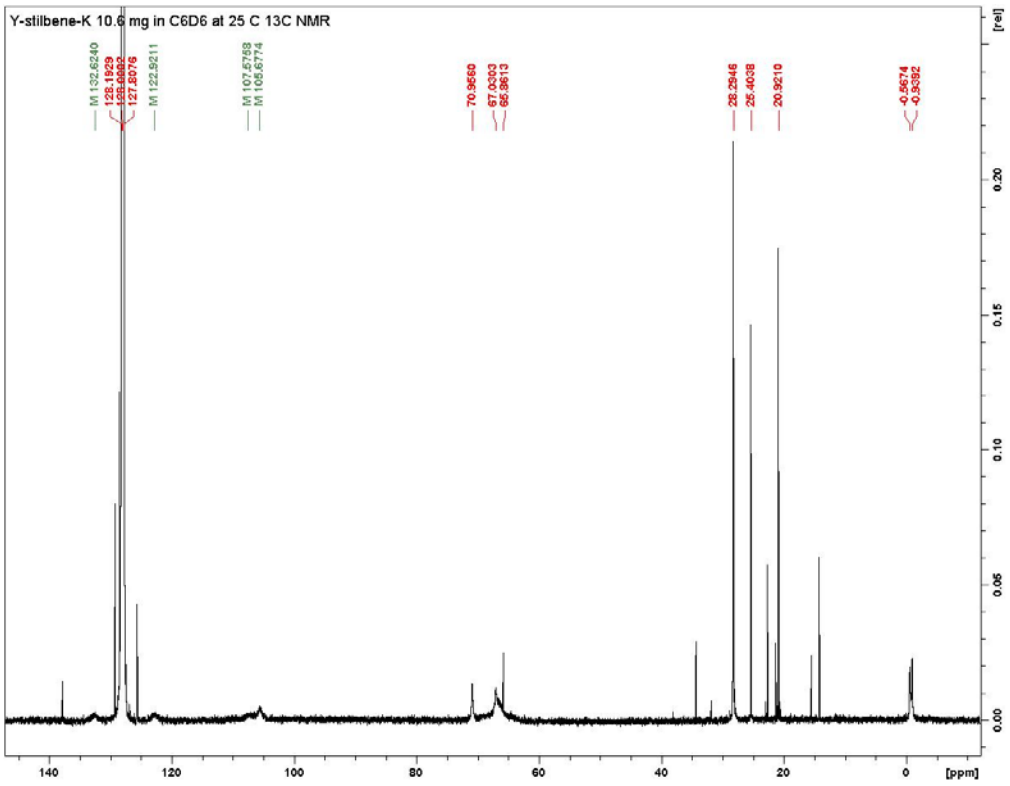
HMBC NMR spectrum of **La_2-stilbene** (500 MHz, C_6D_6, 25 °C)



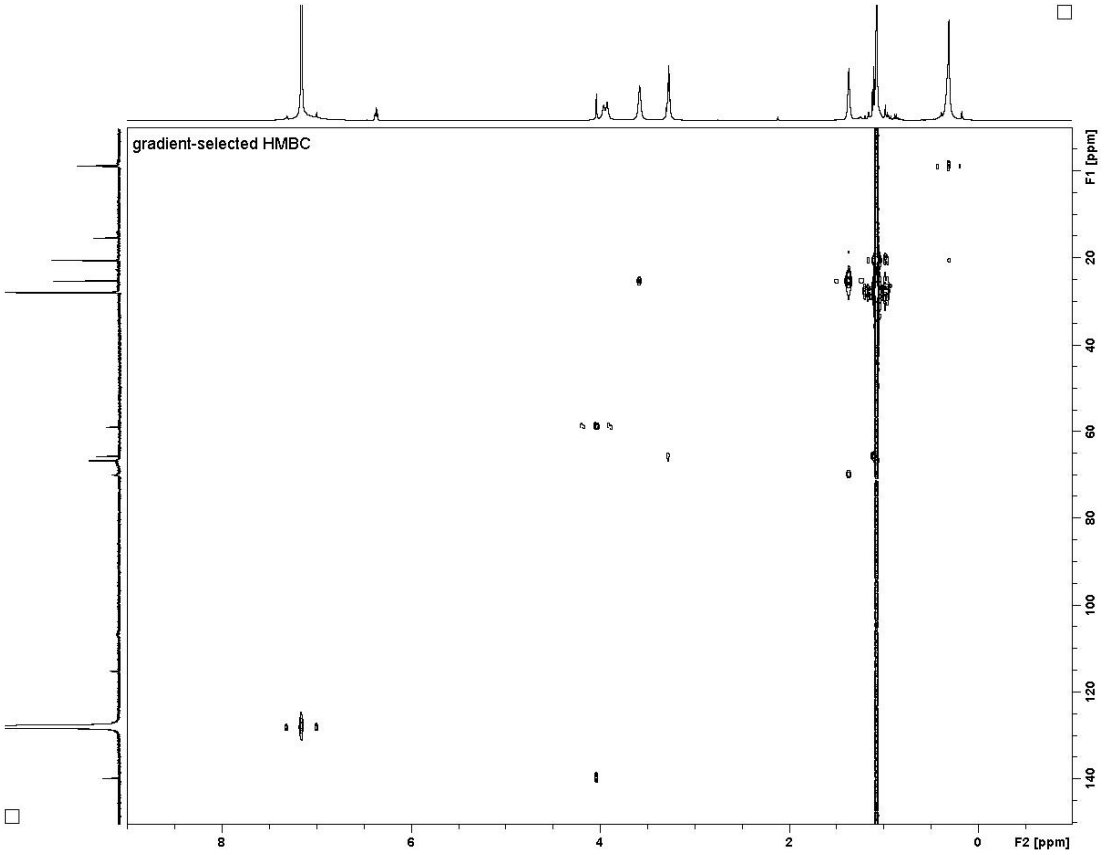
^{1}H NMR spectrum of **Y-stilbene-K** (500 MHz, C_6D_6, 25 °C)



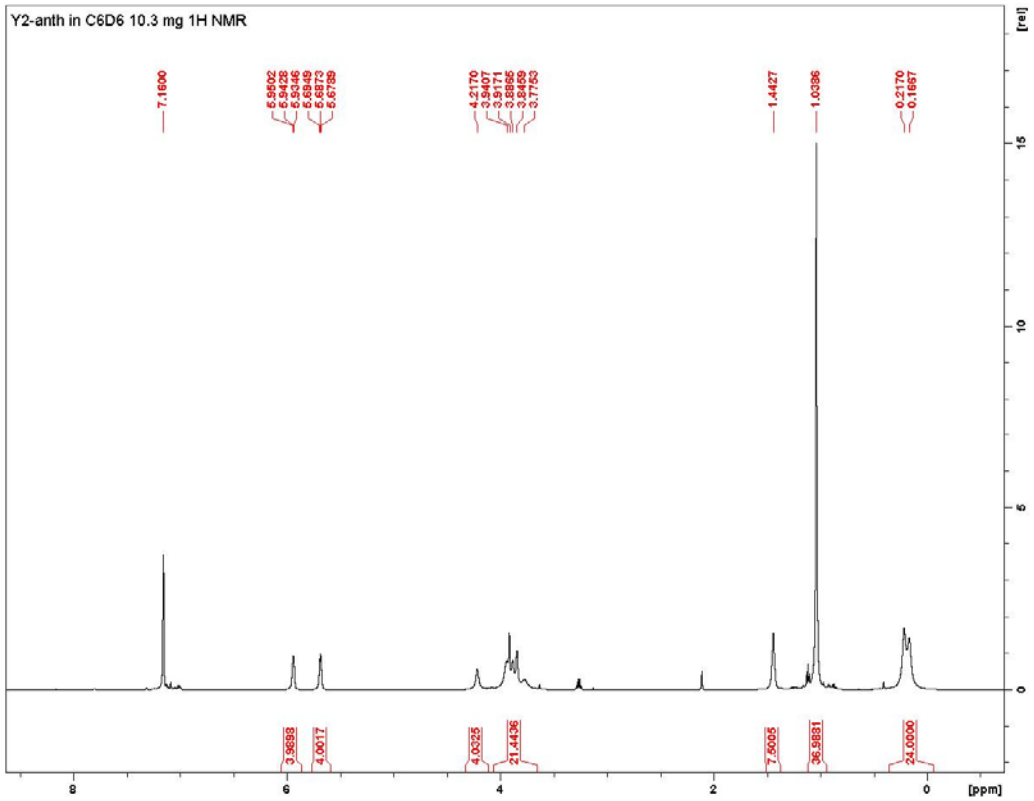
^{13}C NMR spectrum of **Y-stilbene-K** (126 MHz, C_6D_6, 25 °C)



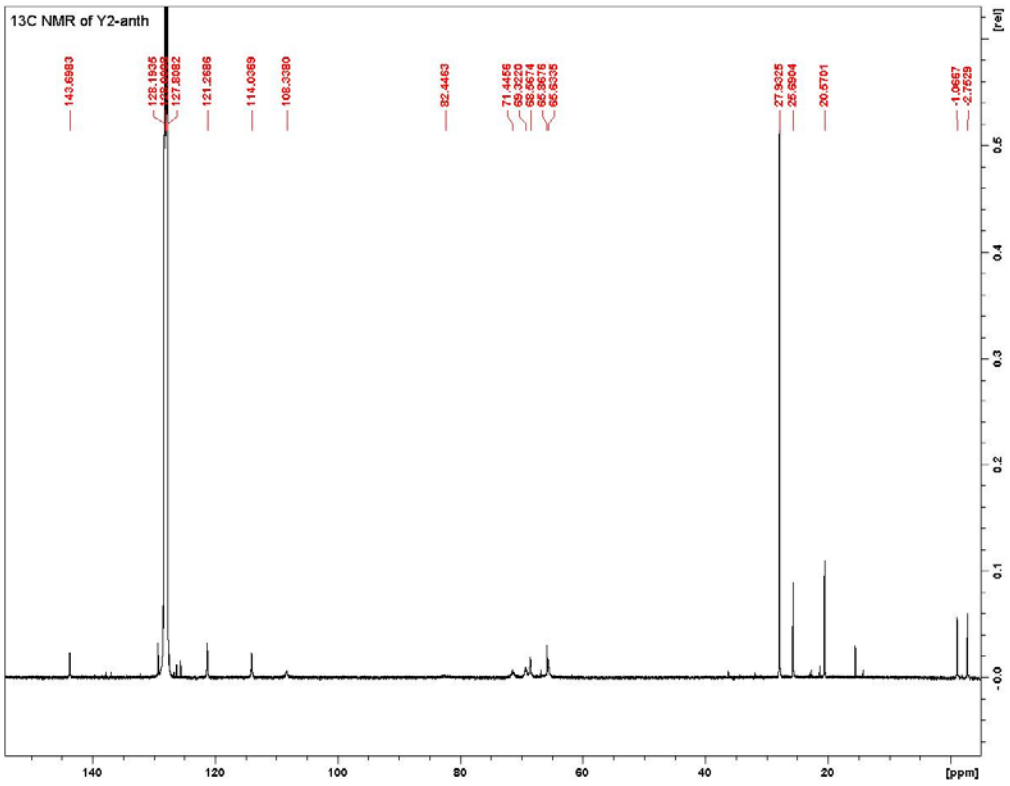
HMBC NMR spectrum of **Y-stilbene-K** (500 MHz, C_6D_6, 25 °C)



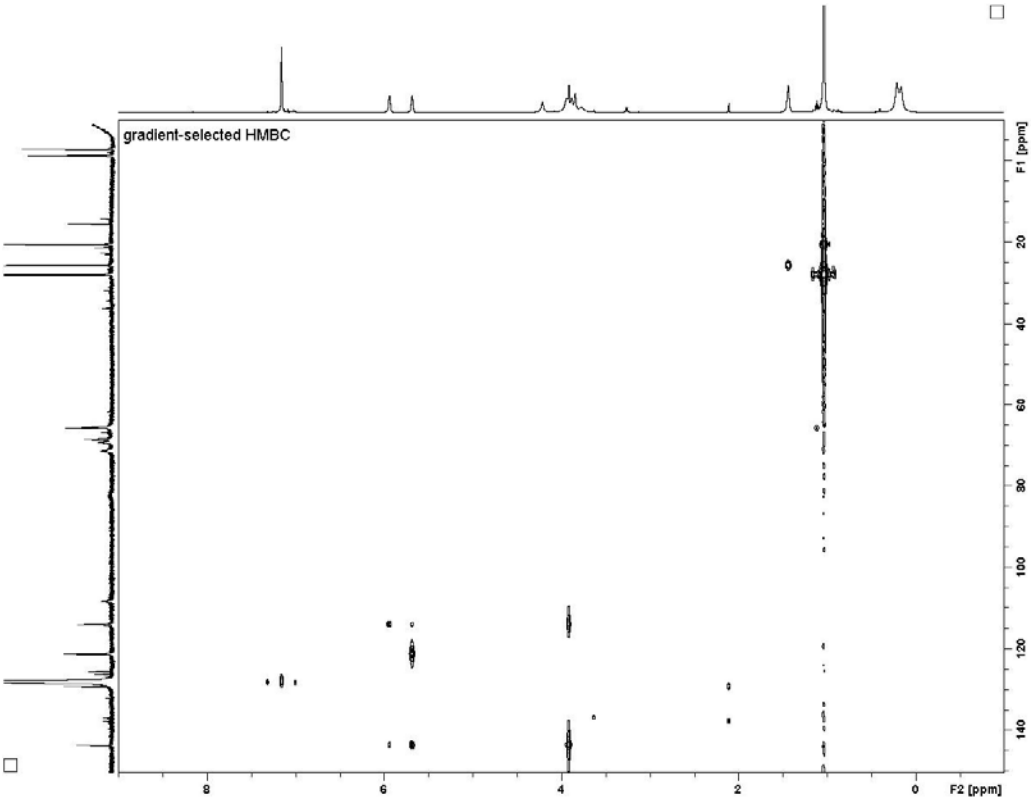
^{1}H NMR spectrum of **Y_2-anth** (C_6D_6, 25 °C)



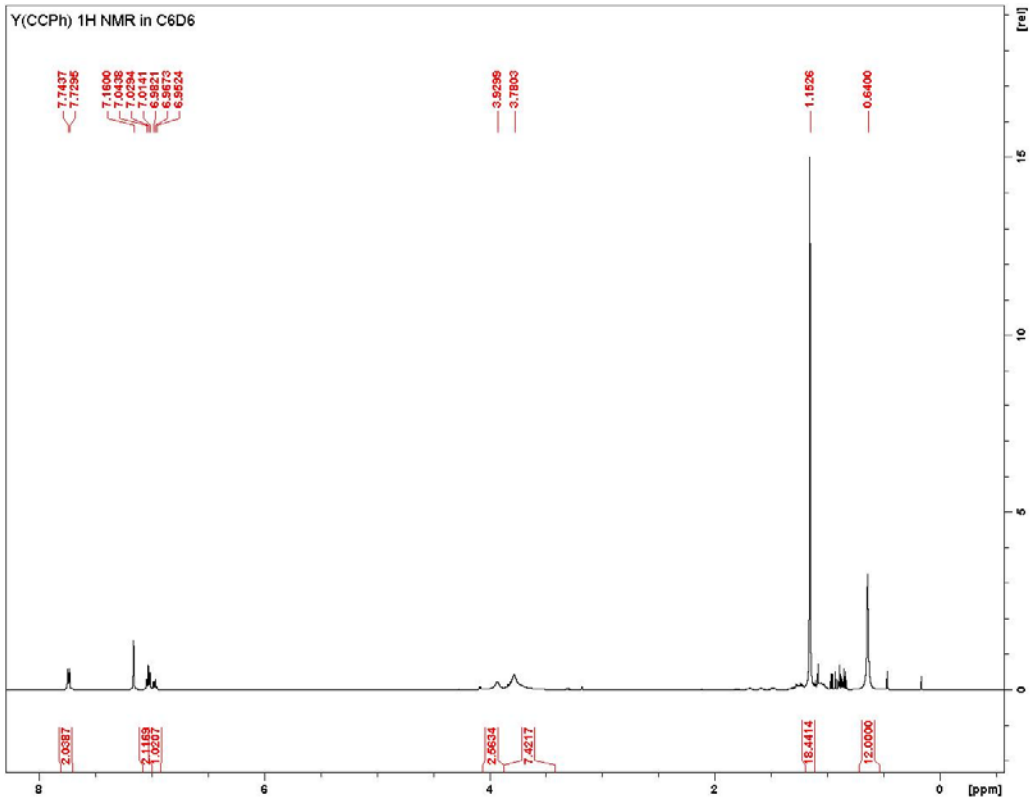
^{13}C NMR spectrum of **Y_2-anth** (C_6D_6, 126 MHz, 25 °C)



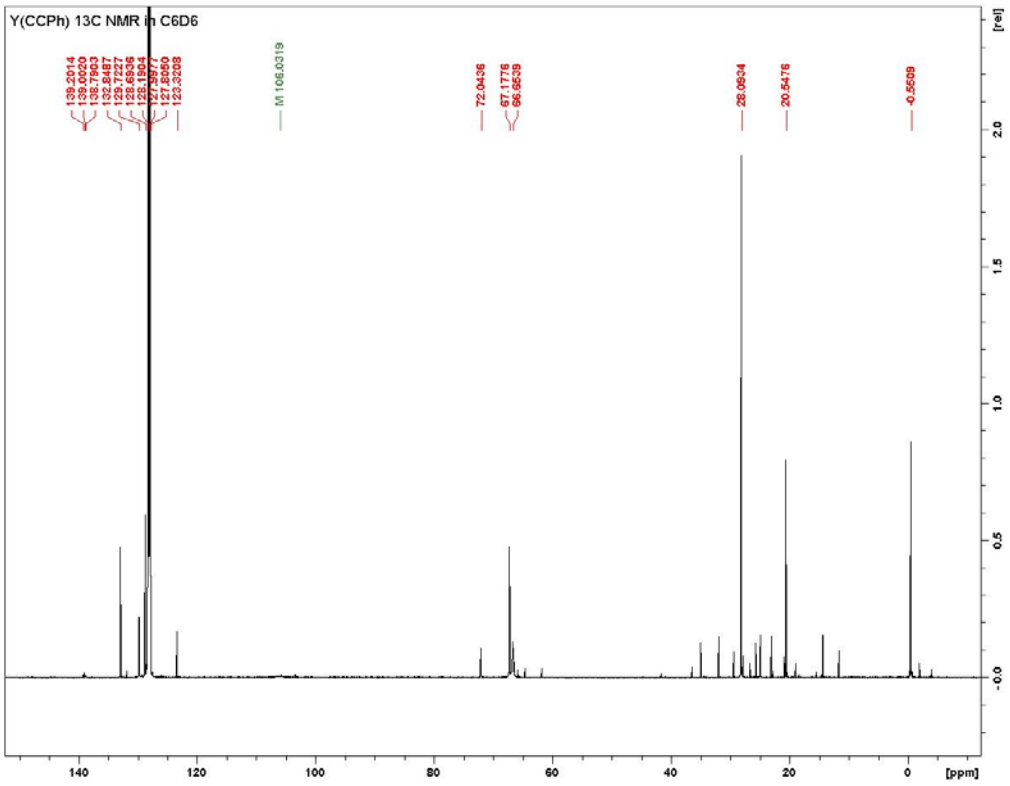
HMBC NMR spectrum of **Y_2-anth** (500 MHz, C_6D_6, 25 °C)



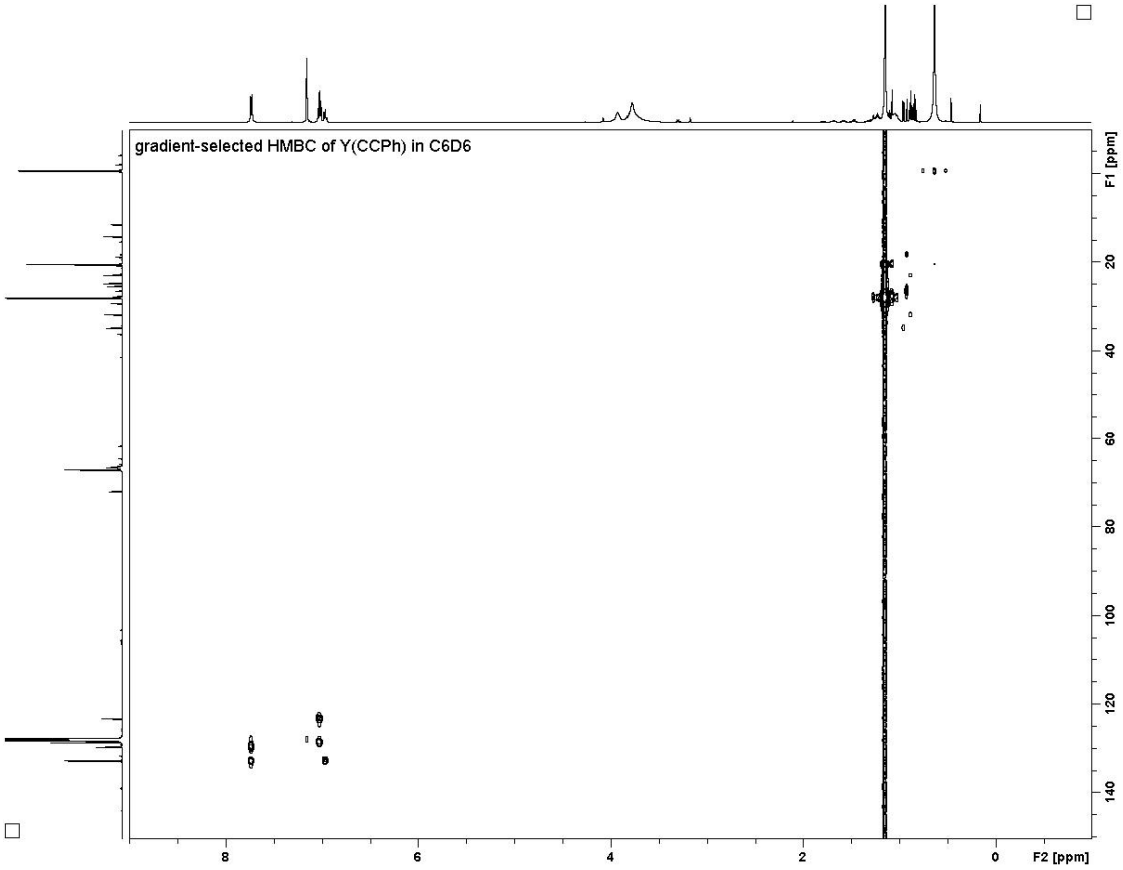
^{1}H NMR spectrum of **[(NN^{TBS})Y(CCPh)]$_2$** (500 MHz, C_6D_6, 25 °C)



^{13}C NMR spectrum of **[(NN^{TBS})Y(CCPh)]$_2$** (126 MHz, C_6D_6, 25 °C)

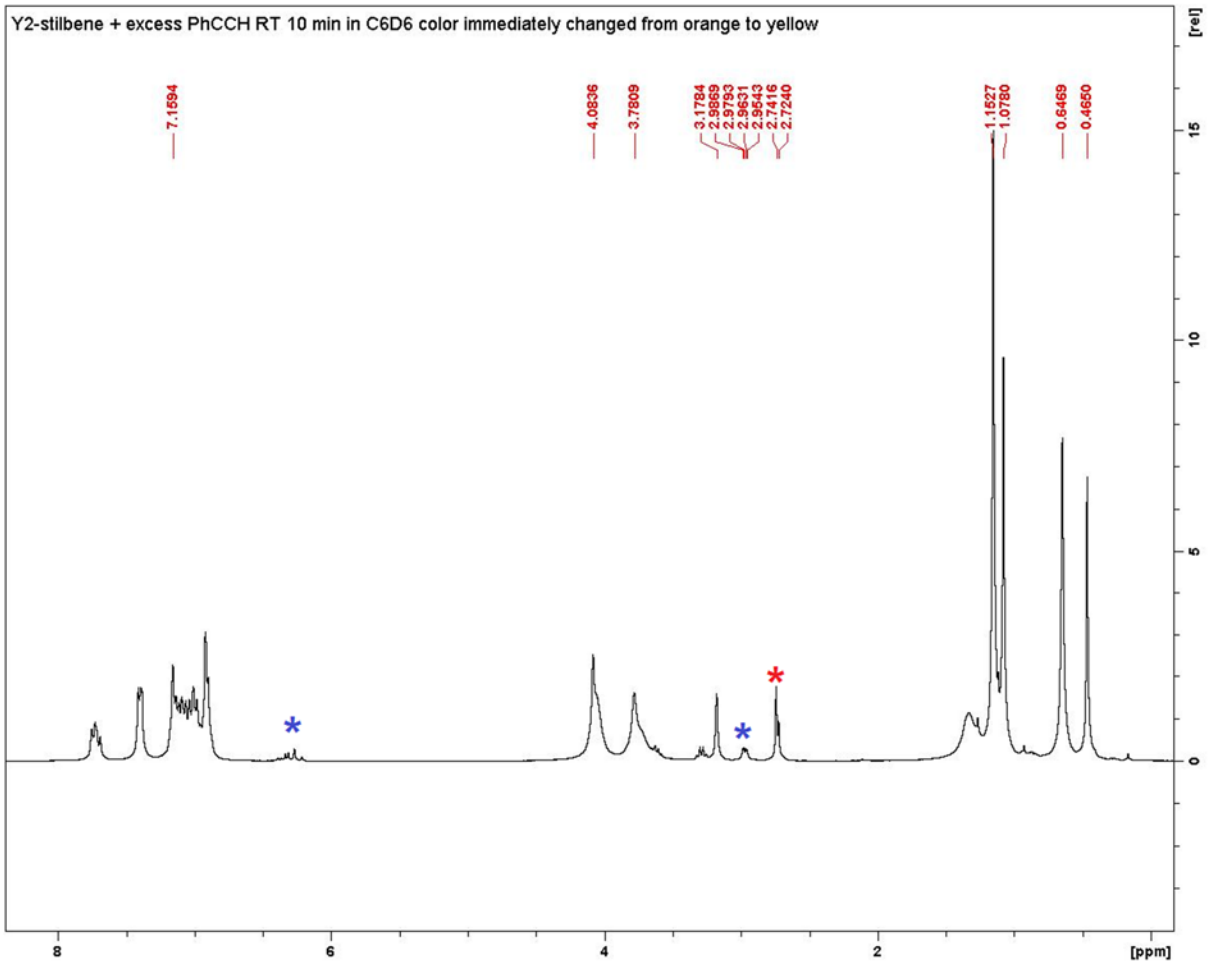


HMBC NMR spectrum of **[(NN^{TBS})Y(CCPh)]$_2$** (500 MHz, C_6D_6, 25 °C)



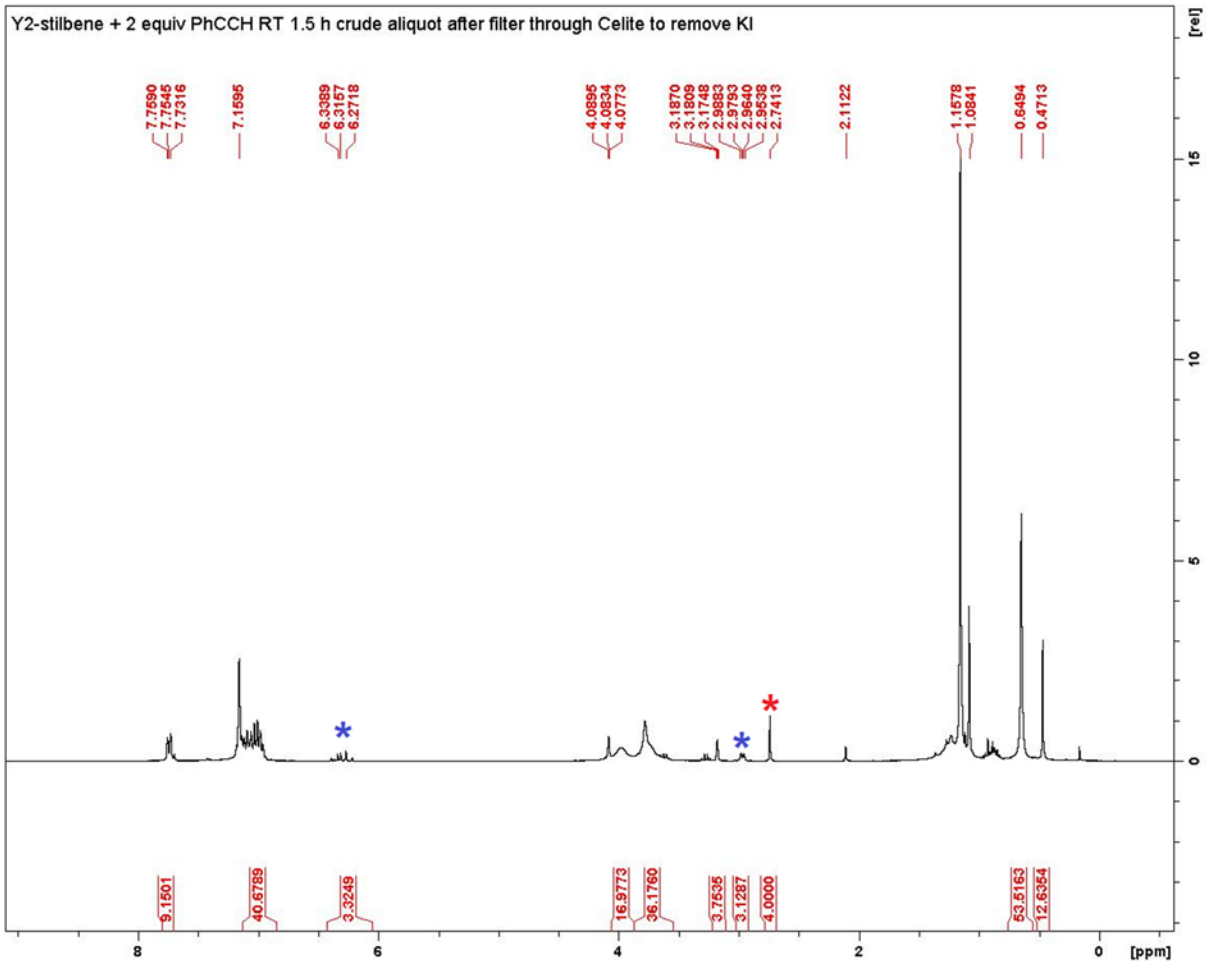
^{1}H NMR spectrum of J-Young scale reaction of **Y_2-stilbene** and excess phenylacetylene (300 MHz, C_6D_6, 25 °C)

Note: The peak at 2.74 ppm labeled with a red star is assigned to bibenzyl. The peaks at 6.3 ppm and 2.9 ppm labeled with blue stars are from other $C_{14}H_{14}$ isomers.

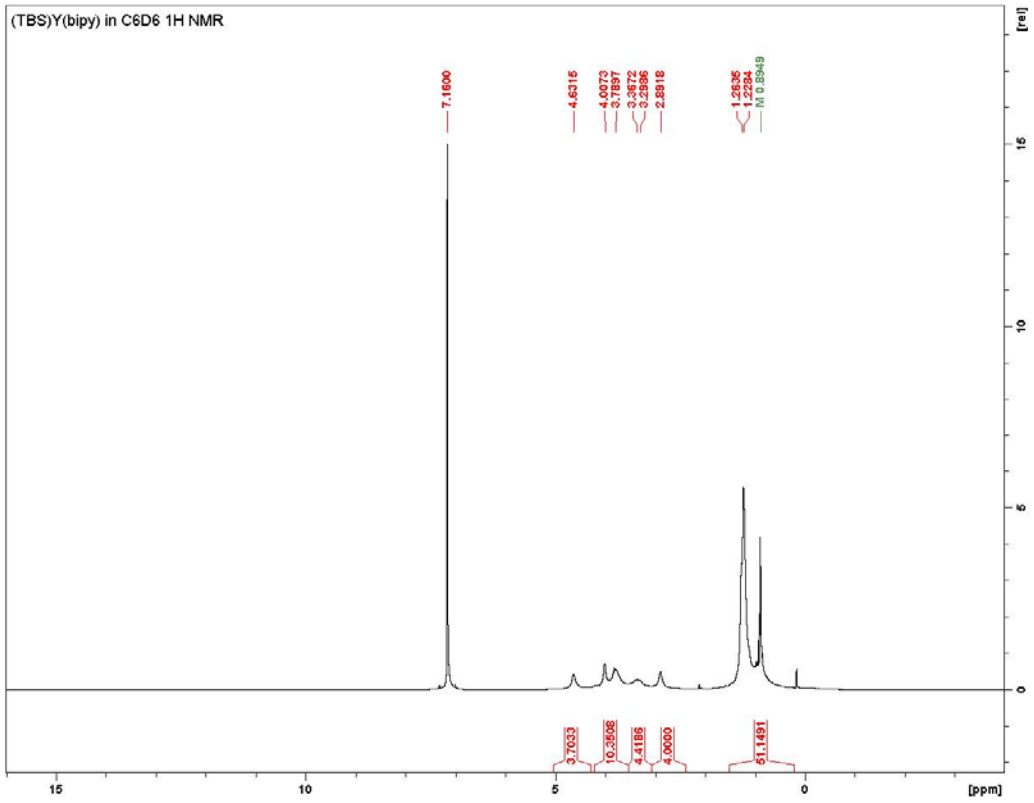


^{1}H NMR spectrum of crude product from a scale-up reaction of **Y_2-stilbene** and excess phenylacetylene (300 MHz, C_6D_6, 25 °C)

Note: Same as for the last spectrum.

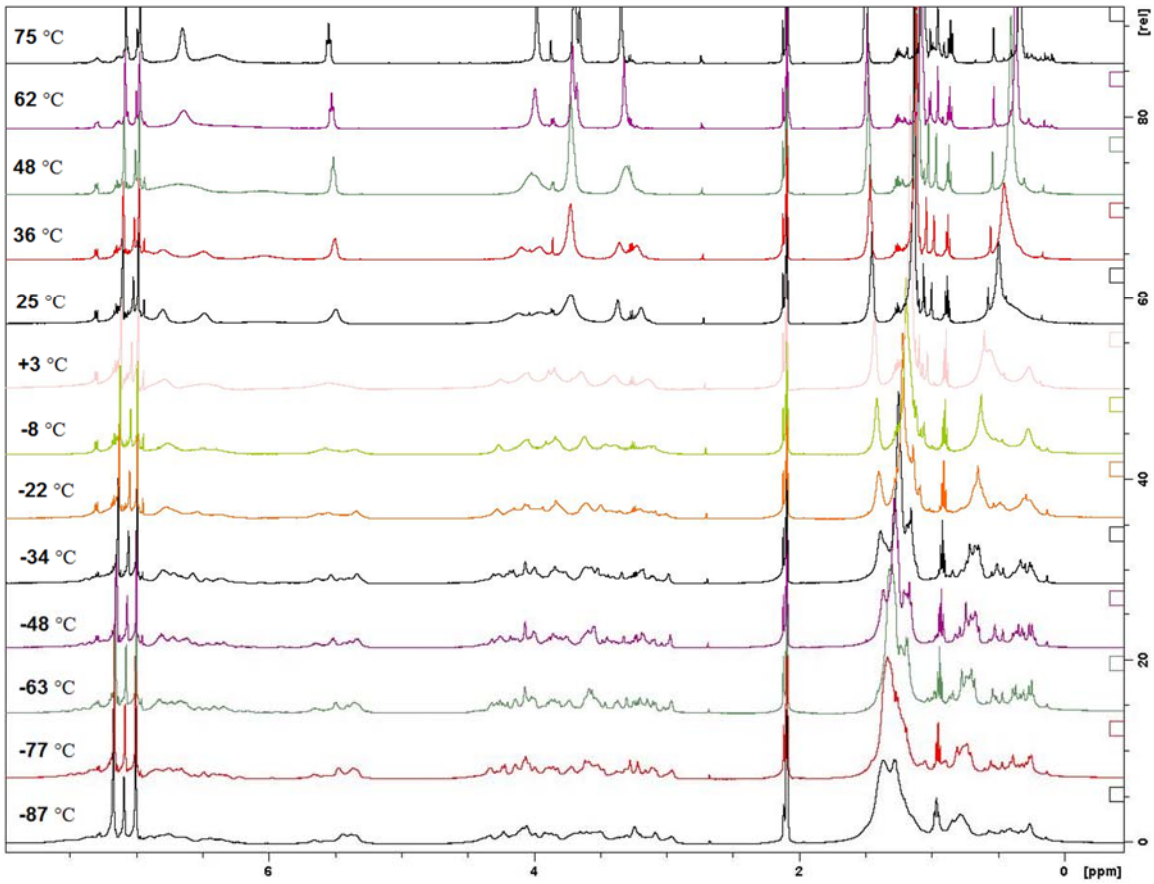


^{1}H NMR spectrum of **(NN^{TBS})Y(THF)(bipy)** (500 MHz, C_6D_6, 25 °C)



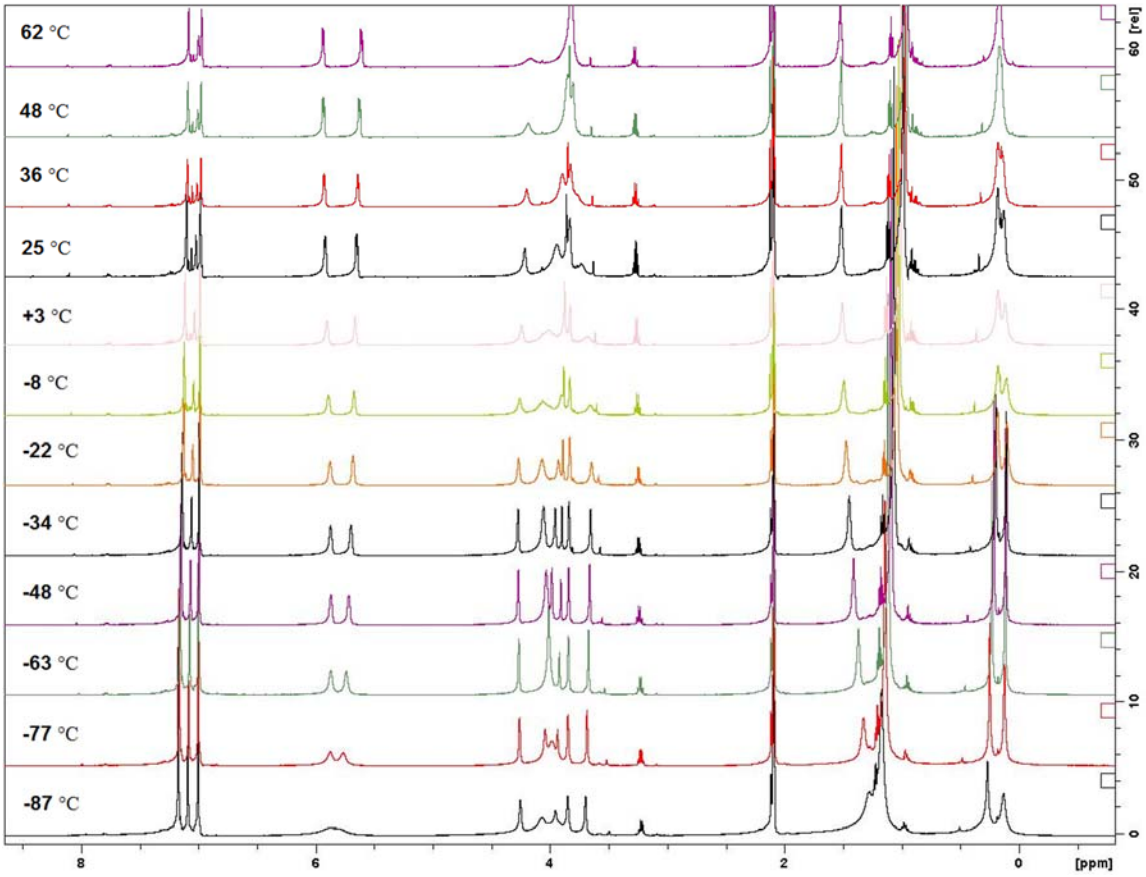
3. Variable temperature NMR spectra

Overlay of ^{1}H NMR spectra of **Y-stilbene-K** (from -87 °C to 75 °C, 500 MHz, C_7D_8)



Discussion: **Y-stilbene-K** formed one or more polymeric species at low temperature as indicated by the complicated spectra below 0 °C. Around room temperature, coalescence was observed as indicated by the broadness of signals. This is likely caused by restricted rotation and/or migration of potassium ion from one phenyl ring to another. At higher temperatures, all signals became sharper, likely the result of a fully equilibrated system.

Overlay of ^{1}H NMR spectra of **Y_2-anth** (from -87 °C to 62 °C, 500 MHz, C_7H_8)



Discussion: At most temperatures studied, **Y_2-anth** presented a symmetric structure in solution. At the low end of the temperature range, some coalescence was observed for peaks related to the [anthracene]$^{2-}$ fragment. This is in contrast to the previously reported variable temperature ^{1}H NMR spectroscopic study of **Sc_2-anth**, which exhibited coalescence around -30 °C and presented an asymmetric structure in solution below -30 °C. The weaker binding between yttrium and the anthracene dianion may explain this difference.

4. X-ray crystallography data

$[(NN^{TBS})Y(THF)]_2(\mu\text{-stilbene})$ (Y_2-stilbene)

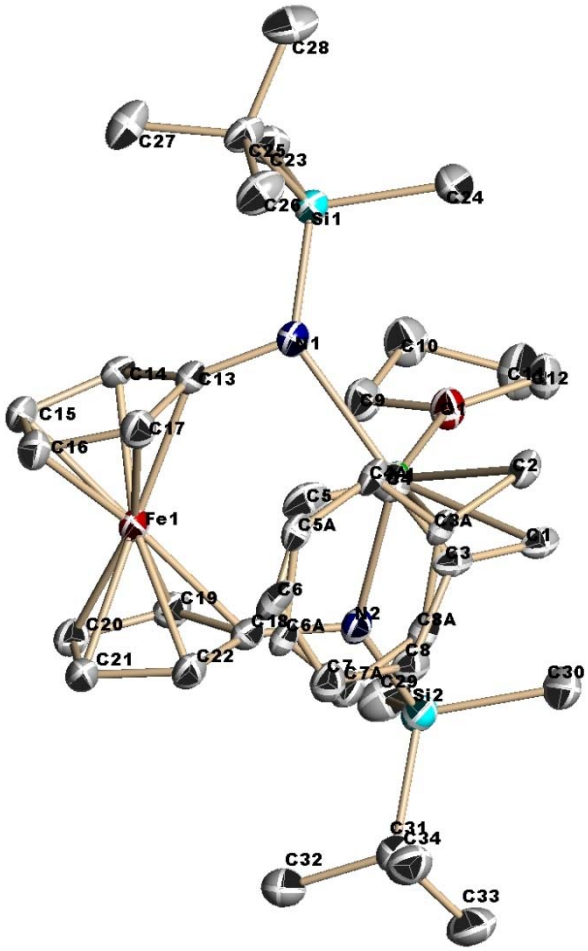


Figure SX1. Thermal-ellipsoid (50% probability) representation of the crystallographically independent atoms in **Y_2-stilbene**. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: Y1-N1 2.242(2), Y1-N2 2.225(2), Y1-C1 2.603(4), Y1-C2 2.581(5), Y1-C3 2.741(7), Y1-C3A 2.717(8), C1-C1A 1.520(7), C2-C2A 1.495(7), C1-C3 1.390(9), C2-C3A 1.456(9), Y1-O1 2.361(2), Y1-Fe1 3.417(1), C3-C1-C1A 123.3(5), C3A-C2-C2A 122.0(5), C1-Y1-C1A 34.1(1), C2-Y1-C2A 33.5(2).

Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with *n*-pentane. The stilbene unit is disordered; this disorder was modeled over two sets of positions (see figure above). A total of 17829 reflections ($-14 \le h \le 14$, $-15 \le k \le 15$, $-22 \le l \le 22$) were collected at $T = 100(2)$ K with $2\theta_{max} = 58.47°$, of which 9520 were unique. The residual peak and hole electron densities were 0.71 and -0.41 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0374$ and GOF = 1.035. Crystal and refinement data for **Y_2-stilbene**: formula $C_{80}H_{103}N_4Si_4Fe_2O_2Y_2 \cdot 2(C_7H_8)$, space group *P*-1, $a = 11.210(1)$, $b = 11.7733(11)$, $c = 16.4895(15)$, $\alpha = 90.787(1)$, $\beta = 109.724(1)$, $\gamma = 106.301(1)°$, $V = 1952.0(3)$ $Å^3$, $Z = 1$, $\mu = 1.945$ mm^{-1}, $F(000) = 830$, $R_1 = 0.0493$ and $wR_2 = 0.0967$ (based on all data, $I > 2\sigma(I)$).

[(NN^{TBS})Y(THF)](μ-stilbene)[K(18-crown-6)] (Y-stilbene-K-crown)

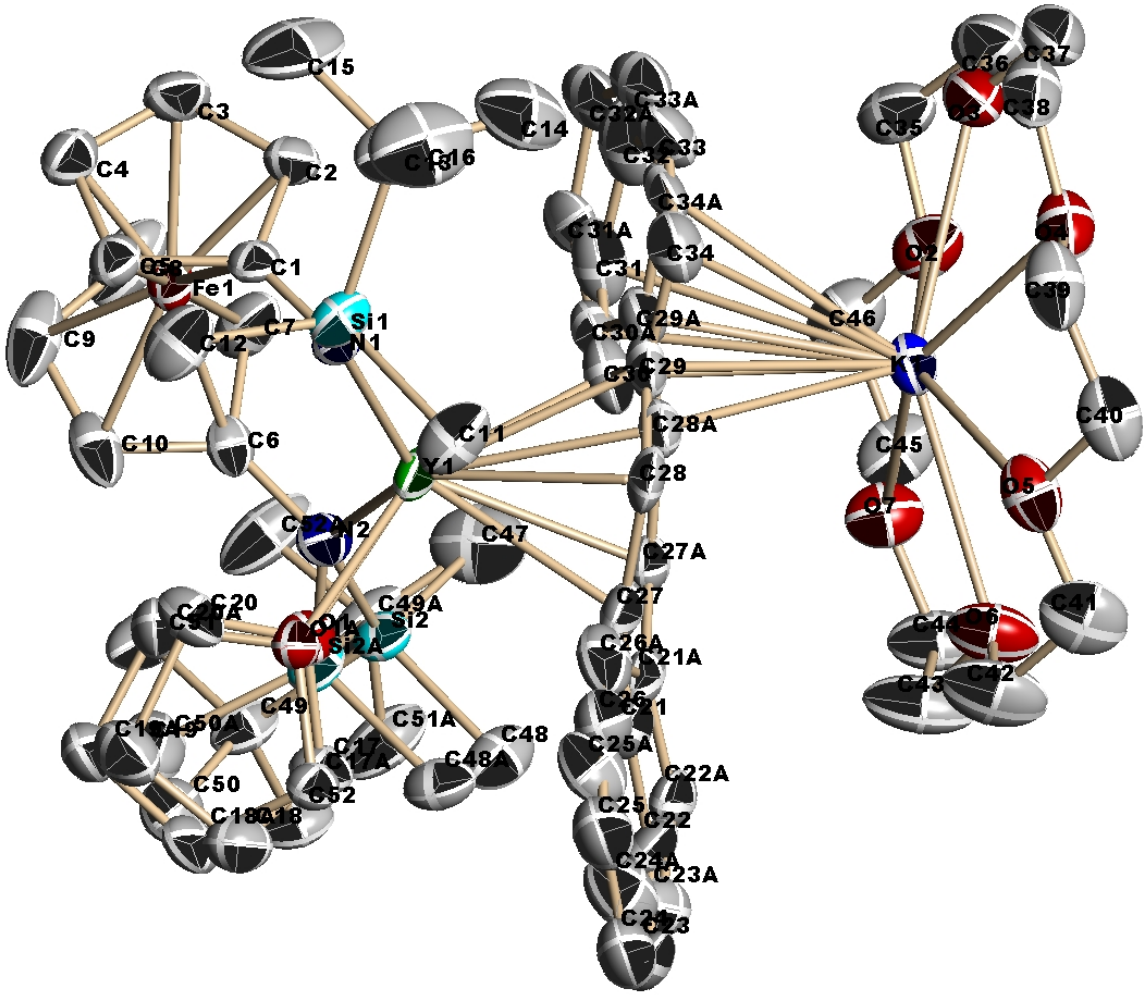


Figure SX2. Thermal-ellipsoid (50% probability) representation of **Y-stilbene-K-crown**. Hydrogen and solvent atoms were omitted for clarity. Selected distances [Å] and angles [°]: Y1-N1 2.276(3), Y1-N2 2.267(3), Y1-C27 2.577(8), Y1-C28 2.545(8), Y1-C29 2.609(5), Y1-C30 2.590(6), C21-C27 1.529(10), C27-C28 1.478(11), C28-C29 1.450(9), C27-C28-C29 120.7(7).

Single crystals suitable for X-ray diffraction were grown from a concentrated hexanes solution. The stilbene unit is disordered; this disorder was modeled over two sets of positions (see figure above). A total of 67858 reflections ($-17 \le h \le 17$, $-18 \le k \le 18$, $-35 \le l \le 35$) were collected at $T = 100(2)$ K with $2\theta_{max} = 52.74°$, of which 12297 were unique. The residual peak and hole electron densities were 0.45 and -0.98 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0498$ and GOF = 1.017. Crystal and refinement data for **Y-stilbene-K-crown**: formula $C_{40}H_{56}N_2Si_2FeOY_2 \cdot C_{12}H_{24}O_6 \cdot K \cdot C_6H_{14}$, space group $P2_1/n$, $a = 14.082(4)$, $b = 15.074(4)$, $c = 28.493(8)$, $\beta = 90.343(4)°$, $V = 6048(3)$ Å^3, $Z = 4$, $\mu = 1.353$ mm^{-1}, $F(000) = 2496$, $R_1 = 0.0840$ and $wR_2 = 0.1197$ (based on all data, $I > 2\sigma(I)$).

$[(NN^{TBS})Y(THF)]_2(\mu\text{-anthracene})$ (Y_2-anth)

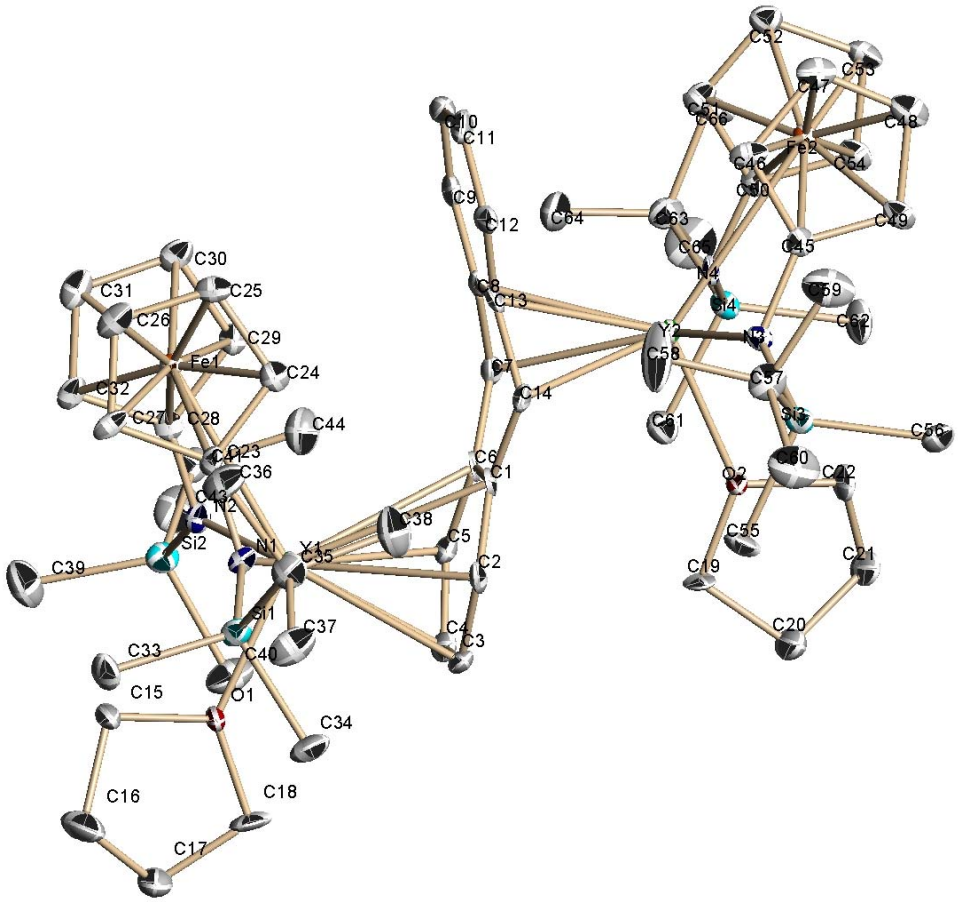


Figure SX3. Thermal-ellipsoid (50% probability) representation of **Y_2-anth**. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: Y1-N1 2.243(8), Y1-N2 2.215(8), Y2-N3 2.238(7), Y2-N4 2.270(8), Y1-C1 3.014(9), Y1-C2 2.793(9), Y1-C3 2.714(9), Y2-C7 2.708(9), Y2-C8 2.705(9), C1-C2 1.419(12), C2-C3 1.441(13), C3-C4 1.426(14), C1-C14 1.432(13), C14-C13 1.454(13), C1-C2-C3 121.7(9), C1-C14-C13 120.1(8).

Single crystals suitable for X-ray diffraction were grown from a concentrated Et_2O solution. The unit cell contains large accessible voids; solvent molecules could not be modeled to fit this space (it is possible that some solvent was lost during crystal handling) and the program SQUEEZE was used. A total of 62347 reflections ($-18 \le h \le 18$, $-33 \le k \le 33$, $-25 \le l \le 25$) were collected at $T = 100(2)$ K with $2\theta_{max} = 52.95°$, of which 16317 were unique. The residual peak and hole electron densities were 1.09 and -0.52 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0479$ and GOF = 1.038. Crystal and refinement data for **Y_2-anth**: formula $C_{66}H_{102}N_4Si_4Fe_2O_2Y_2$, space group $P2_1/c$, $a = 15.097(8)$, $b = 26.925(15)$, $c = 20.626(11)$, $\beta = 108.031(6)°$, $V = 7973(8)$ Å^3, $Z = 4$, $\mu = 1.896$ mm^{-1}, $F(000) = 2912$, $R_1 = 0.0740$ and $wR_2 = 0.1322$ (based on all data, $I > 2\sigma(I)$).

[(NN^{TBS})La(THF)]$_2$(μ-stilbene) (La$_2$-stilbene)

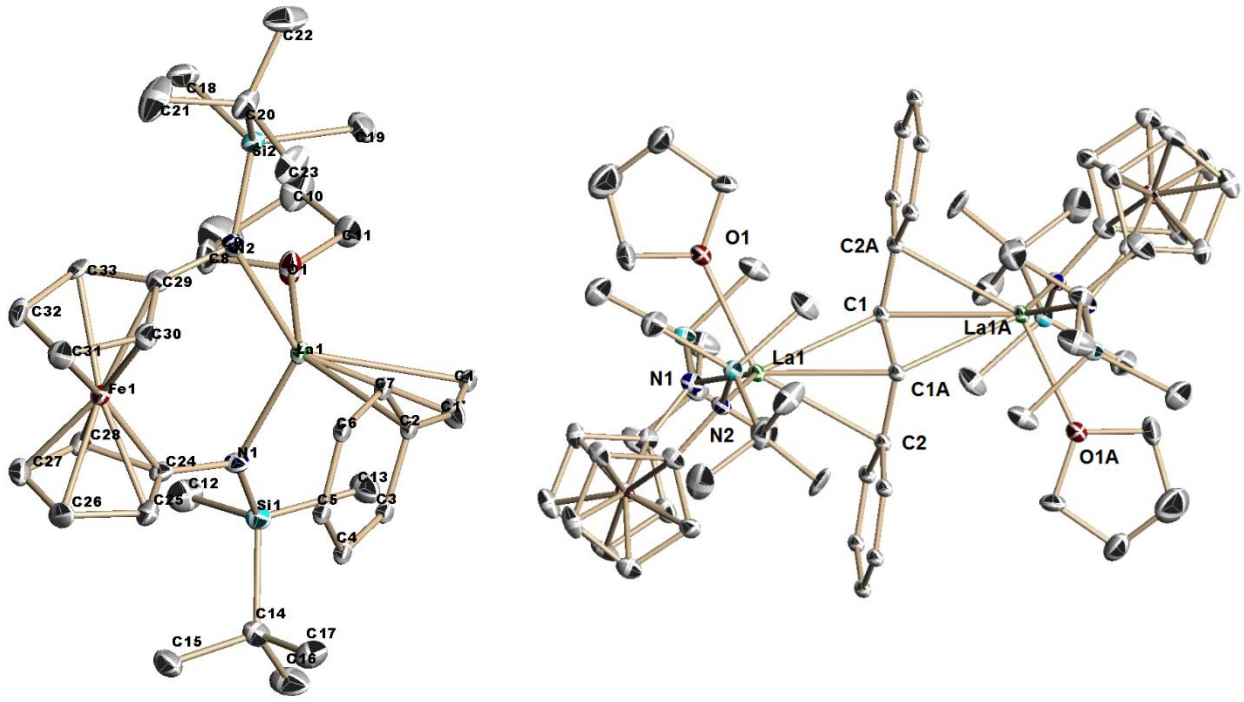


Figure SX4. Thermal-ellipsoid (50% probability) representation of the crystallographically independent atoms in **La$_2$-stilbene** (left) and the full molecule (right). Hydrogen and solvent atoms were omitted for clarity. Selected distances [Å] and angles [°]: La1-N1 2.349(6), La1-N2 2.349(6), La1-C1 2.779(13), La1-C1A 2.696(14), La1-C2 2.822(7), La1-O1 2.543(6), La1-Fe1 3.429(2), C1-C1A 1.4658(240), C1'-C1'A 1.4296(299), C1-C2A 1.4970(148), C1'-C2 1.5108(146), N1-La1-N2 127.02(21), C2A-C1-C1A 114.43(1.34), C2-C1'-C1'A 114.40(1.49), C1-La1-C1A 31.02(49), C1'-La1-C1'A 30.32(61).

Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with n-pentane. The C=C bond in the stilbene unit is disordered; this disorder was modeled over two sets of positions (see figure above). A total of 16042 reflections ($-14 \le h \le 14$, $-14 \le k \le 14$, $-20 \le l \le 20$) were collected at T = 100(2) K with $2\theta_{max}$ = 52.74°, of which 4661 were unique. The residual peak and hole electron densities were 1.74 and -2.30 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0551 and GOF = 1.077. Crystal and refinement data for **La$_2$-stilbene**: formula $C_{66}H_{102}N_4Si_4Fe_2O_2La_2 \cdot 2(C_7H_7)$, space group P-1, a = 11.323(4), b = 11.909(5), c = 16.767(7), α = 89.093(5), β = 70.339(5), γ = 70.830(5)°, V = 1999.6(13) Å^3, Z = 1, μ = 1.508 mm^{-1}, F(000) = 862, R_1 = 0.0614 and wR_2 = 0.1421 (based on all data, I > 2$\sigma(I)$).

(NN^{TBS})Y(THF)(bipy)

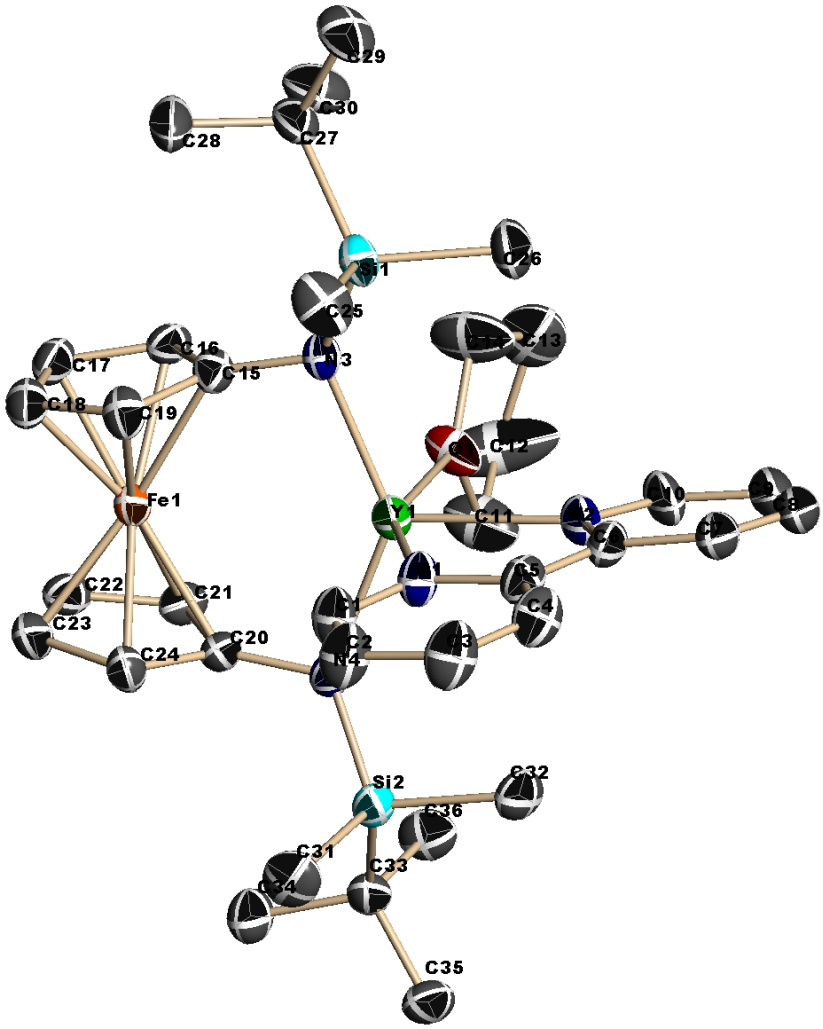


Figure SX5. Thermal-ellipsoid (50% probability) representation of **(NN^{TBS})Y(THF)(bipy)**. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: Y1-N1 2.3411(35), Y1-N2 2.3874(35), Y1-N3 2.2258(34), Y1-N4 2.2140(35), Y1-O1 2.3677(27), Y1-Fe1 3.2612(15), N1-Y1-N2 68.21(12), N3-Y1-N4 137.08(11), N1-Y1-N3 95.85(13), N1-Y1-N4 95.14(12), N1-C5-C6 116.29(37).

Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with *n*-pentane. A total of 40512 reflections ($-13 \le h \le 13$, $-21 \le k \le 21$, $-27 \le l \le 27$) were collected at $T = 100(2)$ K with $2\theta_{max} = 52.74°$, of which 8213 were unique. The residual peak and hole electron densities were 1.68 and -0.75 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0524$ and GOF = 1.045. Crystal and refinement data for **[(NN^{TBS})Y](bipy)**: formula $C_{36}H_{54}N_4Si_2FeOY \cdot 0.5(C_6H_{14})$, space group $P21/c$, $a = 11.115(8)$, $b = 16.898(12)$, $c = 21.869(15)$, $\beta = 84.720(4)°$, V = 4034(5) Å^3, Z = 4, $\mu = 1.885$ mm^{-1}, F(000) = 1696, $R_1 = 0.0842$ and $wR_2 = 0.1460$ (based on all data, $I > 2\sigma(I)$).

[(NN^{TBS})Y(THF)][(NN^{TBS})Y](μ-CCPh)$_2$

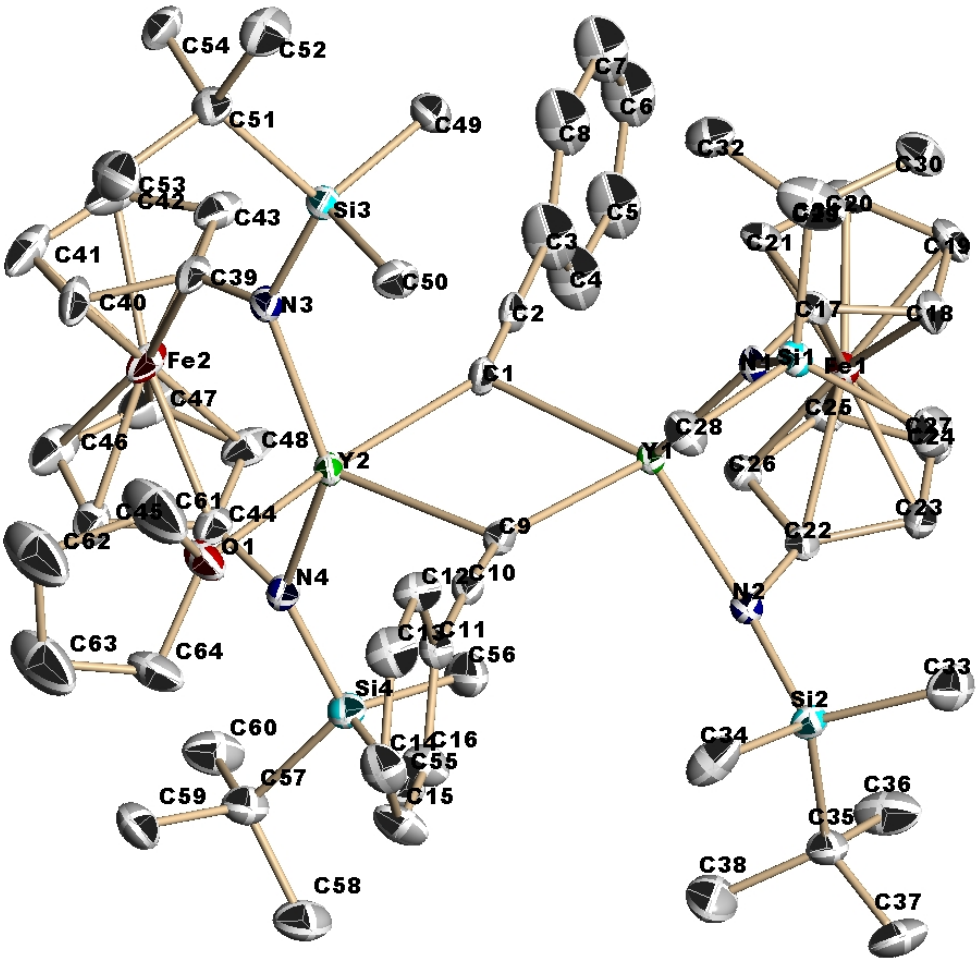


Figure SX6. Thermal-ellipsoid (50% probability) representation of **[(NN^{TBS})Y(THF)][(NN^{TBS})Y](μ-CCPh)$_2$**. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: Y1-N1 2.216(3), Y1-N2 2.237(3), Y2-N3 2.223(3), Y2-N4 2.219(3), Y2-O1 2.367(2), Y1-C1 2.513(3), Y1-C9 2.483(3), Y2-C1 2.522(3), Y2-C9 2.521(3), Y1-Fe1 2.943(1), Y1-Fe2 3.240(1), Y1-Y2 3.826(1), C1-C2 1.210(5), C2-C3 1.446(5), Y1-C1-Y2 98.9(1), C1-C2-C3 180.0(5).

Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with *n*-pentane. The unit cell contains large accessible voids; solvent molecules could not be modeled to fit this space (it is possible that some solvent was lost during crystal handling) and the program SQUEEZE was used. A total of 32725 reflections ($-15 \le h \le 15$, $-21 \le k \le 21$, $-24 \le l \le 24$) were collected at $T = 100(2)$ K with $2\theta_{max} = 52.74°$, of which 4661 were unique. The residual peak and hole electron densities were 1.87 and -1.21 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0463$ and GOF = 1.060. Crystal and refinement data for **[(NN^{TBS})Y(THF)][(NN^{TBS})Y](μ-CCPh)$_2$**: formula $C_{64}H_{92}N_4Si_4Fe_2OY_2$, space group *P*-1, $a = 12.115(4)$, $b = 17.497(6)$, $c = 19.614(6)$, $\alpha = 82.581(4)$, $\beta = 84.720(4)$, $\gamma = 72.458(4)°$, V = 3925(2) Å^3, $Z = 2$, $\mu = 1.922$ mm^{-1}, F(000) = 1396, $R_1 = 0.0581$ and $wR_2 = 0.1367$ (based on all data, $I > 2\sigma(I)$).

5. DFT calculations

General considerations: Computational studies were performed with ADF2013.01. For yttrium, lanthanum, and iron atoms, standard triple-ζ STA basis sets from the ADF database ZORA TZP, while for all the other atoms, standard double-ζ STA basis sets from the ADF database ZORA DZP were employed with the 1s-4p (Y), 1s-5p (La), 1s-3p (Fe), 1s-2p (Si), and 1s (N, C) electrons treated as frozen cores. The generalized gradient approximation (GGA) by Becke-Perdew was used together with the exchange and correlation corrections that are employed by default by the ADF2013.01 program suite. Calculations were carried out using the scalar spin-orbit relativistic formalism. Mayer bond orders and atomic properties were calculated using the defaults implemented in the ADF2013.01 program suite.

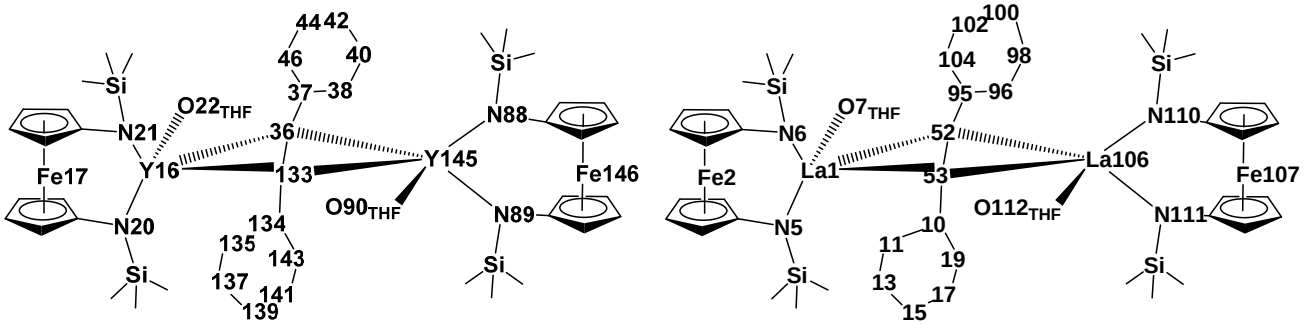


Figure SX7. Atom labeling scheme for **Y_2-stilbene** (left) and **La_2-stilbene** (left) used for computational studies.

Table S1: Comparison of structural parameters derived from X-ray crystallography and DFT calculations, distance [Å] and angles [°].

Y_2-stilbene	***Exp.***	***ADF***	***La_2-stilbene***	***Exp.***	***ADF***
C36-C133	1.51 (av)	1.49	C52-C53	1.45 (av.)	1.47
Y16-C36	2.58	2.62	La1-C52	2.78	2.87
Y16-C9	2.60	2.66	La1-C53	2.70	2.79
Y16-C134	2.74	2.86	La1-C10	2.82	2.94
Y16-O22	2.36	2.45	La1-O7	2.54	2.64
Y16-N20	2.24	2.27	La1-N6	2.35	2.39
Y16-N21	2.23	2.27	La1-N5	2.35	2.40
C36-C37	1.43	1.44	C52-C95	1.50	1.43
C133-C134	1.43	1.44	C53-C10	1.50	1.43
N20Y16N21	128.2	128.9	N6La1N5	127.0	126.7
C36C133C134	122.6 (av.)	122.6	C52C53C10	114.4 (av.)	123.9
C36Y16C133	33.8 (av.)	32.7	C52La1C53	30.7 (av.)	30.0

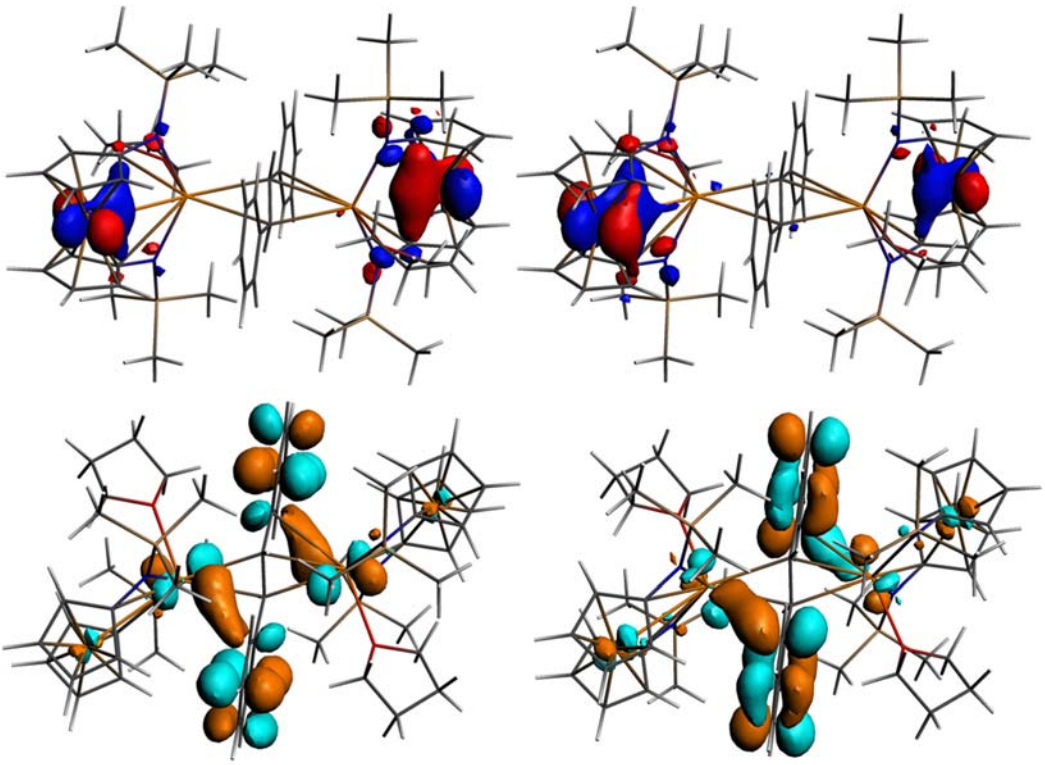


Figure SX8. Frontier molecular orbitals for **Y_2-stilbene**: HOMO-1 (top left), HOMO-2 (top right), LUMO (bottom left), LUMO+1 (bottom right).

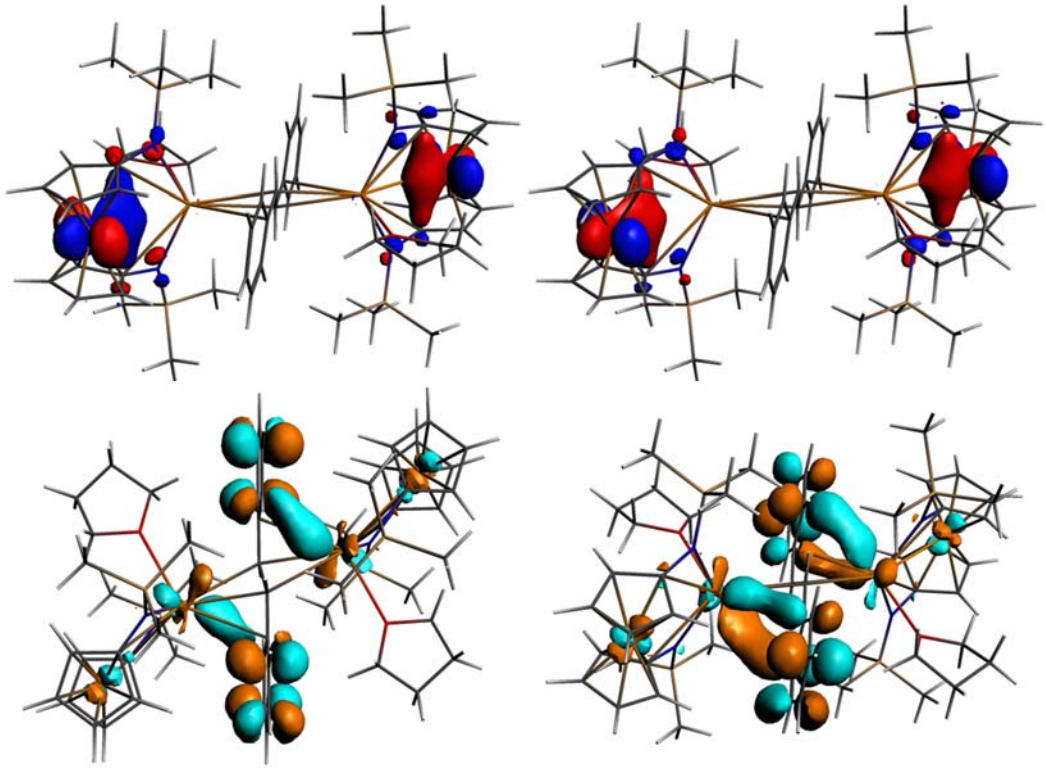


Figure SX9. Frontier molecular orbitals for **La_2-stilbene**: HOMO-1 (top left), HOMO-2 (top right), LUMO (bottom left), LUMO+1 (bottom right).

Optimized parameters for **Y_2-stilbene**

Coordinates

1.H	-1.623252	0.134218	7.931257
2.H	-2.121956	1.820232	8.147310
3.C	0.478338	2.100788	6.221707
4.H	0.997119	2.418063	5.301320
5.C	-1.305545	2.946634	1.418551
6.H	-1.249011	2.639502	0.376810
7.C	-0.708948	4.120059	1.983633
8.H	1.105753	1.337427	6.713858
9.H	-0.126240	4.862200	1.443197
10.C	-1.022920	4.146949	3.374838
11.H	-0.720667	4.908904	4.089213
12.H	0.422045	2.972784	6.894126
13.C	-8.134736	4.197299	2.508798
14.H	-8.161780	3.162107	2.889583
15.H	-9.178639	4.546123	2.418270
16.Y	-4.762293	5.757621	10.004390
17.Fe	-6.090138	5.419924	13.154641
18.Si	-1.709203	4.250833	11.714472
19.Si	-7.603355	8.164088	9.545328
20.N	-3.357177	4.796023	11.499313
21.N	-6.616950	7.003744	10.391414
22.O	-3.495431	7.854668	10.019927
23.C	-2.128540	0.980681	7.435790
24.H	-1.968768	-0.682907	4.622281
25.H	-6.671516	7.118273	1.945420
26.C	-8.017472	5.371725	5.329947
27.H	-7.705706	4.172312	1.493582
28.H	-9.079796	5.633576	5.184418
29.H	-7.589403	6.136595	5.996806
30.C	-7.197834	7.082812	2.913999
31.H	-7.989763	4.403614	5.853954
32.C	-3.869325	4.640288	0.545004
33.H	-6.719921	7.819699	3.580363
34.H	-3.693173	4.242334	-0.451690
35.C	-3.277726	5.823434	1.095541
36.C	-4.365994	4.105490	7.954658
37.C	-5.487807	3.418372	8.551943
38.C	-5.311676	2.186332	9.253033
39.H	-4.304651	1.776758	9.343832
40.C	-6.381231	1.497479	9.789441
41.H	-6.198078	0.552941	10.306201
42.C	-7.694327	1.992873	9.686465
43.H	-8.532371	1.440911	10.111877
44.C	-7.892119	3.208186	9.042212
45.H	-8.898020	3.623352	8.954240
46.C	-6.820926	3.920410	8.495907
47.H	-7.033586	4.851965	7.975035
48.C	-3.786000	8.769365	11.136743
49.H	-4.108617	8.174013	12.000626
50.H	-4.612845	9.412974	10.809178
51.C	-2.496021	9.543968	11.378561
52.H	-1.871168	9.024840	12.121686
53.H	-2.691259	10.562847	11.741030
54.C	-1.817828	9.505724	10.005537
55.H	-0.737508	9.701139	10.047729
56.H	-2.281925	10.232475	9.320268
57.C	-2.128583	8.093558	9.551305
58.H	-2.122503	7.955268	8.464389
59.H	-1.459815	7.363544	10.032350
60.C	-4.138265	4.671708	12.659559
61.C	-4.123745	5.522811	13.827350
62.H	-3.520572	6.421692	13.936209
63.C	-4.975004	4.955151	14.824242
64.H	-5.149261	5.353889	15.820959
65.C	-5.567561	3.771531	14.275806
66.H	-6.271446	3.116825	14.784003
67.C	-5.073877	3.608493	12.947115
68.H	-5.318970	2.803352	12.257580
69.C	-7.054498	6.621693	11.664611
70.C	-6.860826	7.336872	12.904894
71.H	-6.325061	8.277943	13.006421
72.C	-7.543978	6.645173	13.950737
73.H	-7.601613	6.953571	14.992043
74.C	-8.138348	5.470098	13.386859
75.H	-8.719721	4.727476	13.928086
76.C	-7.823869	5.442125	11.995794
77.H	-8.124089	4.678384	11.282543
78.C	-0.713403	5.401852	12.854340
79.H	-0.681024	6.433628	12.464783
80.H	0.328889	5.049639	12.950416
81.H	-1.144738	5.437168	13.868239
82.C	-0.829875	4.212171	10.041132
83.H	-1.257327	3.444565	9.377029
84.H	0.232151	3.950783	10.189668
85.H	-0.856419	5.178128	9.513134
86.C	-1.651088	2.514340	12.465996
87.H	-2.134031	1.774624	11.806396
88.N	-5.492103	4.795501	3.867501
89.N	-2.232133	2.585289	4.977608
90.O	-5.357296	1.737059	5.346708
91.H	-2.172144	2.485079	13.437646
92.C	-5.071263	0.823545	4.227756
93.H	-4.756262	1.420340	3.361989
94.H	-4.240211	0.182497	4.549753
95.H	-0.609196	2.190909	12.632655
96.C	-6.360443	0.045150	3.993906
97.H	-6.991332	0.562246	3.254487
98.H	-6.164428	-0.973226	3.630465
99.C	-7.840630	9.759271	10.549192
100.H	-8.314276	9.553398	11.523501
101.H	-8.491601	10.466737	10.006125
102.H	-6.883419	10.272220	10.742963
103.C	-6.721798	8.604101	7.930554
104.H	-5.675076	8.902321	8.103353

105.H	-7.233726	9.442712	7.428585	127.C	-1.794214	2.968394	3.704843
106.H	-6.719062	7.759916	7.224604	128.C	-1.989879	2.255149	2.463729
107.C	-9.327876	7.484680	9.145887	129.C	-1.010921	-0.170818	4.815375
108.H	-9.845459	7.164839	10.065999	130.H	-2.527667	1.315308	2.361417
109.H	-6.559950	-0.643654	6.053522	131.H	-0.359822	-0.879463	5.356747
110.C	-7.030354	0.081637	5.371014	132.H	-0.538367	0.035885	3.840722
111.H	-8.110327	-0.116933	5.335423	133.C	-4.471894	5.484841	7.410545
112.H	-9.956791	8.248139	8.655868	134.C	-3.348906	6.174464	6.817027
113.C	-6.720894	1.494718	5.823121	135.C	-3.525797	7.406932	6.117514
114.H	-6.721206	1.633594	6.909992	136.H	-4.533420	7.814732	6.024879
115.H	-7.394209	2.222823	5.345504	137.C	-2.456177	8.099001	5.584951
116.H	-9.271114	6.614198	8.471575	138.H	-2.639812	9.044039	5.069300
117.C	-4.710209	4.922068	2.708264	139.C	-1.142558	7.606267	5.691208
118.C	-4.722595	4.071934	1.539753	140.H	-0.304399	8.160640	5.269168
119.H	-5.326006	3.173446	1.428913	141.C	-0.944076	6.390297	6.334309
120.H	-3.178240	0.693062	7.263206	142.H	0.062512	5.977251	6.424501
121.H	-3.380641	3.757844	8.279993	143.C	-2.015265	5.675266	6.876432
122.H	-5.455893	5.826116	7.073936	144.H	-1.802744	4.742569	7.395149
123.H	-2.572924	6.478630	0.589267	145.Y	-4.087458	3.830924	5.360927
124.C	-3.774026	5.985445	2.423374	146.Fe	-2.757114	4.173654	2.216170
125.H	-8.239246	7.405511	2.743268	147.Si	-7.139890	5.342080	3.655514
126.H	-3.530332	6.790121	3.113923	148.Si	-1.246464	1.422915	5.821895

M U L L I K E N P O P U L A T I O N S

The survey below gives for each atom:
a) the total charge (Z minus electrons)
b) the net spin polarization (nr of electrons spin-A minus spin-B)
c) for each spin the atomic electron valence density (integrated) per L-value.

Atom	Charge	Spin density	S	P	D	F
1 H	0.0629		0.8786	0.0585	0.0000	0.0000
2 H	0.1144		0.8218	0.0638	0.0000	0.0000
3 C	-0.4914		1.3176	3.1501	0.0237	0.0000
4 H	0.0663		0.8734	0.0604	0.0000	0.0000
5 C	-0.0351		1.4082	2.5568	0.0701	0.0000
6 H	-0.0161		0.9544	0.0616	0.0000	0.0000
7 C	-0.0416		1.4114	2.5598	0.0704	0.0000
8 H	0.0490		0.8913	0.0597	0.0000	0.0000
9 H	-0.0186		0.9567	0.0619	0.0000	0.0000
10 C	-0.0829		1.4313	2.5847	0.0669	0.0000
11 H	0.0684		0.8678	0.0637	0.0000	0.0000
12 H	0.0823		0.8605	0.0571	0.0000	0.0000
13 C	-0.4907		1.3190	3.1478	0.0240	0.0000
14 H	0.0697		0.8722	0.0581	0.0000	0.0000
15 H	0.0500		0.8903	0.0597	0.0000	0.0000
16 Y	2.1734		0.2362	-0.0155	0.6058	0.0000
17 Fe	0.4689		0.2097	0.3481	6.9733	0.0000
18 Si	1.2451		0.8891	1.4806	0.3852	0.0000
19 Si	1.2500		0.8861	1.4767	0.3872	0.0000
20 N	-1.0406		1.8484	4.1551	0.0370	0.0000
21 N	-1.0356		1.8408	4.1579	0.0369	0.0000
22 O	-0.7638		1.9707	4.7246	0.0685	0.0000
23 C	-0.5786		1.4079	3.1468	0.0239	0.0000
24 H	0.0585		0.8808	0.0607	0.0000	0.0000
25 H	0.0777		0.8623	0.0600	0.0000	0.0000

26 C	-0.5745	1.4072	3.1434	0.0240	0.0000
27 H	0.0657	0.8722	0.0620	0.0000	0.0000
28 H	0.0657	0.8764	0.0579	0.0000	0.0000
29 H	0.1081	0.8289	0.0630	0.0000	0.0000
30 C	-0.4832	1.3006	3.1587	0.0238	0.0000
31 H	0.1012	0.8357	0.0631	0.0000	0.0000
32 C	-0.0354	1.4082	2.5571	0.0700	0.0000
33 H	0.0674	0.8749	0.0577	0.0000	0.0000
34 H	-0.0161	0.9544	0.0617	0.0000	0.0000
35 C	-0.0463	1.4126	2.5634	0.0703	0.0000
36 C	-0.6001	1.5122	3.0291	0.0588	0.0000
37 C	-0.2665	1.4898	2.6871	0.0895	0.0000
38 C	-0.1135	1.4260	2.6266	0.0608	0.0000
39 H	0.0770	0.8718	0.0512	0.0000	0.0000
40 C	-0.0723	1.3897	2.6176	0.0650	0.0000
41 H	0.0267	0.9198	0.0535	0.0000	0.0000
42 C	-0.0906	1.3821	2.6473	0.0613	0.0000
43 H	0.0174	0.9262	0.0564	0.0000	0.0000
44 C	-0.0897	1.4118	2.6121	0.0658	0.0000
45 H	0.0415	0.9066	0.0519	0.0000	0.0000
46 C	-0.2403	1.4739	2.7071	0.0593	0.0000
47 H	0.1157	0.8242	0.0601	0.0000	0.0000
48 C	0.0971	1.3751	2.4501	0.0777	0.0000
49 H	0.1671	0.7908	0.0421	0.0000	0.0000
50 H	0.1554	0.8122	0.0324	0.0000	0.0000
51 C	-0.1944	1.3354	2.8006	0.0584	0.0000
52 H	0.1145	0.8501	0.0354	0.0000	0.0000
53 H	0.0802	0.8724	0.0474	0.0000	0.0000
54 C	-0.1764	1.3163	2.8007	0.0594	0.0000
55 H	0.0823	0.8703	0.0473	0.0000	0.0000
56 H	0.0967	0.8669	0.0365	0.0000	0.0000
57 C	0.1141	1.3642	2.4424	0.0793	0.0000
58 H	0.2166	0.7365	0.0469	0.0000	0.0000
59 H	0.1295	0.8375	0.0330	0.0000	0.0000
60 C	0.0458	1.3665	2.4679	0.1198	0.0000
61 C	-0.0932	1.4255	2.6005	0.0671	0.0000
62 H	0.0064	0.9326	0.0609	0.0000	0.0000
63 C	-0.0356	1.4082	2.5573	0.0700	0.0000
64 H	-0.0162	0.9545	0.0617	0.0000	0.0000
65 C	-0.0464	1.4127	2.5634	0.0703	0.0000
66 H	-0.0183	0.9566	0.0617	0.0000	0.0000
67 C	-0.0746	1.4265	2.5813	0.0669	0.0000
68 H	0.0548	0.8833	0.0619	0.0000	0.0000
69 C	0.0618	1.3635	2.4544	0.1203	0.0000
70 C	-0.0833	1.4179	2.5982	0.0672	0.0000
71 H	0.0055	0.9324	0.0621	0.0000	0.0000
72 C	-0.0353	1.4081	2.5571	0.0701	0.0000
73 H	-0.0162	0.9545	0.0617	0.0000	0.0000
74 C	-0.0416	1.4114	2.5599	0.0704	0.0000
75 H	-0.0187	0.9568	0.0619	0.0000	0.0000
76 C	-0.0830	1.4315	2.5846	0.0669	0.0000
77 H	0.0688	0.8674	0.0638	0.0000	0.0000
78 C	-0.4906	1.3192	3.1474	0.0240	0.0000
79 H	0.0694	0.8723	0.0582	0.0000	0.0000
80 H	0.0499	0.8904	0.0597	0.0000	0.0000
81 H	0.0658	0.8721	0.0621	0.0000	0.0000

82 C	-0.5739	1.4067	3.1432	0.0240	0.0000
83 H	0.1078	0.8292	0.0629	0.0000	0.0000
84 H	0.0655	0.8766	0.0579	0.0000	0.0000
85 H	0.1011	0.8358	0.0631	0.0000	0.0000
86 C	-0.4831	1.3005	3.1587	0.0238	0.0000
87 H	0.0673	0.8750	0.0577	0.0000	0.0000
88 N	-1.0406	1.8482	4.1554	0.0370	0.0000
89 N	-1.0358	1.8409	4.1579	0.0369	0.0000
90 O	-0.7640	1.9706	4.7249	0.0685	0.0000
91 H	0.0777	0.8623	0.0600	0.0000	0.0000
92 C	0.0969	1.3752	2.4502	0.0777	0.0000
93 H	0.1668	0.7912	0.0420	0.0000	0.0000
94 H	0.1559	0.8118	0.0324	0.0000	0.0000
95 H	0.0500	0.8898	0.0602	0.0000	0.0000
96 C	-0.1944	1.3353	2.8007	0.0584	0.0000
97 H	0.1144	0.8502	0.0354	0.0000	0.0000
98 H	0.0804	0.8723	0.0474	0.0000	0.0000
99 C	-0.4890	1.3082	3.1568	0.0240	0.0000
100 H	0.0693	0.8693	0.0614	0.0000	0.0000
101 H	0.0498	0.8902	0.0599	0.0000	0.0000
102 H	0.0586	0.8807	0.0607	0.0000	0.0000
103 C	-0.5787	1.4082	3.1466	0.0239	0.0000
104 H	0.1064	0.8367	0.0569	0.0000	0.0000
105 H	0.0631	0.8784	0.0585	0.0000	0.0000
106 H	0.1149	0.8213	0.0637	0.0000	0.0000
107 C	-0.4914	1.3177	3.1499	0.0237	0.0000
108 H	0.0663	0.8734	0.0604	0.0000	0.0000
109 H	0.0969	0.8666	0.0364	0.0000	0.0000
110 C	-0.1763	1.3163	2.8006	0.0594	0.0000
111 H	0.0824	0.8703	0.0473	0.0000	0.0000
112 H	0.0489	0.8914	0.0597	0.0000	0.0000
113 C	0.1143	1.3638	2.4426	0.0793	0.0000
114 H	0.2167	0.7365	0.0468	0.0000	0.0000
115 H	0.1292	0.8378	0.0330	0.0000	0.0000
116 H	0.0822	0.8607	0.0571	0.0000	0.0000
117 C	0.0464	1.3664	2.4674	0.1198	0.0000
118 C	-0.0927	1.4253	2.6003	0.0671	0.0000
119 H	0.0063	0.9327	0.0610	0.0000	0.0000
120 H	0.1068	0.8362	0.0570	0.0000	0.0000
121 H	0.1260	0.8125	0.0615	0.0000	0.0000
122 H	0.1261	0.8125	0.0615	0.0000	0.0000
123 H	-0.0182	0.9565	0.0617	0.0000	0.0000
124 C	-0.0749	1.4264	2.5817	0.0668	0.0000
125 H	0.0501	0.8898	0.0602	0.0000	0.0000
126 H	0.0547	0.8835	0.0618	0.0000	0.0000
127 C	0.0618	1.3634	2.4545	0.1203	0.0000
128 C	-0.0832	1.4180	2.5980	0.0672	0.0000
129 C	-0.4890	1.3082	3.1568	0.0240	0.0000
130 H	0.0057	0.9323	0.0620	0.0000	0.0000
131 H	0.0500	0.8901	0.0599	0.0000	0.0000
132 H	0.0694	0.8692	0.0614	0.0000	0.0000
133 C	-0.6021	1.5133	3.0299	0.0588	0.0000
134 C	-0.2649	1.4895	2.6860	0.0894	0.0000
135 C	-0.1132	1.4259	2.6265	0.0609	0.0000
136 H	0.0769	0.8719	0.0512	0.0000	0.0000
137 C	-0.0720	1.3897	2.6172	0.0650	0.0000

138 H	0.0267	0.9198	0.0535	0.0000	0.0000
139 C	-0.0903	1.3822	2.6468	0.0613	0.0000
140 H	0.0175	0.9261	0.0564	0.0000	0.0000
141 C	-0.0895	1.4115	2.6122	0.0658	0.0000
142 H	0.0412	0.9068	0.0519	0.0000	0.0000
143 C	-0.2376	1.4736	2.7046	0.0593	0.0000
144 H	0.1153	0.8247	0.0600	0.0000	0.0000
145 Y	2.1691	0.2374	-0.0145	0.6080	0.0000
146 Fe	0.4684	0.2096	0.3486	6.9733	0.0000
147 Si	1.2455	0.8888	1.4805	0.3852	0.0000
148 Si	1.2501	0.8860	1.4767	0.3872	0.0000

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B O N D - O R D E R A N A L Y S I S

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DIST. [A] BOND-ORDERS (THRESHOLD = 0.200)

				MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
H	1 - C	23	1.1033	1.0244	0.9436	1.0109	1.0592	1.0229
H	2 - C	23	1.1005	0.9090	0.9497	1.0064	1.0370	1.0325
C	3 - H	4	1.1031	1.0028	0.9450	1.0110	1.0584	1.0257
C	3 - H	8	1.1039	1.0104	0.9452	1.0113	1.0562	1.0279
C	3 - H	12	1.1026	0.9772	0.9497	1.0120	1.0511	1.0331
C	3 - Si	148	1.8959	0.8320	0.8620	0.9173	1.6431	0.8701
C	5 - H	6	1.0875	1.0897	0.9254	0.9712	0.9931	0.9154
C	5 - C	7	1.4325	1.0877	1.2475	1.2904	1.2095	1.3682
C	5 - C	128	1.4279	1.1062	1.2614	1.3039	1.2139	1.3868
C	5 - Fe	146	2.0613	0.3935	0.3493	0.4840	0.6248	0.4632
C	7 - H	9	1.0874	1.0922	0.9250	0.9710	0.9932	0.9152
C	7 - C	10	1.4264	1.1003	1.2649	1.3070	1.2193	1.3890
C	7 - Fe	146	2.0620	0.3933	0.3460	0.4796	0.6216	0.4590
C	10 - H	11	1.0873	1.0285	0.9192	0.9589	0.9834	0.9060
C	10 - C	127	1.4466	1.0764	1.1803	1.2114	1.2119	1.2449
C	10 - Fe	146	2.0858	0.3944	0.3467	0.4801	0.6339	0.4603
C	13 - H	14	1.1033	0.9807	0.9527	1.0135	1.0469	1.0387
C	13 - H	15	1.1044	1.0109	0.9445	1.0105	1.0556	1.0268
C	13 - H	27	1.1024	1.0025	0.9464	1.0111	1.0561	1.0276
C	13 - Si	147	1.9014	0.8301	0.8519	0.9064	1.6345	0.8597
Y	16 - N	20	2.2658	0.5444	0.7158	0.8821	1.4723	0.8402
Y	16 - N	21	2.2677	0.5352	0.6878	0.8485	1.4474	0.8084
Y	16 - O	22	2.4501	0.1907	0.3067	0.3864	0.7236	0.3576
Y	16 - C	36	2.6623	0.0198	0.1908	0.2258	0.6303	0.2026
Y	16 - C	133	2.6243	0.1037	0.2744	0.3248	0.7124	0.2914
Fe	17 - C	60	2.1482	0.3826	0.2689	0.3708	0.3309	0.3452
Fe	17 - C	61	2.0808	0.3872	0.3475	0.4814	0.6431	0.4621
Fe	17 - C	63	2.0609	0.3911	0.3470	0.4810	0.6230	0.4604
Fe	17 - C	65	2.0609	0.3908	0.3445	0.4775	0.6204	0.4571
Fe	17 - C	67	2.0874	0.3923	0.3463	0.4795	0.6329	0.4597
Fe	17 - C	69	2.1435	0.3761	0.2704	0.3729	0.3284	0.3470
Fe	17 - C	70	2.0811	0.3899	0.3478	0.4818	0.6412	0.4624
Fe	17 - C	72	2.0612	0.3938	0.3493	0.4840	0.6250	0.4633
Fe	17 - C	74	2.0619	0.3907	0.3460	0.4795	0.6216	0.4590
Fe	17 - C	76	2.0855	0.3859	0.3467	0.4801	0.6339	0.4603

Si	18 - N	20	1.7491	0.9646	0.9107	1.0093	1.6083	0.9671
Si	18 - C	78	1.9015	0.8288	0.8517	0.9062	1.6341	0.8595
Si	18 - C	82	1.8907	0.8405	0.8767	0.9331	1.6327	0.8824
Si	18 - C	86	1.8930	0.8371	0.8712	0.9269	1.6498	0.8790
Si	19 - N	21	1.7422	0.9698	0.9154	1.0159	1.6146	0.9737
Si	19 - C	99	1.8996	0.8216	0.8593	0.9143	1.6389	0.8671
Si	19 - C	103	1.8916	0.8425	0.8765	0.9330	1.6371	0.8830
Si	19 - C	107	1.8961	0.8326	0.8618	0.9171	1.6429	0.8700
N	20 - C	60	1.4042	1.0485	1.1280	1.2357	1.1678	1.3608
N	21 - C	69	1.3994	1.0432	1.1330	1.2428	1.1790	1.3676
O	22 - C	48	1.4725	0.7791	0.9092	1.0313	0.9685	1.1150
O	22 - C	57	1.4646	0.7723	0.9133	1.0368	0.9767	1.1201
C	23 - H	120	1.1020	0.9438	0.9453	1.0069	1.0488	1.0243
C	23 - Si	148	1.8916	0.8385	0.8765	0.9331	1.6372	0.8830
H	24 - C	129	1.1032	0.9888	0.9524	1.0139	1.0481	1.0383
H	25 - C	30	1.1029	0.9975	0.9443	1.0099	1.0585	1.0238
C	26 - H	28	1.1038	1.0218	0.9419	1.0090	1.0590	1.0192
C	26 - H	29	1.1013	0.9217	0.9490	1.0064	1.0393	1.0303
C	26 - H	31	1.1012	0.9459	0.9468	1.0055	1.0418	1.0269
C	26 - Si	147	1.8907	0.8367	0.8767	0.9331	1.6327	0.8824
C	30 - H	33	1.1025	0.9913	0.9482	1.0130	1.0559	1.0310
C	30 - H	125	1.1035	1.0104	0.9457	1.0118	1.0566	1.0283
C	30 - Si	147	1.8930	0.8356	0.8711	0.9268	1.6500	0.8790
C	32 - H	34	1.0876	1.0908	0.9254	0.9712	0.9933	0.9156
C	32 - C	35	1.4328	1.0870	1.2492	1.2924	1.2106	1.3707
C	32 - C	118	1.4285	1.1028	1.2609	1.3035	1.2117	1.3872
C	32 - Fe	146	2.0610	0.3833	0.3470	0.4809	0.6228	0.4603
C	35 - H	123	1.0874	1.0938	0.9249	0.9711	0.9935	0.9153
C	35 - C	124	1.4268	1.1040	1.2636	1.3057	1.2177	1.3878
C	35 - Fe	146	2.0612	0.3897	0.3444	0.4773	0.6203	0.4570
C	36 - C	37	1.4448	1.2194	1.1893	1.2500	1.2099	1.3173
C	36 - H	121	1.0944	0.9170	0.9015	0.9479	0.9790	0.9274
C	36 - C	133	1.4866	1.0969	1.0485	1.1248	0.9157	1.2341
C	36 - Y	145	2.6231	0.1138	0.2737	0.3240	0.7111	0.2906
C	37 - C	38	1.4285	1.2032	1.2520	1.2930	1.2798	1.3293
C	37 - C	46	1.4256	1.2339	1.2638	1.3096	1.2898	1.3559
C	38 - H	39	1.0909	0.9837	0.9231	0.9617	0.9766	0.9072
C	38 - C	40	1.3807	1.3649	1.5234	1.5784	1.5294	1.6505
C	40 - H	41	1.0921	1.0495	0.9248	0.9694	0.9829	0.9098
C	40 - C	42	1.4072	1.1936	1.3472	1.3993	1.3431	1.4689
C	42 - H	43	1.0899	1.0563	0.9285	0.9756	0.9947	0.9222
C	42 - C	44	1.3897	1.2856	1.4488	1.5044	1.4508	1.5769
C	44 - H	45	1.0918	1.0314	0.9236	0.9665	0.9784	0.9053
C	44 - C	46	1.3976	1.2924	1.4164	1.4720	1.4122	1.5475
C	46 - H	47	1.0883	0.9199	0.9192	0.9557	0.9764	0.9136
C	48 - H	49	1.0976	0.8780	0.9149	0.9560	0.9574	0.8867
C	48 - H	50	1.0978	0.8860	0.9204	0.9618	0.9636	0.8958
C	48 - C	51	1.5240	0.9133	1.0134	1.0543	1.0095	1.1079
C	51 - H	52	1.1010	0.9425	0.9264	0.9677	0.9957	0.9277
C	51 - H	53	1.0989	1.0194	0.9257	0.9730	1.0033	0.9249
C	51 - C	54	1.5319	0.9428	1.0059	1.0443	0.9170	1.1253
C	54 - H	55	1.0987	1.0156	0.9245	0.9722	1.0023	0.9233
C	54 - H	56	1.1014	0.9631	0.9239	0.9663	0.9942	0.9253
C	54 - C	57	1.5156	0.9106	1.0188	1.0610	1.0193	1.1134
C	57 - H	58	1.0957	0.8974	0.9141	0.9601	0.9590	0.8818
C	57 - H	59	1.1007	0.8722	0.9195	0.9577	0.9596	0.8992

C	60 - C	61	1.4451	1.0861	1.1840	1.2158	1.2139	1.2522
C	60 - C	67	1.4452	1.0853	1.1827	1.2136	1.2124	1.2480
C	61 - H	62	1.0880	1.0575	0.9258	0.9660	0.9909	0.9180
C	61 - C	63	1.4285	1.1021	1.2609	1.3034	1.2116	1.3872
C	63 - H	64	1.0876	1.0897	0.9254	0.9712	0.9934	0.9156
C	63 - C	65	1.4328	1.0908	1.2493	1.2925	1.2106	1.3709
C	65 - H	66	1.0874	1.0948	0.9250	0.9711	0.9935	0.9154
C	65 - C	67	1.4268	1.1059	1.2634	1.3055	1.2176	1.3875
C	67 - H	68	1.0880	1.0415	0.9198	0.9606	0.9852	0.9068
C	69 - C	70	1.4447	1.0843	1.1848	1.2168	1.2169	1.2516
C	69 - C	76	1.4467	1.0750	1.1803	1.2114	1.2119	1.2448
C	70 - H	71	1.0876	1.0654	0.9263	0.9662	0.9906	0.9184
C	70 - C	72	1.4279	1.1021	1.2614	1.3039	1.2138	1.3869
C	72 - H	73	1.0875	1.0897	0.9254	0.9712	0.9932	0.9155
C	72 - C	74	1.4325	1.0833	1.2476	1.2905	1.2096	1.3684
C	74 - H	75	1.0874	1.0944	0.9250	0.9710	0.9932	0.9152
C	74 - C	76	1.4264	1.0985	1.2648	1.3069	1.2192	1.3890
C	76 - H	77	1.0873	1.0296	0.9191	0.9588	0.9833	0.9060
C	78 - H	79	1.1033	0.9805	0.9527	1.0134	1.0468	1.0388
C	78 - H	80	1.1044	1.0113	0.9445	1.0104	1.0556	1.0268
C	78 - H	81	1.1024	1.0013	0.9465	1.0111	1.0560	1.0276
C	82 - H	83	1.1013	0.9216	0.9490	1.0065	1.0394	1.0304
C	82 - H	84	1.1038	1.0207	0.9419	1.0090	1.0590	1.0193
C	82 - H	85	1.1012	0.9467	0.9468	1.0055	1.0419	1.0268
C	86 - H	87	1.1025	0.9914	0.9482	1.0130	1.0559	1.0310
C	86 - H	91	1.1029	0.9975	0.9443	1.0100	1.0585	1.0238
C	86 - H	95	1.1036	1.0106	0.9457	1.0118	1.0565	1.0283
N	88 - C	117	1.4040	1.0538	1.1283	1.2361	1.1682	1.3613
N	88 - Y	145	2.2658	0.5619	0.7152	0.8815	1.4723	0.8396
N	88 - Si	147	1.7490	0.9638	0.9106	1.0094	1.6086	0.9672
N	89 - C	127	1.3995	1.0491	1.1329	1.2427	1.1790	1.3676
N	89 - Y	145	2.2673	0.5340	0.6882	0.8492	1.4482	0.8090
N	89 - Si	148	1.7423	0.9646	0.9151	1.0155	1.6144	0.9733
O	90 - C	92	1.4725	0.7767	0.9092	1.0312	0.9684	1.1149
O	90 - C	113	1.4646	0.7710	0.9132	1.0366	0.9764	1.1199
O	90 - Y	145	2.4489	0.1894	0.3073	0.3873	0.7243	0.3583
C	92 - H	93	1.0977	0.8766	0.9149	0.9561	0.9575	0.8868
C	92 - H	94	1.0978	0.8860	0.9203	0.9618	0.9636	0.8958
C	92 - C	96	1.5240	0.9113	1.0134	1.0543	1.0095	1.1079
C	96 - H	97	1.1010	0.9427	0.9264	0.9677	0.9957	0.9277
C	96 - H	98	1.0989	1.0191	0.9256	0.9730	1.0034	0.9249
C	96 - C	110	1.5318	0.9444	1.0059	1.0443	0.9170	1.1253
C	99 - H	100	1.1027	1.0025	0.9451	1.0105	1.0577	1.0252
C	99 - H	101	1.1042	1.0120	0.9448	1.0109	1.0563	1.0269
C	99 - H	102	1.1031	0.9890	0.9524	1.0139	1.0481	1.0383
C	103 - H	104	1.1020	0.9446	0.9453	1.0070	1.0490	1.0244
C	103 - H	105	1.1033	1.0256	0.9436	1.0109	1.0592	1.0229
C	103 - H	106	1.1005	0.9087	0.9496	1.0063	1.0369	1.0325
C	107 - H	108	1.1031	1.0051	0.9451	1.0110	1.0584	1.0257
C	107 - H	112	1.1039	1.0110	0.9452	1.0113	1.0562	1.0279
C	107 - H	116	1.1026	0.9767	0.9498	1.0120	1.0510	1.0332
H	109 - C	110	1.1014	0.9626	0.9238	0.9663	0.9942	0.9252
C	110 - H	111	1.0987	1.0152	0.9245	0.9722	1.0022	0.9232
C	110 - C	113	1.5156	0.9104	1.0188	1.0611	1.0194	1.1135
C	113 - H	114	1.0957	0.8975	0.9141	0.9601	0.9591	0.8818
C	113 - H	115	1.1007	0.8727	0.9195	0.9577	0.9596	0.8992

C	117 - C	118	1.4451	1.0798	1.1840	1.2158	1.2139	1.2521
C	117 - C	124	1.4451	1.0771	1.1827	1.2137	1.2125	1.2481
C	117 - Fe	146	2.1487	0.3811	0.2685	0.3703	0.3303	0.3448
C	118 - H	119	1.0880	1.0579	0.9258	0.9660	0.9909	0.9180
C	118 - Fe	146	2.0811	0.3806	0.3474	0.4812	0.6429	0.4619
H	122 - C	133	1.0945	0.9258	0.9012	0.9475	0.9786	0.9273
C	124 - H	126	1.0880	1.0396	0.9198	0.9606	0.9852	0.9068
C	124 - Fe	146	2.0880	0.3916	0.3460	0.4791	0.6326	0.4593
C	127 - C	128	1.4448	1.0864	1.1846	1.2166	1.2167	1.2514
C	127 - Fe	146	2.1438	0.3776	0.2702	0.3726	0.3281	0.3467
C	128 - H	130	1.0877	1.0654	0.9263	0.9662	0.9906	0.9183
C	128 - Fe	146	2.0810	0.3899	0.3480	0.4820	0.6413	0.4625
C	129 - H	131	1.1042	1.0119	0.9448	1.0109	1.0563	1.0269
C	129 - H	132	1.1027	1.0027	0.9451	1.0105	1.0577	1.0252
C	129 - Si	148	1.8996	0.8235	0.8593	0.9144	1.6390	0.8671
C	133 - C	134	1.4453	1.2117	1.1878	1.2485	1.2084	1.3158
C	133 - Y	145	2.6616	0.0234	0.1914	0.2266	0.6319	0.2033
C	134 - C	135	1.4281	1.2074	1.2534	1.2945	1.2813	1.3308
C	134 - C	143	1.4252	1.2337	1.2654	1.3112	1.2916	1.3573
C	135 - H	136	1.0910	0.9842	0.9231	0.9617	0.9767	0.9072
C	135 - C	137	1.3808	1.3640	1.5223	1.5774	1.5283	1.6494
C	137 - H	138	1.0921	1.0496	0.9248	0.9695	0.9830	0.9098
C	137 - C	139	1.4070	1.1942	1.3483	1.4005	1.3443	1.4701
C	139 - H	140	1.0899	1.0564	0.9285	0.9756	0.9947	0.9222
C	139 - C	141	1.3898	1.2846	1.4480	1.5035	1.4500	1.5760
C	141 - H	142	1.0918	1.0316	0.9237	0.9666	0.9785	0.9055
C	141 - C	143	1.3974	1.2962	1.4175	1.4731	1.4135	1.5486
C	143 - H	144	1.0882	0.9219	0.9195	0.9559	0.9765	0.9137
Sum :			157.0638	168.0680	180.6360	180.6360	180.6360	

List of selected MOs, ordered by energy, with the most significant SFO gross populations

Each percentage contribution in the table below corresponds to the indicated SFO. In general, a SFO may be a linear combination of several Fragment Orbitals on the same, or on symmetry-related Fragments. Only the first 'member' of such a combination is specified here. A full definition of all SFOs is given in an earlier part of the output. The numbering of the SFOs in this table does NOT include the Core Orbitals, and starts from one for each symmetry representation, as in the SFO definition list earlier.

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-4.430	2.00	179 A	23.46%	1 D:yz	-7.682	1.20	138 Fe
			14.12%	1 D:z2	-7.682	1.20	138 Fe
			9.80%	1 D:xy	-7.682	1.20	138 Fe
			8.94%	1 D:yz	-7.682	1.20	137 Fe
			5.68%	1 D:z2	-7.682	1.20	137 Fe
			4.18%	1 D:xy	-7.682	1.20	137 Fe
			3.11%	1 D:xz	-7.682	1.20	138 Fe
			1.81%	1 P:y	-7.403	1.00	145 N
			1.52%	1 P:x	-5.608	0.67	124 C
			1.25%	1 D:yz	-2.564	0.20	136 Y
			1.17%	1 P:x	-5.608	0.67	83 C
			1.14%	1 D:xz	-7.682	1.20	137 Fe
			1.05%	1 P:x	-5.608	0.67	89 C
			1.03%	1 P:y	-7.403	1.00	146 N
-4.416	2.00	180 A	25.33%	1 D:yz	-7.682	1.20	137 Fe

			13.31%	1 D:z2	-7.682	1.20	137	Fe
			10.38%	1 D:yz	-7.682	1.20	138	Fe
			8.54%	1 D:xy	-7.682	1.20	137	Fe
			5.04%	1 D:z2	-7.682	1.20	138	Fe
			3.62%	1 D:xz	-7.682	1.20	137	Fe
			3.09%	1 D:xy	-7.682	1.20	138	Fe
			1.62%	1 P:y	-7.403	1.00	143	N
			1.56%	1 P:x	-5.608	0.67	106	C
			1.53%	1 D:xz	-7.682	1.20	138	Fe
			1.29%	1 P:y	-7.403	1.00	144	N
			1.14%	1 P:x	-5.608	0.67	110	C
			1.04%	1 P:x	-5.608	0.67	104	C
-4.309	2.00	181 A	13.36%	1 D:yz	-7.682	1.20	138	Fe
			9.33%	1 D:xz	-7.682	1.20	138	Fe
			8.57%	1 D:z2	-7.682	1.20	138	Fe
			8.53%	1 D:yz	-7.682	1.20	137	Fe
			7.55%	1 D:xy	-7.682	1.20	138	Fe
			6.85%	1 D:x2-y2	-7.682	1.20	138	Fe
			5.63%	1 D:xz	-7.682	1.20	137	Fe
			4.78%	1 D:z2	-7.682	1.20	137	Fe
			4.60%	1 D:xy	-7.682	1.20	137	Fe
			4.28%	1 D:x2-y2	-7.682	1.20	137	Fe
			1.33%	1 P:x	-5.608	0.67	125	C
			1.30%	1 P:y	-7.403	1.00	145	N
-4.285	2.00	182 A	11.71%	1 D:z2	-7.682	1.20	137	Fe
			11.22%	1 D:yz	-7.682	1.20	137	Fe
			9.51%	1 D:xz	-7.682	1.20	137	Fe
			7.59%	1 D:z2	-7.682	1.20	138	Fe
			7.58%	1 D:xy	-7.682	1.20	137	Fe
			6.75%	1 D:yz	-7.682	1.20	138	Fe
			6.49%	1 D:x2-y2	-7.682	1.20	137	Fe
			6.01%	1 D:xz	-7.682	1.20	138	Fe
			4.68%	1 D:xy	-7.682	1.20	138	Fe
			3.85%	1 D:x2-y2	-7.682	1.20	138	Fe
			1.52%	1 P:x	-5.608	0.67	107	C
			1.34%	1 P:y	-7.403	1.00	143	N
			1.16%	1 P:x	-7.403	1.00	144	N
-3.862	2.00	183 A	12.64%	1 P:z	-5.608	0.67	128	C
			12.60%	1 P:z	-5.608	0.67	91	C
			5.03%	1 P:z	-5.608	0.67	132	C
			5.02%	1 P:z	-5.608	0.67	95	C
			4.75%	1 P:z	-5.608	0.67	97	C
			4.71%	1 P:z	-5.608	0.67	134	C
			4.56%	1 P:y	-5.608	0.67	128	C
			4.52%	1 P:y	-5.608	0.67	91	C
			3.16%	1 P:z	-5.608	0.67	93	C
			3.15%	1 P:z	-5.608	0.67	130	C
			2.19%	1 D:z2	-7.682	1.20	137	Fe
			2.14%	1 D:z2	-7.682	1.20	138	Fe
			1.84%	1 D:yz	-2.564	0.20	136	Y
			1.80%	1 D:yz	-2.564	0.20	135	Y
			1.64%	1 P:x	-7.403	1.00	144	N
			1.59%	1 P:x	-7.403	1.00	146	N
			1.57%	1 P:y	-5.608	0.67	95	C
			1.57%	1 P:y	-5.608	0.67	132	C
			1.46%	1 P:y	-5.608	0.67	97	C

			1.44%	1 P:y	-5.608	0.67	134	C
			1.34%	1 D:z2	-2.564	0.20	136	Y
			1.33%	1 D:z2	-2.564	0.20	135	Y
			1.15%	1 P:y	-5.608	0.67	93	C
			1.12%	1 P:y	-5.608	0.67	130	C
-1.917	0.00	184 A	8.25%	1 P:z	-5.608	0.67	96	C
			7.83%	1 P:z	-5.608	0.67	93	C
			7.80%	1 P:z	-5.608	0.67	133	C
			7.65%	1 D:xz	-2.564	0.20	136	Y
			7.64%	1 D:xz	-2.564	0.20	135	Y
			7.50%	1 P:z	-5.608	0.67	130	C
			3.72%	1 P:z	-5.608	0.67	94	C
			3.22%	1 P:z	-5.608	0.67	131	C
			2.71%	1 P:y	-5.608	0.67	93	C
			2.60%	1 P:y	-5.608	0.67	130	C
			2.38%	1 P:y	-5.608	0.67	96	C
			2.25%	1 P:y	-5.608	0.67	133	C
			1.94%	1 P:x	-1.145	0.00	135	Y
			1.93%	1 P:x	-1.145	0.00	136	Y
			1.81%	1 P:z	-5.608	0.67	97	C
			1.76%	1 P:z	-5.608	0.67	132	C
			1.69%	1 P:z	-5.608	0.67	95	C
			1.49%	1 P:z	-5.608	0.67	134	C
			1.23%	1 P:y	-5.608	0.67	94	C
			1.05%	1 P:y	-5.608	0.67	131	C
-1.816	0.00	185 A	7.63%	1 P:z	-5.608	0.67	131	C
			7.33%	1 P:z	-5.608	0.67	94	C
			7.16%	1 P:z	-5.608	0.67	134	C
			6.94%	1 P:z	-5.608	0.67	97	C
			5.21%	1 D:x2-y2	-2.564	0.20	135	Y
			5.12%	1 D:x2-y2	-2.564	0.20	136	Y
			3.44%	1 P:z	-5.608	0.67	133	C
			3.09%	1 P:z	-5.608	0.67	96	C
			2.52%	1 P:y	-5.608	0.67	131	C
			2.44%	1 P:y	-5.608	0.67	94	C
			2.30%	1 P:y	-5.608	0.67	134	C
			2.26%	1 P:y	-5.608	0.67	97	C
			2.20%	1 P:z	-5.608	0.67	130	C
			1.93%	1 P:z	-5.608	0.67	93	C
			1.77%	1 P:z	-5.608	0.67	92	C
			1.75%	1 D:xz	-7.682	1.20	138	Fe
			1.66%	1 P:z	-5.608	0.67	129	C
			1.53%	1 D:xz	-7.682	1.20	137	Fe
			1.27%	1 D:yz	-7.682	1.20	138	Fe
			1.12%	1 D:z2	-7.682	1.20	138	Fe
			1.08%	1 D:yz	-7.682	1.20	137	Fe
			1.06%	1 P:z	-5.608	0.67	95	C
			1.02%	1 P:y	-5.608	0.67	133	C
			1.01%	1 D:z2	-7.682	1.20	137	Fe
-1.694	0.00	186 A	30.79%	1 D:x2-y2	-7.682	1.20	138	Fe
			10.72%	1 D:xz	-7.682	1.20	138	Fe
			10.34%	1 D:xy	-7.682	1.20	138	Fe
			4.53%	1 P:x	-5.608	0.67	84	C
			4.18%	1 P:x	-5.608	0.67	123	C
			4.07%	1 P:x	-5.608	0.67	126	C
			3.97%	1 P:x	-5.608	0.67	124	C

			2.57%	1 P:x	-5.608	0.67	82	C
			2.14%	1 P:y	-5.608	0.67	124	C
			2.04%	1 D:z2	-7.682	1.20	138	Fe
			1.88%	1 P:y	-5.608	0.67	126	C
			1.63%	1 P:y	-5.608	0.67	84	C
			1.62%	1 P:y	-5.608	0.67	123	C
			1.52%	1 P:x	-5.608	0.67	83	C
			1.35%	1 P:y	-5.608	0.67	89	C
			1.21%	1 P:x	-5.608	0.67	90	C
			1.03%	1 P:x	-5.608	0.67	89	C
-1.687	0.00	187 A	31.72%	1 D:x2-y2	-7.682	1.20	137	Fe
			10.30%	1 D:xy	-7.682	1.20	137	Fe
			9.86%	1 D:xz	-7.682	1.20	137	Fe
			4.49%	1 P:x	-5.608	0.67	111	C
			4.15%	1 P:x	-5.608	0.67	108	C
			4.15%	1 P:x	-5.608	0.67	103	C
			3.94%	1 P:x	-5.608	0.67	106	C
			2.35%	1 P:x	-5.608	0.67	109	C
			2.02%	1 P:y	-5.608	0.67	106	C
			1.95%	1 P:y	-5.608	0.67	108	C
			1.75%	1 D:z2	-7.682	1.20	137	Fe
			1.74%	1 P:x	-5.608	0.67	110	C
			1.65%	1 P:y	-5.608	0.67	103	C
			1.60%	1 P:y	-5.608	0.67	111	C
			1.38%	1 D:x2-y2	-7.682	1.20	138	Fe
			1.34%	1 P:x	-5.608	0.67	105	C
			1.28%	1 P:y	-5.608	0.67	104	C
-1.648	0.00	188 A	9.94%	1 D:xz	-7.682	1.20	138	Fe
			8.76%	1 D:x2-y2	-7.682	1.20	138	Fe
			8.63%	1 D:yz	-7.682	1.20	138	Fe
			5.39%	1 D:x2-y2	-7.682	1.20	137	Fe
			4.99%	1 D:z2	-7.682	1.20	138	Fe
			4.10%	1 D:yz	-7.682	1.20	137	Fe
			4.01%	1 D:xz	-7.682	1.20	137	Fe
			2.97%	1 P:x	-5.608	0.67	83	C
			2.89%	1 P:x	-5.608	0.67	125	C
			2.30%	1 P:x	-5.608	0.67	89	C
			2.18%	1 D:z2	-7.682	1.20	137	Fe
			2.16%	1 P:x	-5.608	0.67	122	C
			2.08%	1 P:x	-5.608	0.67	90	C
			1.77%	1 P:x	-5.608	0.67	82	C
			1.61%	1 P:x	-5.608	0.67	110	C
			1.56%	1 P:y	-5.608	0.67	90	C
			1.45%	1 P:y	-5.608	0.67	82	C
			1.36%	1 P:x	-5.608	0.67	107	C
			1.21%	1 P:y	-5.608	0.67	122	C
			1.13%	1 P:x	-5.608	0.67	105	C
			1.05%	1 P:y	-5.608	0.67	125	C
			1.01%	1 P:x	-5.608	0.67	102	C

Optimized parameters for **La_2-stilbene**

Atom	X	Y	Z (Angstrom)
1.La	12.007158	9.462224	5.320762
2.Fe	10.629211	9.674745	2.144844
3.Si	9.081320	6.958035	5.811820
4.Si	15.119412	10.826302	3.469729
5.N	10.039299	8.140928	4.972746
6.N	13.459295	10.334381	3.633410
7.O	13.564282	7.329275	5.319237
8.H	11.284822	9.434257	8.411142
9.H	11.663297	12.179912	14.435154
10.C	11.465003	11.838049	6.959877
11.C	10.085021	11.465538	7.030458
12.H	9.781944	10.595189	7.612467
13.C	9.089270	12.241293	6.432105
14.H	8.048728	11.927482	6.535846
15.C	9.398626	13.394420	5.718145
16.H	8.617080	13.992067	5.250038
17.C	10.753432	13.756382	5.597179
18.H	11.027248	14.644832	5.024369
19.C	11.752473	13.005825	6.184412
20.H	12.793913	13.312682	6.071947
21.C	13.735281	6.679675	4.015948
22.H	14.583186	7.165982	3.512020
23.H	12.821339	6.840786	3.427874
24.C	14.015750	5.217811	4.327356
25.H	13.071903	4.664105	4.450559
26.H	14.605319	4.731649	3.537665
27.C	14.751684	5.313255	5.667823
28.H	15.793526	5.635544	5.512197
29.H	14.757649	4.370140	6.231388
30.C	13.966580	6.400362	6.379841
31.H	13.057445	5.995576	6.850318
32.H	14.544915	6.964026	7.122260
33.C	9.121159	5.263734	4.955192
34.H	10.149793	4.871925	4.884923
35.H	8.713379	5.324498	3.932419
36.H	8.517346	4.523573	5.508955
37.C	9.802755	6.758495	7.551490
38.H	10.883095	6.542374	7.536565
39.H	9.308674	5.924437	8.078239
40.H	9.643922	7.663422	8.158980
41.C	7.269691	7.487643	5.962621
42.H	6.828422	7.663809	4.967149
43.C	12.187497	10.368951	13.203959
44.C	13.141281	9.316755	13.476221
45.H	13.336329	8.475768	12.813550
46.H	6.664558	6.713647	6.465312
47.C	13.709084	9.527910	14.768396
48.H	14.432503	8.885520	15.264518
49.C	13.154391	10.737245	15.300198
50.H	7.172970	8.421320	6.540565
51.H	13.383084	11.171821	16.270454
52.C	12.304947	9.742954	8.166479
53.C	12.512111	11.058162	7.549105
54.C	16.100155	9.720940	2.275547
55.H	16.139250	8.675267	2.624039
56.H	17.141037	10.075952	2.176369
57.H	15.652271	9.724824	1.267876
58.C	15.913576	10.695123	5.182026
59.H	15.789468	9.692344	5.622680
60.H	15.485235	11.434697	5.877239
61.H	16.996674	10.896305	5.124403
62.C	15.270796	12.606987	2.844183
63.H	14.781921	12.720355	1.861991
64.H	9.172353	11.064512	14.453964
65.C	8.908210	10.101136	10.538180
66.H	9.029824	11.104997	10.099300
67.H	16.327621	12.903113	2.729030
68.H	9.337440	9.363779	9.841158
69.H	7.825615	9.897495	10.596514
70.C	9.558065	8.186049	12.871477
71.H	14.792726	13.317789	3.537974
72.H	10.048265	8.071980	13.852928
73.C	15.184878	12.297749	12.021983
74.C	15.922293	11.105757	12.380833
75.C	9.635673	8.505844	3.689575
76.C	8.900237	9.698777	3.329800
77.H	8.598929	10.473519	4.032027
78.C	8.581322	9.645941	1.940049
79.H	8.006893	10.383454	1.384778
80.C	9.153921	8.447930	1.401871
81.H	9.087367	8.116634	0.368238
82.C	9.831414	7.770695	2.461233
83.H	10.356161	6.820837	2.381974
84.C	12.637045	10.430601	2.512438
85.C	11.685352	11.484081	2.237922
86.H	11.490413	12.325683	2.899835
87.C	11.119644	11.273214	0.944779
88.H	10.398158	11.916488	0.446988
89.C	11.673480	10.062785	0.414571
90.H	11.445929	9.628096	-0.555904
91.C	12.570639	9.526389	1.387593
92.H	13.160567	8.618106	1.283188
93.H	13.532255	11.366881	7.304041
94.C	12.254597	11.272715	14.329118
95.C	13.351822	8.963007	8.755943
96.C	14.731901	9.335630	8.686306
97.H	15.035289	10.205998	8.104505
98.C	15.727395	8.559791	9.285070
99.H	16.768006	8.873501	9.181694
100.C	15.417743	7.406438	9.998468
101.H	16.199074	6.808699	10.466817
102.C	14.062890	7.044210	10.118345
103.H	13.788834	6.155601	10.690794
104.C	13.064104	7.795046	9.531114
105.H	12.022608	7.488207	9.643107
106.La	12.812031	11.338574	10.394924
107.Fe	14.194927	11.127598	13.568151

108.Si	15.737018	13.843556	9.897989	129.C	15.013227	14.042814	8.159272
109.Si	9.704532	9.968352	12.249357	130.H	13.933154	14.260115	8.175618
110.N	14.779134	12.662086	10.739301	131.H	15.507496	14.875999	7.631321
111.N	11.363201	10.464648	12.084482	132.H	15.170149	13.137343	7.552092
112.O	11.249955	13.467698	10.400431	133.C	17.547842	13.311893	9.744614
113.C	11.075192	14.111553	11.706097	134.H	17.990485	13.135793	10.739487
114.H	10.226063	13.622889	12.205611	135.H	16.223555	10.331297	11.678271
115.H	11.987471	13.948183	12.296160	136.H	8.502089	7.887084	12.987146
116.C	10.795154	15.574632	11.400225	137.C	16.243018	11.159066	13.770140
117.H	11.739162	16.129149	11.282041	138.H	18.152994	14.084980	9.240500
118.H	10.203260	16.057176	12.190389	139.H	16.819104	10.422293	14.324676
119.C	10.062925	15.484802	10.057315	140.C	15.669626	12.356395	14.309024
120.H	9.020743	15.161597	10.208679	141.H	10.037190	7.477779	12.175833
121.H	10.058262	16.430324	9.497788	142.H	17.642718	12.377801	9.167058
122.C	10.850158	14.400928	9.342681	143.H	15.737196	12.687845	15.342541
123.H	11.760415	14.807985	8.876336	144.C	14.989883	13.032742	13.250533
124.H	10.273881	13.840224	8.596430	145.H	14.464136	13.982003	13.330295
125.C	15.700443	15.538304	10.753829	146.C	8.722472	11.068634	13.447174
126.H	14.672425	15.931476	10.825305	147.H	8.679243	12.114781	13.100623
127.H	16.109526	15.477477	11.776079	148.H	7.682963	10.710037	13.547807
128.H	16.304484	16.277393	10.198888				

M U L L I K E N P O P U L A T I O N S

The survey below gives for each atom:
a) the total charge (Z minus electrons)
b) the net spin polarization (nr of electrons spin-A minus spin-B)
c) for each spin the atomic electron valence density (integrated) per L-value.

Atom	Charge	Spin density	S	P	D	F
1 La	2.1100		0.2615	-0.2383	0.5717	0.2951
2 Fe	0.4278		0.2330	0.3665	6.9726	0.0000
3 Si	1.2370		0.8824	1.4891	0.3914	0.0000
4 Si	1.2379		0.8836	1.4878	0.3907	0.0000
5 N	-0.9646		1.8343	4.0929	0.0374	0.0000
6 N	-0.9634		1.8345	4.0915	0.0374	0.0000
7 O	-0.7496		1.9708	4.7114	0.0674	0.0000
8 H	0.0757		0.8566	0.0678	0.0000	0.0000
9 H	0.0085		0.9307	0.0609	0.0000	0.0000
10 C	-0.2693		1.4968	2.6819	0.0906	0.0000
11 C	-0.2509		1.4566	2.7354	0.0589	0.0000
12 H	0.0820		0.8575	0.0605	0.0000	0.0000
13 C	-0.0798		1.4064	2.6070	0.0663	0.0000
14 H	0.0378		0.9105	0.0518	0.0000	0.0000
15 C	-0.1003		1.3844	2.6550	0.0610	0.0000
16 H	0.0174		0.9260	0.0566	0.0000	0.0000
17 C	-0.0714		1.3964	2.6096	0.0654	0.0000
18 H	0.0305		0.9165	0.0530	0.0000	0.0000
19 C	-0.1396		1.4320	2.6466	0.0610	0.0000
20 H	0.0736		0.8756	0.0508	0.0000	0.0000
21 C	0.1076		1.3569	2.4564	0.0790	0.0000
22 H	0.1466		0.8211	0.0323	0.0000	0.0000
23 H	0.1489		0.8097	0.0414	0.0000	0.0000
24 C	-0.1926		1.3376	2.7962	0.0588	0.0000
25 H	0.1162		0.8494	0.0345	0.0000	0.0000
26 H	0.0806		0.8722	0.0471	0.0000	0.0000

27 C	-0.1799	1.3188	2.8020	0.0592	0.0000
28 H	0.0983	0.8653	0.0364	0.0000	0.0000
29 H	0.0846	0.8684	0.0470	0.0000	0.0000
30 C	0.1362	1.3412	2.4436	0.0789	0.0000
31 H	0.1257	0.8411	0.0331	0.0000	0.0000
32 H	0.1980	0.7586	0.0433	0.0000	0.0000
33 C	-0.4925	1.3145	3.1541	0.0239	0.0000
34 H	0.0701	0.8725	0.0574	0.0000	0.0000
35 H	0.0682	0.8705	0.0613	0.0000	0.0000
36 H	0.0500	0.8904	0.0597	0.0000	0.0000
37 C	-0.5814	1.4049	3.1524	0.0241	0.0000
38 H	0.1070	0.8323	0.0607	0.0000	0.0000
39 H	0.0654	0.8760	0.0586	0.0000	0.0000
40 H	0.1057	0.8343	0.0600	0.0000	0.0000
41 C	-0.4861	1.3021	3.1603	0.0237	0.0000
42 H	0.0737	0.8665	0.0598	0.0000	0.0000
43 C	0.0854	1.3513	2.4430	0.1203	0.0000
44 C	-0.0876	1.4250	2.5957	0.0668	0.0000
45 H	0.0417	0.8958	0.0626	0.0000	0.0000
46 H	0.0502	0.8900	0.0598	0.0000	0.0000
47 C	-0.0457	1.4157	2.5595	0.0704	0.0000
48 H	-0.0170	0.9552	0.0618	0.0000	0.0000
49 C	-0.0363	1.4112	2.5547	0.0703	0.0000
50 H	0.0695	0.8729	0.0575	0.0000	0.0000
51 H	-0.0156	0.9539	0.0617	0.0000	0.0000
52 C	-0.4859	1.4881	2.9374	0.0604	0.0000
53 C	-0.4860	1.4881	2.9376	0.0604	0.0000
54 C	-0.4936	1.3151	3.1546	0.0240	0.0000
55 H	0.0665	0.8725	0.0610	0.0000	0.0000
56 H	0.0511	0.8894	0.0594	0.0000	0.0000
57 H	0.0675	0.8714	0.0611	0.0000	0.0000
58 C	-0.5754	1.3990	3.1525	0.0239	0.0000
59 H	0.1033	0.8377	0.0589	0.0000	0.0000
60 H	0.1064	0.8330	0.0606	0.0000	0.0000
61 H	0.0713	0.8705	0.0582	0.0000	0.0000
62 C	-0.4854	1.3023	3.1593	0.0238	0.0000
63 H	0.0721	0.8680	0.0599	0.0000	0.0000
64 H	0.0675	0.8714	0.0611	0.0000	0.0000
65 C	-0.5754	1.3990	3.1524	0.0239	0.0000
66 H	0.1034	0.8377	0.0589	0.0000	0.0000
67 H	0.0498	0.8904	0.0599	0.0000	0.0000
68 H	0.1064	0.8330	0.0606	0.0000	0.0000
69 H	0.0713	0.8705	0.0582	0.0000	0.0000
70 C	-0.4854	1.3024	3.1592	0.0238	0.0000
71 H	0.0716	0.8710	0.0574	0.0000	0.0000
72 H	0.0721	0.8680	0.0599	0.0000	0.0000
73 C	0.0813	1.3545	2.4438	0.1204	0.0000
74 C	-0.0896	1.4259	2.5968	0.0668	0.0000
75 C	0.0814	1.3544	2.4437	0.1204	0.0000
76 C	-0.0895	1.4259	2.5968	0.0668	0.0000
77 H	0.0428	0.8945	0.0627	0.0000	0.0000
78 C	-0.0462	1.4158	2.5600	0.0705	0.0000
79 H	-0.0169	0.9551	0.0618	0.0000	0.0000
80 C	-0.0367	1.4111	2.5553	0.0703	0.0000
81 H	-0.0160	0.9542	0.0618	0.0000	0.0000
82 C	-0.0956	1.4243	2.6042	0.0671	0.0000

83 H	0.0060	0.9330	0.0610	0.0000	0.0000
84 C	0.0853	1.3513	2.4431	0.1203	0.0000
85 C	-0.0875	1.4249	2.5957	0.0668	0.0000
86 H	0.0414	0.8960	0.0625	0.0000	0.0000
87 C	-0.0457	1.4157	2.5596	0.0704	0.0000
88 H	-0.0170	0.9552	0.0618	0.0000	0.0000
89 C	-0.0363	1.4113	2.5547	0.0703	0.0000
90 H	-0.0156	0.9539	0.0617	0.0000	0.0000
91 C	-0.0923	1.4225	2.6028	0.0670	0.0000
92 H	0.0085	0.9306	0.0608	0.0000	0.0000
93 H	0.0756	0.8567	0.0677	0.0000	0.0000
94 C	-0.0922	1.4223	2.6028	0.0670	0.0000
95 C	-0.2695	1.4968	2.6820	0.0906	0.0000
96 C	-0.2515	1.4567	2.7359	0.0589	0.0000
97 H	0.0821	0.8574	0.0605	0.0000	0.0000
98 C	-0.0799	1.4065	2.6071	0.0663	0.0000
99 H	0.0378	0.9105	0.0518	0.0000	0.0000
100 C	-0.1003	1.3843	2.6550	0.0610	0.0000
101 H	0.0174	0.9260	0.0566	0.0000	0.0000
102 C	-0.0715	1.3964	2.6097	0.0654	0.0000
103 H	0.0305	0.9165	0.0530	0.0000	0.0000
104 C	-0.1396	1.4321	2.6465	0.0610	0.0000
105 H	0.0736	0.8756	0.0508	0.0000	0.0000
106 La	2.1111	0.2614	-0.2386	0.5711	0.2950
107 Fe	0.4274	0.2333	0.3667	6.9726	0.0000
108 Si	1.2369	0.8825	1.4892	0.3914	0.0000
109 Si	1.2378	0.8836	1.4879	0.3907	0.0000
110 N	-0.9646	1.8344	4.0929	0.0374	0.0000
111 N	-0.9633	1.8344	4.0915	0.0374	0.0000
112 O	-0.7496	1.9708	4.7114	0.0675	0.0000
113 C	0.1074	1.3571	2.4564	0.0790	0.0000
114 H	0.1470	0.8206	0.0323	0.0000	0.0000
115 H	0.1487	0.8098	0.0414	0.0000	0.0000
116 C	-0.1926	1.3375	2.7963	0.0588	0.0000
117 H	0.1161	0.8495	0.0345	0.0000	0.0000
118 H	0.0807	0.8721	0.0471	0.0000	0.0000
119 C	-0.1799	1.3188	2.8019	0.0592	0.0000
120 H	0.0983	0.8653	0.0364	0.0000	0.0000
121 H	0.0846	0.8684	0.0470	0.0000	0.0000
122 C	0.1362	1.3410	2.4439	0.0789	0.0000
123 H	0.1255	0.8414	0.0331	0.0000	0.0000
124 H	0.1980	0.7587	0.0433	0.0000	0.0000
125 C	-0.4923	1.3142	3.1542	0.0239	0.0000
126 H	0.0698	0.8728	0.0574	0.0000	0.0000
127 H	0.0682	0.8704	0.0613	0.0000	0.0000
128 H	0.0500	0.8903	0.0597	0.0000	0.0000
129 C	-0.5814	1.4049	3.1524	0.0241	0.0000
130 H	0.1068	0.8325	0.0606	0.0000	0.0000
131 H	0.0654	0.8760	0.0586	0.0000	0.0000
132 H	0.1058	0.8341	0.0601	0.0000	0.0000
133 C	-0.4862	1.3022	3.1602	0.0237	0.0000
134 H	0.0737	0.8665	0.0598	0.0000	0.0000
135 H	0.0428	0.8945	0.0627	0.0000	0.0000
136 H	0.0497	0.8904	0.0599	0.0000	0.0000
137 C	-0.0463	1.4158	2.5600	0.0705	0.0000
138 H	0.0503	0.8900	0.0598	0.0000	0.0000

139 H	-0.0169	0.9551	0.0618	0.0000	0.0000
140 C	-0.0368	1.4112	2.5553	0.0703	0.0000
141 H	0.0718	0.8708	0.0574	0.0000	0.0000
142 H	0.0696	0.8729	0.0575	0.0000	0.0000
143 H	-0.0159	0.9542	0.0618	0.0000	0.0000
144 C	-0.0955	1.4242	2.6042	0.0671	0.0000
145 H	0.0060	0.9331	0.0609	0.0000	0.0000
146 C	-0.4936	1.3150	3.1546	0.0240	0.0000
147 H	0.0665	0.8725	0.0610	0.0000	0.0000
148 H	0.0511	0.8895	0.0594	0.0000	0.0000

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B O N D - O R D E R A N A L Y S I S

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DIST. [A] BOND-ORDERS (THRESHOLD = 0.200)

				MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
La	1 - Fe	2	3.4685	0.1598	0.1833	0.2810	-0.5187	0.2316
La	1 - N	5	2.3957	0.5978	0.6886	0.8618	1.4734	0.8179
La	1 - N	6	2.3909	0.6066	0.7049	0.8811	1.4832	0.8353
La	1 - O	7	2.6409	0.1901	0.2669	0.3431	0.7120	0.3177
La	1 - C	52	2.8750	0.0778	0.1994	0.2394	0.6308	0.2136
La	1 - C	53	2.7870	0.0464	0.2110	0.2533	0.6422	0.2260
Fe	2 - C	75	2.1771	0.3944	0.2548	0.3511	0.3044	0.3265
Fe	2 - C	76	2.0962	0.4065	0.3454	0.4779	0.6348	0.4584
Fe	2 - C	78	2.0583	0.3876	0.3478	0.4816	0.6238	0.4611
Fe	2 - C	80	2.0576	0.3835	0.3510	0.4860	0.6267	0.4652
Fe	2 - C	82	2.0885	0.3942	0.3475	0.4809	0.6425	0.4617
Fe	2 - C	84	2.1767	0.3930	0.2543	0.3504	0.3043	0.3259
Fe	2 - C	85	2.0971	0.4001	0.3440	0.4759	0.6330	0.4565
Fe	2 - C	87	2.0581	0.3952	0.3485	0.4825	0.6250	0.4620
Fe	2 - C	89	2.0579	0.3946	0.3493	0.4836	0.6243	0.4629
Fe	2 - C	91	2.0892	0.3926	0.3477	0.4812	0.6424	0.4619
Si	3 - N	5	1.7381	0.9852	0.9219	1.0231	1.6188	0.9795
Si	3 - C	33	1.8990	0.8257	0.8536	0.9089	1.6426	0.8620
Si	3 - C	37	1.8939	0.8391	0.8725	0.9293	1.6359	0.8788
Si	3 - C	41	1.8935	0.8323	0.8640	0.9200	1.6526	0.8727
Si	4 - N	6	1.7392	0.9843	0.9185	1.0178	1.6091	0.9735
Si	4 - C	54	1.8999	0.8231	0.8524	0.9075	1.6381	0.8605
Si	4 - C	58	1.8921	0.8414	0.8742	0.9311	1.6425	0.8813
Si	4 - C	62	1.8934	0.8291	0.8670	0.9231	1.6524	0.8755
N	5 - C	75	1.3938	1.0553	1.1457	1.2561	1.1954	1.3812
N	6 - C	84	1.3935	1.0551	1.1452	1.2538	1.1938	1.3776
O	7 - C	21	1.4662	0.7775	0.9189	1.0481	0.9818	1.1362
O	7 - C	30	1.4662	0.7668	0.9150	1.0446	0.9803	1.1318
H	8 - C	52	1.0935	0.9656	0.9067	0.9514	0.9801	0.9305
H	9 - C	94	1.0881	1.0660	0.9259	0.9667	0.9917	0.9181
C	10 - C	11	1.4311	1.2372	1.2369	1.2830	1.2609	1.3307
C	10 - C	19	1.4310	1.2028	1.2416	1.2836	1.2680	1.3227
C	10 - C	53	1.4324	1.2465	1.2221	1.2831	1.2442	1.3494
C	11 - H	12	1.0900	0.9698	0.9217	0.9599	0.9816	0.9190
C	11 - C	13	1.3969	1.3075	1.4300	1.4866	1.4240	1.5647

C	13 - H	14	1.0918	1.0351	0.9238	0.9672	0.9789	0.9060
C	13 - C	15	1.3911	1.2769	1.4396	1.4956	1.4401	1.5692
C	15 - H	16	1.0896	1.0542	0.9289	0.9766	0.9967	0.9246
C	15 - C	17	1.4075	1.1912	1.3450	1.3979	1.3396	1.4689
C	17 - H	18	1.0920	1.0437	0.9248	0.9692	0.9825	0.9097
C	17 - C	19	1.3807	1.3627	1.5242	1.5801	1.5273	1.6551
C	19 - H	20	1.0915	0.9857	0.9243	0.9630	0.9797	0.9118
C	21 - H	22	1.0997	0.8846	0.9186	0.9586	0.9607	0.8952
C	21 - H	23	1.0987	0.9018	0.9158	0.9581	0.9593	0.8881
C	21 - C	24	1.5208	0.9120	1.0159	1.0566	1.0123	1.1100
C	24 - H	25	1.1012	0.9399	0.9255	0.9664	0.9941	0.9269
C	24 - H	26	1.0989	1.0181	0.9255	0.9728	1.0030	0.9246
C	24 - C	27	1.5322	0.9432	1.0058	1.0439	0.9169	1.1248
C	27 - H	28	1.1016	0.9606	0.9248	0.9669	0.9947	0.9266
C	27 - H	29	1.0987	1.0136	0.9249	0.9725	1.0027	0.9236
C	27 - C	30	1.5183	0.9092	1.0186	1.0604	1.0179	1.1131
C	30 - H	31	1.1008	0.8920	0.9208	0.9606	0.9624	0.8998
C	30 - H	32	1.0970	0.9063	0.9161	0.9622	0.9615	0.8850
C	33 - H	34	1.1030	0.9849	0.9516	1.0138	1.0500	1.0374
C	33 - H	35	1.1027	1.0018	0.9460	1.0113	1.0571	1.0275
C	33 - H	36	1.1041	1.0104	0.9448	1.0110	1.0558	1.0280
C	37 - H	38	1.1018	0.9347	0.9489	1.0075	1.0422	1.0303
C	37 - H	39	1.1033	1.0242	0.9436	1.0111	1.0601	1.0225
C	37 - H	40	1.1014	0.9356	0.9499	1.0087	1.0432	1.0317
C	41 - H	42	1.1030	0.9994	0.9446	1.0111	1.0594	1.0257
C	41 - H	46	1.1036	1.0085	0.9457	1.0121	1.0567	1.0293
C	41 - H	50	1.1023	0.9919	0.9486	1.0137	1.0559	1.0328
C	43 - C	44	1.4460	1.0833	1.1822	1.2136	1.2148	1.2472
C	43 - C	94	1.4447	1.0842	1.1853	1.2175	1.2185	1.2523
C	43 - Fe	107	2.1767	0.3856	0.2543	0.3503	0.3043	0.3259
C	43 - N	111	1.3935	1.0607	1.1453	1.2539	1.1939	1.3777
C	44 - H	45	1.0883	1.0537	0.9207	0.9624	0.9876	0.9092
C	44 - C	47	1.4271	1.0984	1.2620	1.3042	1.2145	1.3870
C	44 - Fe	107	2.0971	0.3977	0.3440	0.4758	0.6329	0.4565
C	47 - H	48	1.0873	1.0938	0.9251	0.9709	0.9932	0.9155
C	47 - C	49	1.4328	1.0847	1.2459	1.2889	1.2077	1.3667
C	47 - Fe	107	2.0581	0.3939	0.3485	0.4825	0.6250	0.4620
C	49 - H	51	1.0875	1.0885	0.9254	0.9709	0.9928	0.9154
C	49 - C	94	1.4281	1.1012	1.2602	1.3027	1.2116	1.3860
C	49 - Fe	107	2.0579	0.3958	0.3493	0.4836	0.6243	0.4628
C	52 - C	53	1.4676	1.1322	1.0823	1.1579	0.9685	1.2644
C	52 - C	95	1.4324	1.2556	1.2222	1.2833	1.2444	1.3496
C	52 - La	106	2.7873	0.0317	0.2108	0.2531	0.6419	0.2258
C	53 - H	93	1.0936	0.9611	0.9067	0.9514	0.9801	0.9305
C	53 - La	106	2.8753	0.0699	0.1993	0.2393	0.6307	0.2135
C	54 - H	55	1.1029	0.9820	0.9523	1.0133	1.0469	1.0386
C	54 - H	56	1.1042	1.0085	0.9443	1.0106	1.0563	1.0267
C	54 - H	57	1.1027	1.0009	0.9462	1.0115	1.0573	1.0274
C	58 - H	59	1.1023	0.9520	0.9454	1.0070	1.0479	1.0257
C	58 - H	60	1.1017	0.9285	0.9500	1.0082	1.0405	1.0334
C	58 - H	61	1.1031	1.0184	0.9435	1.0112	1.0603	1.0232
C	62 - H	63	1.1030	0.9996	0.9446	1.0110	1.0595	1.0252
C	62 - H	67	1.1036	1.0088	0.9457	1.0119	1.0566	1.0290
C	62 - H	71	1.1023	0.9900	0.9486	1.0135	1.0558	1.0322
H	64 - C	146	1.1027	1.0010	0.9462	1.0115	1.0573	1.0274
C	65 - H	66	1.1023	0.9519	0.9454	1.0070	1.0479	1.0257

C	65 - H	68	1.1017	0.9288	0.9500	1.0082	1.0404	1.0334
C	65 - H	69	1.1031	1.0187	0.9435	1.0112	1.0603	1.0232
C	65 - Si	109	1.8921	0.8414	0.8742	0.9311	1.6425	0.8813
C	70 - H	72	1.1030	1.0002	0.9446	1.0110	1.0595	1.0252
C	70 - Si	109	1.8934	0.8314	0.8670	0.9230	1.6524	0.8755
C	70 - H	136	1.1036	1.0089	0.9457	1.0119	1.0566	1.0290
C	70 - H	141	1.1023	0.9905	0.9487	1.0135	1.0558	1.0322
C	73 - C	74	1.4469	1.0820	1.1791	1.2104	1.2119	1.2438
C	73 - Fe	107	2.1771	0.3986	0.2548	0.3510	0.3044	0.3265
C	73 - N	110	1.3938	1.0559	1.1456	1.2561	1.1954	1.3811
C	73 - C	144	1.4448	1.0812	1.1852	1.2173	1.2184	1.2520
C	74 - Fe	107	2.0962	0.4073	0.3454	0.4779	0.6348	0.4585
C	74 - H	135	1.0882	1.0524	0.9208	0.9620	0.9871	0.9093
C	74 - C	137	1.4268	1.1018	1.2629	1.3051	1.2156	1.3879
C	75 - C	76	1.4469	1.0786	1.1791	1.2104	1.2119	1.2439
C	75 - C	82	1.4448	1.0804	1.1852	1.2173	1.2184	1.2520
C	76 - H	77	1.0882	1.0531	0.9208	0.9620	0.9871	0.9093
C	76 - C	78	1.4269	1.0925	1.2629	1.3051	1.2156	1.3879
C	78 - H	79	1.0873	1.0933	0.9250	0.9709	0.9931	0.9154
C	78 - C	80	1.4327	1.0794	1.2458	1.2887	1.2076	1.3664
C	80 - H	81	1.0875	1.0898	0.9254	0.9709	0.9929	0.9154
C	80 - C	82	1.4282	1.0974	1.2589	1.3013	1.2100	1.3847
C	82 - H	83	1.0881	1.0645	0.9259	0.9666	0.9915	0.9184
C	84 - C	85	1.4460	1.0810	1.1822	1.2136	1.2148	1.2473
C	84 - C	91	1.4447	1.0853	1.1854	1.2175	1.2185	1.2523
C	85 - H	86	1.0883	1.0510	0.9208	0.9624	0.9876	0.9092
C	85 - C	87	1.4271	1.0984	1.2620	1.3042	1.2145	1.3870
C	87 - H	88	1.0873	1.0920	0.9251	0.9709	0.9932	0.9155
C	87 - C	89	1.4328	1.0866	1.2460	1.2889	1.2077	1.3667
C	89 - H	90	1.0875	1.0870	0.9254	0.9709	0.9928	0.9154
C	89 - C	91	1.4281	1.1032	1.2601	1.3026	1.2116	1.3860
C	91 - H	92	1.0881	1.0651	0.9259	0.9667	0.9917	0.9181
C	94 - Fe	107	2.0893	0.3934	0.3476	0.4811	0.6424	0.4619
C	95 - C	96	1.4312	1.2288	1.2367	1.2827	1.2607	1.3304
C	95 - C	104	1.4310	1.1995	1.2415	1.2835	1.2678	1.3225
C	96 - H	97	1.0900	0.9669	0.9217	0.9598	0.9816	0.9190
C	96 - C	98	1.3969	1.3080	1.4298	1.4864	1.4237	1.5645
C	98 - H	99	1.0918	1.0346	0.9238	0.9672	0.9789	0.9060
C	98 - C	100	1.3911	1.2751	1.4397	1.4957	1.4402	1.5693
C	100 - H	101	1.0896	1.0546	0.9289	0.9765	0.9967	0.9246
C	100 - C	102	1.4076	1.1903	1.3448	1.3977	1.3394	1.4687
C	102 - H	103	1.0920	1.0439	0.9248	0.9692	0.9825	0.9097
C	102 - C	104	1.3806	1.3618	1.5244	1.5803	1.5274	1.6552
C	104 - H	105	1.0915	0.9871	0.9243	0.9630	0.9797	0.9118
La	106 - Fe	107	3.4679	0.1590	0.1834	0.2812	-0.5185	0.2318
La	106 - N	110	2.3958	0.5919	0.6886	0.8618	1.4734	0.8179
La	106 - N	111	2.3911	0.6000	0.7045	0.8806	1.4829	0.8349
La	106 - O	112	2.6407	0.1900	0.2669	0.3431	0.7120	0.3177
Fe	107 - C	137	2.0583	0.3942	0.3478	0.4816	0.6237	0.4611
Fe	107 - C	140	2.0576	0.3964	0.3510	0.4860	0.6267	0.4652
Fe	107 - C	144	2.0886	0.3936	0.3475	0.4809	0.6425	0.4617
Si	108 - N	110	1.7382	0.9880	0.9218	1.0231	1.6187	0.9795
Si	108 - C	125	1.8989	0.8244	0.8537	0.9090	1.6427	0.8621
Si	108 - C	129	1.8939	0.8441	0.8725	0.9293	1.6358	0.8788
Si	108 - C	133	1.8935	0.8307	0.8639	0.9200	1.6525	0.8727
Si	109 - N	111	1.7392	0.9867	0.9186	1.0179	1.6093	0.9736

Si	109 - C	146	1.9000	0.8203	0.8524	0.9075	1.6380	0.8605
O	112 - C	113	1.4662	0.7790	0.9188	1.0481	0.9818	1.1361
O	112 - C	122	1.4661	0.7673	0.9150	1.0446	0.9803	1.1318
C	113 - H	114	1.0997	0.8865	0.9186	0.9586	0.9607	0.8952
C	113 - H	115	1.0987	0.8988	0.9158	0.9580	0.9592	0.8880
C	113 - C	116	1.5207	0.9134	1.0159	1.0566	1.0123	1.1100
C	116 - H	117	1.1012	0.9395	0.9255	0.9664	0.9941	0.9269
C	116 - H	118	1.0989	1.0186	0.9255	0.9728	1.0030	0.9246
C	116 - C	119	1.5322	0.9422	1.0058	1.0439	0.9169	1.1249
C	119 - H	120	1.1016	0.9613	0.9248	0.9669	0.9947	0.9266
C	119 - H	121	1.0987	1.0137	0.9249	0.9725	1.0027	0.9236
C	119 - C	122	1.5183	0.9104	1.0186	1.0604	1.0179	1.1131
C	122 - H	123	1.1008	0.8898	0.9208	0.9607	0.9625	0.8999
C	122 - H	124	1.0970	0.9075	0.9161	0.9622	0.9616	0.8850
C	125 - H	126	1.1030	0.9847	0.9516	1.0139	1.0501	1.0374
C	125 - H	127	1.1027	1.0012	0.9460	1.0113	1.0572	1.0275
C	125 - H	128	1.1041	1.0096	0.9448	1.0110	1.0558	1.0280
C	129 - H	130	1.1018	0.9351	0.9489	1.0075	1.0423	1.0303
C	129 - H	131	1.1033	1.0247	0.9436	1.0111	1.0601	1.0224
C	129 - H	132	1.1014	0.9352	0.9499	1.0087	1.0431	1.0317
C	133 - H	134	1.1030	0.9981	0.9446	1.0111	1.0594	1.0257
C	133 - H	138	1.1036	1.0078	0.9457	1.0121	1.0567	1.0293
C	133 - H	142	1.1023	0.9914	0.9487	1.0137	1.0559	1.0328
C	137 - H	139	1.0873	1.0921	0.9250	0.9709	0.9931	0.9154
C	137 - C	140	1.4327	1.0823	1.2457	1.2886	1.2076	1.3664
C	140 - H	143	1.0875	1.0898	0.9254	0.9709	0.9929	0.9154
C	140 - C	144	1.4282	1.0997	1.2590	1.3013	1.2101	1.3847
C	144 - H	145	1.0881	1.0632	0.9258	0.9666	0.9915	0.9184
C	146 - H	147	1.1029	0.9819	0.9523	1.0133	1.0468	1.0386
C	146 - H	148	1.1042	1.0090	0.9443	1.0106	1.0563	1.0266
Sum :			157.7670	168.0639	180.8038	180.8038	180.8038	

List of all MOs, ordered by energy, with the most significant SFO gross populations

Each percentage contribution in the table below corresponds to the indicated SFO.
In general, a SFO may be a linear combination of several Fragment Orbitals on the same, or on symmetry-related Fragments. Only the first 'member' of such a combination is specified here. A full definition of all SFOs is given in an earlier part of the output.
The numbering of the SFOs in this table does NOT include the Core Orbitals, and starts from one for each symmetry representation, as in the SFO definition list earlier.

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-4.439	2.00	179 A	19.91%	1 D:yz	-7.682	1.20	4 Fe
			15.82%	1 D:yz	-7.682	1.20	3 Fe
			9.83%	1 D:z2	-7.682	1.20	4 Fe
			7.72%	1 D:z2	-7.682	1.20	3 Fe
			7.41%	1 D:xy	-7.682	1.20	4 Fe
			5.80%	1 D:xy	-7.682	1.20	3 Fe
			2.09%	1 D:xz	-7.682	1.20	4 Fe
			1.65%	1 D:xz	-7.682	1.20	3 Fe
			1.27%	1 P:y	-7.403	1.00	12 N
			1.25%	1 P:x	-5.608	0.67	109 C

-4.432	2.00	180 A	19.60%	1 D:yz	-7.682	1.20	3 Fe
			15.37%	1 D:yz	-7.682	1.20	4 Fe
			9.92%	1 D:z2	-7.682	1.20	3 Fe
			7.86%	1 D:z2	-7.682	1.20	4 Fe
			7.59%	1 D:xy	-7.682	1.20	3 Fe
			6.04%	1 D:xy	-7.682	1.20	4 Fe
			2.19%	1 D:xz	-7.682	1.20	3 Fe
			1.74%	1 D:xz	-7.682	1.20	4 Fe
			1.31%	1 P:y	-7.403	1.00	10 N
			1.25%	1 P:x	-5.608	0.67	127 C
			1.06%	1 P:y	-7.403	1.00	9 N
			1.04%	1 P:y	-7.403	1.00	12 N
-4.248	2.00	181 A	9.59%	1 D:yz	-7.682	1.20	4 Fe
			9.43%	1 D:z2	-7.682	1.20	4 Fe
			8.58%	1 D:xz	-7.682	1.20	4 Fe
			8.22%	1 D:yz	-7.682	1.20	3 Fe
			8.06%	1 D:z2	-7.682	1.20	3 Fe
			7.25%	1 D:xz	-7.682	1.20	3 Fe
			6.99%	1 D:x2-y2	-7.682	1.20	4 Fe
			6.01%	1 D:x2-y2	-7.682	1.20	3 Fe
			5.87%	1 D:xy	-7.682	1.20	4 Fe
			5.05%	1 D:xy	-7.682	1.20	3 Fe
			1.41%	1 P:x	-5.608	0.67	119 C
			1.07%	1 P:y	-7.403	1.00	12 N
			1.07%	1 P:x	-5.608	0.67	121 C
-4.237	2.00	182 A	10.16%	1 D:z2	-7.682	1.20	3 Fe
			9.44%	1 D:yz	-7.682	1.20	3 Fe
			9.02%	1 D:xz	-7.682	1.20	3 Fe
			8.73%	1 D:z2	-7.682	1.20	4 Fe
			8.03%	1 D:yz	-7.682	1.20	4 Fe
			7.83%	1 D:xz	-7.682	1.20	4 Fe
			6.70%	1 D:x2-y2	-7.682	1.20	3 Fe
			5.73%	1 D:x2-y2	-7.682	1.20	4 Fe
			5.32%	1 D:xy	-7.682	1.20	3 Fe
			4.55%	1 D:xy	-7.682	1.20	4 Fe
			1.40%	1 P:x	-5.608	0.67	121 C
			1.20%	1 P:x	-5.608	0.67	119 C
			1.03%	1 P:x	-7.403	1.00	9 N
-3.707	2.00	183 A	12.38%	1 P:z	-5.608	0.67	113 C
			12.07%	1 P:z	-5.608	0.67	112 C
			5.46%	1 P:z	-5.608	0.67	98 C
			5.45%	1 P:z	-5.608	0.67	135 C
			4.90%	1 P:z	-5.608	0.67	133 C
			4.87%	1 P:z	-5.608	0.67	96 C
			4.20%	1 P:y	-5.608	0.67	113 C
			4.14%	1 P:y	-5.608	0.67	112 C
			3.18%	1 P:z	-5.608	0.67	137 C
			3.17%	1 P:z	-5.608	0.67	100 C
			2.28%	1 P:y	-5.608	0.67	98 C
			2.27%	1 P:y	-5.608	0.67	135 C
			2.18%	1 P:y	-5.608	0.67	133 C
			2.17%	1 P:y	-5.608	0.67	96 C
			1.97%	1 D:yz	-3.140	0.20	1 La
			1.96%	1 D:yz	-3.140	0.20	2 La
			1.67%	1 P:y	-5.608	0.67	137 C
			1.66%	1 P:y	-5.608	0.67	100 C

			1.09%	1 P:x	-7.403	1.00	9 N
			1.03%	1 P:x	-7.403	1.00	11 N
-1.917	0.00	184 A	7.08%	1 P:z	-5.608	0.67	134 C
			6.28%	1 P:z	-5.608	0.67	97 C
			6.22%	1 P:z	-5.608	0.67	137 C
			5.69%	1 P:z	-5.608	0.67	100 C
			5.09%	1 D:xz	-3.140	0.20	2 La
			4.95%	1 D:xz	-3.140	0.20	1 La
			3.92%	1 P:z	-5.608	0.67	136 C
			3.03%	1 P:z	-5.608	0.67	99 C
			2.89%	1 P:y	-5.608	0.67	137 C
			2.74%	1 P:y	-5.608	0.67	134 C
			2.67%	1 P:y	-5.608	0.67	100 C
			2.44%	1 P:y	-5.608	0.67	97 C
			1.95%	1 P:z	-5.608	0.67	133 C
			1.78%	1 D:xz	-7.682	1.20	4 Fe
			1.71%	1 P:y	-5.608	0.67	136 C
			1.54%	1 D:yz	-7.682	1.20	4 Fe
			1.52%	1 D:xz	-7.682	1.20	3 Fe
			1.37%	1 P:z	-5.608	0.67	96 C
			1.31%	1 P:y	-5.608	0.67	99 C
			1.30%	1 D:yz	-7.682	1.20	3 Fe
			1.09%	1 P:z	-5.608	0.67	98 C
			1.03%	1 P:x	-1.074	0.00	2 La
			1.01%	1 D:yz	-3.140	0.20	2 La
			1.00%	1 P:x	-1.074	0.00	1 La
-1.907	0.00	185 A	6.92%	1 P:z	-5.608	0.67	99 C
			6.14%	1 P:z	-5.608	0.67	96 C
			6.08%	1 P:z	-5.608	0.67	136 C
			5.58%	1 P:z	-5.608	0.67	133 C
			5.28%	1 D:x2-y2	-3.140	0.20	1 La
			5.18%	1 D:x2-y2	-3.140	0.20	2 La
			3.38%	1 P:z	-5.608	0.67	97 C
			3.11%	1 P:y	-5.608	0.67	99 C
			2.79%	1 P:y	-5.608	0.67	96 C
			2.74%	1 P:y	-5.608	0.67	136 C
			2.57%	1 P:z	-5.608	0.67	134 C
			2.53%	1 P:y	-5.608	0.67	133 C
			1.77%	1 P:z	-5.608	0.67	100 C
			1.62%	1 D:xz	-7.682	1.20	3 Fe
			1.49%	1 D:z2	-7.682	1.20	3 Fe
			1.44%	1 P:z	-5.608	0.67	132 C
			1.41%	1 F:y	-3.824	0.00	1 La
			1.35%	1 F:y	-3.824	0.00	2 La
			1.35%	1 P:y	-5.608	0.67	97 C
			1.33%	1 D:z2	-7.682	1.20	4 Fe
			1.32%	1 D:xz	-7.682	1.20	4 Fe
			1.31%	1 P:z	-5.608	0.67	95 C
			1.27%	1 D:yz	-7.682	1.20	3 Fe
			1.23%	1 P:z	-5.608	0.67	137 C
			1.05%	1 P:z	-5.608	0.67	135 C
			1.04%	1 D:yz	-7.682	1.20	4 Fe
			1.03%	1 P:y	-5.608	0.67	134 C
-1.725	0.00	186 A	10.70%	1 D:xz	-7.682	1.20	4 Fe
			8.80%	1 D:x2-y2	-7.682	1.20	4 Fe
			7.70%	1 D:xz	-7.682	1.20	3 Fe

			6.73%	1	D:xy	-7.682	1.20	4	Fe
			6.25%	1	D:x2-y2	-7.682	1.20	3	Fe
			4.85%	1	D:xy	-7.682	1.20	3	Fe
			4.15%	1	D:z2	-7.682	1.20	4	Fe
			3.12%	1	P:x	-5.608	0.67	120	C
			3.02%	1	D:z2	-7.682	1.20	3	Fe
			2.32%	1	P:x	-5.608	0.67	146	C
			2.28%	1	P:x	-5.608	0.67	109	C
			2.21%	1	P:x	-5.608	0.67	122	C
			1.70%	1	P:x	-5.608	0.67	131	C
			1.68%	1	P:x	-5.608	0.67	124	C
			1.64%	1	P:x	-5.608	0.67	127	C
			1.52%	1	P:x	-5.608	0.67	147	C
			1.36%	1	P:x	-5.608	0.67	111	C
			1.33%	1	P:y	-5.608	0.67	109	C
			1.24%	1	P:x	-5.608	0.67	130	C
			1.10%	1	P:x	-5.608	0.67	125	C
			1.05%	1	P:y	-5.608	0.67	111	C
-1.720	0.00	187 A	10.66%	1	D:xz	-7.682	1.20	3	Fe
			8.85%	1	D:x2-y2	-7.682	1.20	3	Fe
			7.62%	1	D:xz	-7.682	1.20	4	Fe
			6.72%	1	D:xy	-7.682	1.20	3	Fe
			6.36%	1	D:x2-y2	-7.682	1.20	4	Fe
			4.78%	1	D:xy	-7.682	1.20	4	Fe
			3.70%	1	D:z2	-7.682	1.20	3	Fe
			3.07%	1	P:x	-5.608	0.67	122	C
			2.61%	1	D:z2	-7.682	1.20	4	Fe
			2.39%	1	P:x	-5.608	0.67	124	C
			2.19%	1	P:x	-5.608	0.67	120	C
			2.17%	1	P:x	-5.608	0.67	127	C
			1.73%	1	P:x	-5.608	0.67	130	C
			1.72%	1	P:x	-5.608	0.67	146	C
			1.53%	1	P:x	-5.608	0.67	109	C
			1.52%	1	P:x	-5.608	0.67	125	C
			1.34%	1	P:x	-5.608	0.67	129	C
			1.30%	1	P:y	-5.608	0.67	127	C
			1.23%	1	P:x	-5.608	0.67	131	C
			1.08%	1	P:x	-5.608	0.67	147	C
			1.01%	1	P:y	-5.608	0.67	129	C

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