Supplementary Information for

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

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Contents:

1. Experimental details S2
2. NMR spectra S6
3. Variable temperature NMR spectra S19
4. X-ray crystallography data S21
5. DFT calculations S27
6. References S51

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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 (Et₂O), and tetrahydrofuran (THF) were purified using a two-column solid-state purification system by the method of Grubbs¹ 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-δ₆ (C₆D₆), THF-δ₈ (C₄D₈O) and toluene-δ₈ (C₇D₈) 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. (NN⁵¹TB₃S)YI(THF)₂,² (NN⁵¹TB₃S)Lal(THF),² [(NN⁵¹TB₃S)Y(THF)]₂(μ-C₁₀H₈)(Y₂-naph),³ and [(NN⁵¹TB₃S)Y₂(μ-C₆H₅Ph)(K(OEt₂))]₂ (Y₂K₂-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 C₆D₆ or C₇D₈ unless otherwise specified. Chemical shifts are reported with respect to internal solvent (C₆D₆ at 7.16 ppm or C₇D₈ at 2.09 ppm). CHN analyses were performed in house on a CE-440 Elemental Analyzer manufactured by Exeter Analytical, INC.

**Synthesis of Y₂-stilbene:** (NN⁵¹TB₃S)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 / isopropanol bath. 1.25 equiv KC₈ (0.1280 g, 0.377 mmol) were weighed in a scintillation vial. THF (10 mL) was added to make a yellow solution which was warmed 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 Et₂O and an orange solid was collected at 50 °C. 1H NMR (500 MHz, C₆D₆, 50 °C) 2.50 (δ, s, 2H, PhCH₂OPh), 3.00 (δ, br s, 8H, C₆H of Cp rings), 3.58 (δ, br s, 8H, C₆H of Cp rings), 3.92 (δ, br s, 8H, C₆H of Cp rings) ppm. ¹³C NMR (126 MHz, C₆D₆, 50 °C) δ, ppm: 134.9 (ipso-C of (E)-stilbene), 115.3 (para-C of (E)-stilbene), 107.0 (CN of Cp rings), 70.1, 67.7 and 66.8 (CH of Cp rings), 66.8 (CH₂O of THF), 58.9 (PhCHCHPh), 28.0 ((CH₃)₃C), 25.4 (CH₂CH₂O of THF), 20.6 ((CH₃)₃C), and -0.9 and -1.1 (SiCH₃). 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 C₆₆H₁₀₄N₄O₂Fe₂Y₂Si₄, Mₘ = 1387.430: C, 57.14; H, 7.56; N, 4.04. Found: C, 57.03; H, 7.54; N, 3.74.
Synthesis of La2-stilbene: (NN\textsuperscript{TBS})La(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/isopropanol bath. 1.25 equiv KC\textsubscript{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 La2-stilbene in aromatic solvents is higher than that of Y2-stilbene. The residual KI could be removed by extraction of La2-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\textsubscript{2}O and a brown solid was collected on a medium frit after filtration. Yield: 0.0927 g, 48.6%. Single crystals of La2-stilbene were grown from a toluene solution layerd with hexanes stored in a -35 °C freezer. Due to the lability of coordinating solvent molecules, La2-stilbene contained both Et\textsubscript{2}O and THF with a total amount of one solvent molecule per lanthanum. 1H NMR (500 MHz, C\textsubscript{6}D\textsubscript{6}, 25 °C) δ, ppm: 7.28 and 6.90 (t, 2H each, H\textsubscript{rings}), 3.27 and 3.14 (br s, 4H each, Cs of Cp rings), 1.33 (br s, C\textsubscript{Et\textsubscript{2}O}), 1.40 (br s, 4H, C\textsubscript{Et\textsubscript{2}O} of THF), 20.9 ((CH\textsubscript{3})\textsubscript{3}C), 25.3 (CH\textsubscript{2}CH\textsubscript{2}O of THF), 20.6 ((CH\textsubscript{3})\textsubscript{3}C), 14.6 (CH\textsubscript{2}CH\textsubscript{2}O of Et\textsubscript{2}O), and -1.7 and -2.0 (Si(CH\textsubscript{3})\textsubscript{3}). Anal. (%): Calcd. for C\textsubscript{66}H\textsubscript{108}N\textsubscript{4}O\textsubscript{2}Fe\textsubscript{2}La\textsubscript{2}Si\textsubscript{4}, M\textsubscript{w} = 1491.462: C, 53.15; H, 7.08; N, 3.38. Found: C, 52.22; H, 6.94; N, 3.72.

Synthesis of Y-stilbene-K: (NN\textsuperscript{TBS})YI(THF)\textsubscript{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 (6 mL) was added to make a yellow solution which was cooled down to -78 °C with a dry ice/isopropanol bath. 2.5 equiv KC\textsubscript{8} (0.1350 g, 0.0794 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 remaining solid was extracted with Et\textsubscript{2}O. All volatiles were removed under reduced pressure. The solubility of Y-stilbene-K in aromatic solvents is higher than that of Y\textsubscript{2}-stilbene. 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\textsubscript{2}-stilbene-K as determined by 1H NMR spectroscopy. Yield: 0.1650 g, 53.5%. Attempts to grow single crystals of Y\textsubscript{2}-stilbene-K-crown were not successful due to loss of solvent upon crytallization. The crown ether version of Y\textsubscript{2}-stilbene-K was grown from a concentrated hexanes solution with a formula of [(NN\textsuperscript{TBS})YI(THF)](18-crown-6)(\mu-stilbene) as determined by 1H NMR spectroscopy. Yield: 0.1650 g, 53.5%. Attempts to grow single crystals of Y\textsubscript{2}-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\textsubscript{2}-stilbene-K to afford the crown ether version Y\textsubscript{2}-stilbene-K-crown to increase crystallinity. Single crystals of Y\textsubscript{2}-stilbene-K-crown were grown from a concentrated hexanes solution with a formula of [(NN\textsuperscript{TBS})YI(THF)][(18-crown-6)](\mu-stilbene). 1H NMR (500 MHz, C\textsubscript{6}D\textsubscript{6}, 25 °C) δ, ppm: 7.00, 6.82, 6.49, 6.08, and 5.50 (br s, 2H each, CH of phenyl rings of (E)-stilbene), 3.74 (br s, overlapped by THF peaks, 2H, PhCH\textsubscript{2}CH\textsubscript{Ph}), 4.13, 3.99, 3.41, and 3.26 (br s, 2H each, CH of Cp rings), 3.74 (br s, 4H, CH\textsubscript{2}O of THF), 1.40 (br s, 4H, CH\textsubscript{2}CH\textsubscript{2}O of THF), 1.20 (s, 36H, (CH\textsubscript{3})\textsubscript{3}C), and 0.54 and 0.46 (br s, 12H total, Si(CH\textsubscript{3})\textsubscript{3}). 13C NMR (126 MHz, C\textsubscript{6}D\textsubscript{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 (CN of Cp rings), 70.9, 67.0 and 66.2 (CH of Cp rings), 97.7 (CH\textsubscript{2}O of THF), 66.2 (CH\textsubscript{2}O of Et\textsubscript{2}O), 65.2 (PhCH\textsubscript{2}CH\textsubscript{2}O of THF), 27.7 ((CH\textsubscript{3})\textsubscript{3}C), 25.3 (CH\textsubscript{2}CH\textsubscript{2}O of THF), 20.6 ((CH\textsubscript{3})\textsubscript{3}C), 14.6 (CH\textsubscript{2}CH\textsubscript{2}O of Et\textsubscript{2}O), and -1.7 and -2.0 (Si(CH\textsubscript{3})\textsubscript{3}). Anal. (%): Calcd. for C\textsubscript{60}H\textsubscript{108}O\textsubscript{2}FeLa\textsubscript{2}Si\textsubscript{4}, M\textsubscript{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\textsubscript{2}-anth: (NN\textsuperscript{TBS})YI(THF)\textsubscript{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 / isopropanol bath. 1.25 equiv KC₈ (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 Et₂O and was collected on a medium frit after filtration. Yield: 0.1091 g, 62.3%. Single crystals of Y₂-anth were grown from a Et₂O solution in a -35 °C freezer. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ, ppm: 5.94 and 5.69 (t, 4H each, CᵥHᵥ-CᵥHᵥ of anthracene), 3.92 (s, 2H, CᵥHᵥ-CᵥHᵥ of anthracene), 4.22, 3.89, 3.85, and 3.76 (br s, 4H each, CᵥHᵥ of Cp rings), 3.94 (br s, 8H, CH₂O of THF), 1.44 (br s, 8H, CH₃CH₂O of THF), 1.04 (s, 36H, (C₆H₃)₃C), and 0.22 and 0.17 (br s, 12H each, SiCᵥH₃). ¹³C NMR (126 MHz, C₆D₆, 50 °C) δ, ppm: 143.7, 121.3, 114.0, and 82.4 (C and CᵥH of anthracene), 108.3 (CN of Cp rings), 71.4, 69.3 and 65.6 (CH of Cp rings), 68.6 (CH₂O of THF), 27.9 ((CH₃)₃C), 25.7 (CH₂CH₂O of THF), 20.6 ((CH₃)₃C), and -1.1 and -2.8 (SiCH₃). Anal. (%): Calcd. for C₆₆H₁₀₂N₄O₂Fe₂Y₂Si₄, Mw = 1385.414: C, 57.22; H, 7.42; N, 4.04. Found: C, 56.64; H, 7.21; N, 3.97.

**Reaction of Y₂-stilbene and KC₈:** Y₂-stilbene (0.0335 g, 0.024 mmol) was dissolved in THF (3 mL) and cooled down to -78 °C with a dry ice / isopropanol bath. 2.5 equiv KC₈ (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 KC₈. The volatiles were removed under reduced pressure. The crude product was identified as Y-stilbene-K by ¹H NMR spectroscopy.

**Reaction of Y₂K₂-biph and (E)-stilbene:** Y₂K₂-biph (0.0250 g, 0.017 mmol) was dissolved in cold THF (3 mL) and cooled down to -78 °C with a dry ice / isopropanol bath. (E)-stilbene (0.0062 g, 0.034 mmol) was dissolved in THF (1 mL) and added dropwise to Y₂K₂-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 ¹H NMR spectroscopy and biphenyl was identified as a byproduct.

**Reaction of Y₂-naph and (E)-stilbene:** Y₂-naph (0.0065 g, 0.005 mmol) and excess (E)-stilbene (0.0026 g, 0.014 mmol) were dispersed in ca. 0.5 mL C₆D₆ in a J-Young tube. The reaction was monitored by routine ¹H NMR spectroscopy. The formation of Y₂-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 Y₂-naph to Y₂-stilbene.

**Reaction of Y₂-stilbene and anthracene:** Y₂-stilbene (0.0079 g, 0.006 mmol) and excess anthracene (0.0024 g, 0.013 mmol) were dispersed in ca. 0.5 mL C₆D₆ in a J-Young tube. The reaction was monitored by routine ¹H NMR spectroscopy. The formation of Y₂-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 Y₂-stilbene to Y₂-anth.

**Thermodecomposition of Y₂-stilbene:** Y₂-stilbene (0.0125 g, 0.009 mmol) was dispersed in ca. 0.5 mL C₆D₆ 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 Y₂-stilbene was transformed. Bibenzyl
was identified as a decomposition product but we were not able to identify the yttrium decomposition products.

**Reaction of Y₂-stilbene and phenylacetylene: Y₂-stilbene** (0.1600 g, 0.115 mmol) was dispersed in toluene (6 mL) and was cooled down to -78 °C with a dry ice / isopropanol 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 C₁₄H₁₄ isomers (the majority was bibenzyl) by ¹H NMR spectroscopy. Single crystals of the product were grown from a concentrated toluene solution layered with n-pentane with the formula of [(NNTBS)₃Y(THF)][(NNTBS)₃Y(µ-CCPh)]₂. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ, ppm: 7.73 (d, 2H, ortho-C₆H₆ of phenyl ring), 7.03 (t, 2H, meta-C₆H₆ of phenyl ring), 6.98 (t, 1H, para-C₆H₆ of phenyl ring), 3.93 (br s, 2H, CH of Cp rings), 3.78 (br s, 6H, CH of Cp rings), 1.15 (s, 18H, (C₆H₃)₃C), and 0.64 (s, 12H, SiC₆H₃). ¹³C NMR (126 MHz, C₆D₆, 50 °C) δ, ppm: 139.0 (t, C₆C₆Ph), 132.8, 129.7, 128.7, and 123.3 (C and CH of phenyl ring), 106.0 (CN of Cp rings), 72.0 (CCPh), 67.2 and 66.7 (CH of Cp rings), 28.1 ((CH₃)₃C), 20.5 ((CH₃)₃C), and -0.6 (SiCH₃). Anal. (%): Calcd. for C₆₄H₉₄N₄OFe₂Y₂Si₄, Mₑw = 1337.329, with two hexanes molecule (2*C₆H₁₄, Mₑw = 2*86.178): C, 60.47; H, 8.15; N, 3.71. Found: C, 60.27; H, 7.84; N, 4.02.

*Note:* The ¹H 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 C₆D₆), 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 C₁₄H₁₄ 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 Sc₂-naph with phenylacetylene: mixtures of C₁₀H₁₀ isomers were present.

**Reaction of Y₂-stilbene and 2,2’-bipyridine: Y₂-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 ¹H 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%. ¹H NMR (500 MHz, C₆D₆, 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 (NNTBS)₂Y(bipy) was confirmed by comparison to the analogous (NNTBS)₃Sc(bipy) complex.⁴ Anal. (%): Calcd. for C₃₆H₅₄N₄OFe₂Y₂Si₄, Mₑw = 759.778, with one hexanes molecule (C₆H₁₄, Mₑw = 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 $\text{Y}_2$-stilbene (500 MHz, $\text{C}_6\text{D}_6$, 50 °C)

$^{13}$C NMR spectrum of $\text{Y}_2$-stilbene (126 MHz, $\text{C}_6\text{D}_6$, 50 °C)
HMBC NMR spectrum of Y₂-stilbene (500 MHz, C₆D₆, 50 °C)
$^1$H NMR spectrum of La$_2$-stilbene (500 MHz, C$_6$D$_6$, 25 °C)

$^{13}$C NMR spectrum of La$_2$-stilbene (126 MHz, C$_6$D$_6$, 25 °C)
HMBC NMR spectrum of La₂-stilbene (500 MHz, C₆D₆, 25 °C)
$^1$H NMR spectrum of Y-stilbene-K (500 MHz, C$_6$D$_6$, 25 °C)

$^{13}$C NMR spectrum of Y-stilbene-K (126 MHz, C$_6$D$_6$, 25 °C)
HMBC NMR spectrum of **Y-stilbene-K** (500 MHz, C$_6$D$_6$, 25 °C)
$^1$H NMR spectrum of $\text{Y}_2$-anth (500 MHz, C$_6$D$_6$, 25 °C)

$^{13}$C NMR spectrum of $\text{Y}_2$-anth (126 MHz, C$_6$D$_6$, 25 °C)
HMBC NMR spectrum of **Y₂-anth** (500 MHz, C₆D₆, 25 °C)
$^1$H NMR spectrum of [(NN$^\text{TBS}$)Y(CCPh)]$_2$ (500 MHz, C$_6$D$_6$, 25 °C)

$^{13}$C NMR spectrum of [(NN$^\text{TBS}$)Y(CCPh)]$_2$ (126 MHz, C$_6$D$_6$, 25 °C)
HMBC NMR spectrum of [(NNTBS)Y(CCPh)]₂ (500 MHz, C₆D₆, 25 °C)
$^1$H NMR spectrum of J-Young scale reaction of Y$_2$-stilbene and excess phenylacetylene (300 MHz, C$_6$D$_6$, 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$_6$D$_6$, 25 °C)

*Note:* Same as for the last spectrum.
\(^1\)H NMR spectrum of \((\text{NN}^{\text{TBS}})\text{Y(THF)(bipy)}\) (500 MHz, \(\text{C}_6\text{D}_6\), 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$_7$D$_8$)

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 $^\circ$C to 62 $^\circ$C, 500 MHz, C$_7$H$_8$)

**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 $^\circ$C and presented an asymmetric structure in solution below -30 $^\circ$C. The weaker binding between yttrium and the anthracene dianion may explain this difference.
4. X-ray crystallography data

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

**Figure SX1.** Thermal-ellipsoid (50% probability) representation of the crystallographically independent atoms in \textbf{Y}_2\text{-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 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 \textit{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 ≤ h ≤ 14, -15 ≤ k ≤ 15, -22 ≤ l ≤ 22) were collected at \(T = 100(2)\) K with \(2\theta_{\text{max}} = 58.47°\), of which 9520 were unique. The residual peak and hole electron densities were 0.71 and -0.41 eÅ\(^{-3}\). The least-squares refinement converged normally with residuals of \(R_1 = 0.0374\) and GOF = 1.035. Crystal and refinement data for \textbf{Y}_2\text{-stilbene}: formula \(\text{C}_{80}\text{H}_{103}\text{N}_{4}\text{Si}_{4}\text{Fe}_{2}\text{O}_{2}\text{Y}_{2}\cdot 2(\text{C}_7\text{H}_8)\), space group \text{P}-1, \(a = 11.210(1)\), \(b = 11.7733(11)\), \(c = 16.4895(15)\), \(\alpha = 90.787(1)\), \(\beta = 109.724(1)\), \(\gamma = 106.301(1)°\), \(V = 1952.0(3) \text{Å}^3\), \(Z = 1\), \(\mu = 1.945 \text{ mm}^{-1}\), \(F(000) = 830\), \(R_1 = 0.0493\) and \(wR_2 = 0.0967\) (based on all data, \(I > 2\sigma(I)\)).
[(NN^{TBS})Y(THF)][(\mu\text{-stilbene})[K(18\text{-crown-6})]] (Y\text{-stilbene}-K\text{-crown})

Figure SX2. Thermal-ellipsoid (50% probability) representation of Y\text{-stilbene}-K\text{-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 ≤ h ≤ 17, -18 ≤ k ≤ 18, -35 ≤ l ≤ 35) were collected at T = 100(2) K with 2θ_{max} = 52.74°, of which 12297 were unique. The residual peak and hole electron densities were 0.45 and -0.98 eÅ^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0498 and GOF = 1.017. Crystal and refinement data for Y\text{-stilbene}-K\text{-crown}: formula C_{40}H_{56}N_{2}Si_{2}FeO_{2}\cdot C_{12}H_{24}O_{6}\cdot K\cdot C_{6}H_{14}, space group P2_1/n, a = 14.082(4), b = 15.074(4), c = 28.493(8), β = 90.343(4)°, V = 6048(3) Å³, Z = 4, μ = 1.353 mm^{-1}, F(000) = 2496, R_1 = 0.0840 and wR_2 = 0.1197 (based on all data, I > 2σ(I)).
Figure SX3. Thermal-ellipsoid (50% probability) representation of \( \text{Y}_2\text{-anth} \). 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 ≤ h ≤ 18, -33 ≤ k ≤ 33, -25 ≤ l ≤ 25) were collected at \( T = 100(2) \) K with \( 2\theta_{\text{max}} = 52.95° \), of which 16317 were unique. The residual peak and hole electron densities were 1.09 and -0.52 eÅ\(^{-3}\). The least-squares refinement converged normally with residuals of \( R_1 = 0.0479 \) and GOF = 1.038. Crystal and refinement data for \( \text{Y}_2\text{-anth} \): formula \( \text{C}_{66}\text{H}_{102}\text{N}_4\text{Si}_4\text{Fe}_2\text{O}_2\text{Y}_2 \), space group \( P2_1/c \), \( a = 15.097(8) \), \( b = 26.925(15) \), \( c = 20.626(11) \), \( \beta = 108.031(6)° \), \( V = 7973(8) \text{ Å}^3 \), \( Z = 4 \), \( \mu = 1.896 \text{ mm}^{-1} \), \( F(000) = 2912 \), \( R_1 = 0.0740 \) and \( wR_2 = 0.1322 \) (based on all data, \( I > 2\sigma(I) \)).
[(NN\textsuperscript{TBS})La(THF)]\textsubscript{2}(\mu\text{-stilbene}) (La\textsubscript{2}-stilbene)

Figure SX4. Thermal-ellipsoid (50% probability) representation of the crystallographically independent atoms in La\textsubscript{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 ≤ h ≤ 14, -14 ≤ k ≤ 14, -20 ≤ l ≤ 20) were collected at \(T = 100(2)\) K with 2\(\theta\)\textsubscript{max} = 52.74°, of which 4661 were unique. The residual peak and hole electron densities were 1.74 and -2.30 eÅ\(^{-3}\). The least-squares refinement converged normally with residuals of \(R\textsubscript{1} = 0.0551\) and \(\text{GOF} = 1.077\). Crystal and refinement data for La\textsubscript{2}-stilbene: formula C\textsubscript{66}H\textsubscript{102}N\textsubscript{4}Si\textsubscript{4}Fe\textsubscript{2}O\textsubscript{2}La\textsubscript{2}·2(C\textsubscript{7}H\textsubscript{7}), space group P-1, \(a = 11.323(4)\), \(b = 11.909(5)\), \(c = 16.767(7)\), \(\alpha = 89.093(5)\), \(\beta = 70.339(5)\), \(\gamma = 70.830(5)°\), \(V = 1999.6(13)\) Å\(^3\), \(Z = 1\), \(\mu = 1.508\) mm\(^{-1}\), F(000) = 862, \(R\textsubscript{1} = 0.0614\) and \(wR\textsubscript{2} = 0.1421\) (based on all data, \(I > 2\sigma(I)\)).
(NN\textsuperscript{TBS})Y(THF)(bipy)

**Figure SX5.** Thermal-ellipsoid (50% probability) representation of (\textit{NN}\textsuperscript{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 \textit{n}-pentane. A total of 40512 reflections (-13 ≤ \textit{h} ≤ 13, -21 ≤ \textit{k} ≤ 21, -27 ≤ \textit{l} ≤ 27) were collected at \textit{T} = 100(2) K with 2\textit{θ}_{\text{max}} = 52.74°, of which 8213 were unique. The residual peak and hole electron densities were 1.68 and -0.75 eÅ\textsuperscript{-3}. The least-squares refinement converged normally with residuals of \textit{R}_1 = 0.0524 and \textit{GOF} = 1.045. Crystal and refinement data for [\textit{NN}\textsuperscript{TBS})Y](bipy): formula C\textsubscript{36}H\textsubscript{54}N\textsubscript{4}Si\textsubscript{2}FeOY·0.5(C\textsubscript{6}H\textsubscript{14}), space group \textit{P2}_1/c, \textit{a} = 11.115(8), \textit{b} = 16.898(12), \textit{c} = 21.869(15), \textit{β} = 84.720(4)°, \textit{V} = 4034(5) Å\textsuperscript{3}, \textit{Z} = 4, \mu = 1.885 mm\textsuperscript{-1}, \textit{F}(000) = 1696, \textit{R}_1 = 0.0842 and \textit{wR}_2 = 0.1460 (based on all data, \textit{I} > 2\sigma(\textit{I})).
Figure SX6. Thermal-ellipsoid (50% probability) representation of \( [(\text{NNTBS})\text{Y(THF)}][(\text{NNTBS})\text{Y}](\mu\text{-CCPh})_2] \). 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 1.446(5), Y1-C1-Y2 98.9(1), C1-C2-C3 1.80.0(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 ≤ h ≤ 15, -21 ≤ k ≤ 21, -24 ≤ l ≤ 24) were collected at \( T = 100(2) \) K with \( 2θ_{\text{max}} = 52.74° \), of which 4661 were unique. The residual peak and hole electron densities were 1.87 and -1.21 eÅ\(^{-3}\). The least-squares refinement converged normally with residuals of \( R_1 = 0.0463 \) and GOF = 1.060. Crystal and refinement data for \( [(\text{NNTBS})\text{Y(THF)}][(\text{NNTBS})\text{Y}](\mu\text{-CCPh})_2] \): formula \( \text{C}_64\text{H}_{92}\text{N}_4\text{Si}_4\text{Fe}_2\text{O}_2\text{Y}_2 \), space group \( P-1 \), \( a = 12.115(4) \), \( b = 17.497(6) \), \( c = 19.614(6) \), \( α = 82.581(4) \), \( β = 84.720(4) \), \( γ = 72.458(4) ° \), \( V = 3925(2) \) Å\(^3\), \( Z = 2 \), \( μ = 1.922 \text{ mm}^{-1} \), \( F(000) = 1396 \), \( R_1 = 0.0581 \) and \( wR_2 = 0.1367 \) (based on all data, \( I > 2σ(I) \)).
5. DFT calculations

General considerations: Computational studies were performed with ADF2013.01. For yttrium, lanthanum, and iron atoms, standard triple-\(\zeta\) STA basis sets from the ADF database ZORA TZP, while for all the other atoms, standard double-\(\zeta\) 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](image)

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 [°].

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Figure SX8. Frontier molecular orbitals for Y₂-stilbene: HOMO-1 (top left), HOMO-2 (top right), LUMO (bottom left), LUMO+1 (bottom right).

Figure SX9. Frontier molecular orbitals for La₂-stilbene: HOMO-1 (top left), HOMO-2 (top right), LUMO (bottom left), LUMO+1 (bottom right).
## Optimized parameters for \( \text{Y}_2\text{-stilbene} \)

### Coordinates

| 1.H | -1.623252 | 0.134218 | 7.931257 |
| 2.H | -2.121956 | 1.820232 | 8.147310 |
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| 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 |
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| 48.C| -3.786000 | 8.769365 | 11.136743 |
| 49.H| -4.108617 | 8.174013 | 12.006626 |
| 51.C| -2.496021 | 9.543968 | 11.378561 |
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**Note:** The coordinates are given in Angstroms (Å).
## Mulliken Populations

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.

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### BOND-ORDER ANALYSIS

**DIST. [Å]**

**BOND-ORDERS**

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**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.

<table>
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<th>E(eV)</th>
<th>Occ</th>
<th>MO</th>
<th>%</th>
<th>SFO (first member)</th>
<th>E(eV)</th>
<th>Occ</th>
<th>Fragment</th>
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<td>138 Fe</td>
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<tr>
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<td></td>
<td></td>
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<td>1 D:z2</td>
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<td>1.20</td>
<td>138 Fe</td>
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<tr>
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<td></td>
<td></td>
<td>9.80%</td>
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<td></td>
<td></td>
<td>8.94%</td>
<td>1 D:yz</td>
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<td>1.20</td>
<td>137 Fe</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5.68%</td>
<td>1 D:z2</td>
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<td>1.20</td>
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<tr>
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<td></td>
<td></td>
<td>4.18%</td>
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<td></td>
<td>3.11%</td>
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<tr>
<td></td>
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<td>1.81%</td>
<td>1 P:y</td>
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<td>1.00</td>
<td>145 N</td>
</tr>
<tr>
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<td></td>
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<td>1.52%</td>
<td>1 P:x</td>
<td>-5.608</td>
<td>0.67</td>
<td>124 C</td>
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<tr>
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<tr>
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<td>1 P:x</td>
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<td>137 Fe</td>
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<tr>
<td></td>
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<tr>
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<td>1 P:y</td>
<td>-7.403</td>
<td>1.00</td>
<td>146 N</td>
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</table>

**Sum:**

157.0638 168.0680 180.6360 180.6360 180.6360 180.6360
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:zx  -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:zx  -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
 8.75%  1 D:xz  -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:zx  -7.682  1.20  137 Fe
 4.78%  1 D:xz  -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:zx  -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:zx  -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
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<th>Energy</th>
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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
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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
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1.65%  1 P:y  -5.608  0.67   103 C
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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
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4.10%  1 D:yz  -7.682  1.20   137 Fe
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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
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1.13%  1 P:x  -5.608  0.67  105 C
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1.01%  1 P:x  -5.608  0.67  102 C
### Optimized parameters for La2-stilbene

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Optimized parameters for La2-stilbene
### Mulliken Populations

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.

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**Bond-Order Analysis**

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Electronic Supplementary Material (ESI) for Chemical Communications
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