**Supporting information for**

# Mechanistic Insight into N=N Cleavage by a Low-Coordinate Iron(II) Hydride Complex

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**Kinetic Experiments.**

1. Thermolysis of $L^{tBu}FeNPhNHPh$ at different temperatures. A J. Young resealable NMR tube was charged with $L^{tBu}FeNPhNHPh$ (8.5 mg) and $C_7D_8$ or $C_6D_6$ (0.30 mL). The NMR tube was placed into the NMR probe, which was already equilibrated at the appropriate temperature (358 K unless otherwise specified). After the sample had equilibrated for 2 min, $^1H$ NMR spectra were recorded at preset times using an automated program. Fourier transform, phasing, calibrating and integrating of each spectrum was done using MestReC. The plot of normalized $L^{tBu}FeNPhNHPh$ concentration (y) *vs.* time (M0) was fit to the general, integrated equation: y = m1 + m2*exp(-M0*M3), where m1, m2 and M3 are variables, M3 being the first order rate constant. For this purpose, KaleidaGraph 3.51 was used. The error bars on the rate constant came either from the least-squares fit to the data (Method A) or the range of values seen in multiple experiments (Method B). Temperatures in the NMR probe were calibrated using 100% ethylene glycol.[1]

2. Thermolysis of $L^{tBu}FeNPhNHPh$ in the presence of PhN=NPh. A solution of $L^{tBu}FeNPhNHPh$ (10.0 mg), PhN=NPh (2.5 mg), and $C_6D_6$ (0.30 mL) was heated to 358 K. First order rate constant obtained was $7.0 \pm 0.1 \times 10^{-4}$ $s^{-1}$. Error estimation used Method A. Therefore, *added diazene does not inhibit the rate of the reaction.*

3. Thermolysis of $L^{tBu}FeNPhNHPh$ in the presence of $[L^{tBu}FeH]_2$. A solution of $L^{tBu}FeNPhNHPh$ (8.8 mg), $[L^{tBu}FeH]_2$ (4.0 mg), and $C_6D_6$ (0.30 mL) was heated to 358 K. First order rate constant obtained was $5.3 \pm 0.7 \times 10^{-4}$ $s^{-1}$. Error estimation used Method B.

4. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of $L^{tBu}$FeCl. A solution of $L^{tBu}$FeNPhNHPh (8.3 mg), $L^{tBu}$FeCl (2.2 mg), and $C_7D_8$ (0.30 mL) was heated to 315 K. Kinetic plot showed the presence of an induction period.

5. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of $L^{tBu}$FeNPhNPh. A solution of $L^{tBu}$FeNPhNHPh (8.1 mg), $L^{tBu}$FeNPhNPh (3.1 mg), and $C_7D_8$ (0.30 mL) was heated to 315 K. Kinetic plot showed the absence of induction period.

6. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of $L^{tBu}$FeKCl(solvent)$_x$. A solution of $L^{tBu}$FeNPhNHPh (8.0 mg) and $L^{tBu}$FeKCl(solvent)$_x$ (prepared *in situ* by reacting $L^{tBu}$FeCl (2.5 mg) with $KC_8$ (0.6 mg) in $C_7D_8$ (0.30 mL)[2]) was heated to 315 K. Kinetic plot showed the absence of induction period.

7. Thermolysis of $L^{tBu}$FeNPhNHPh in THF-$d_8$. A solution of $L^{tBu}$FeNPhNHPh (8.5 mg) and THF-$d_8$ (0.3 mL) was heated to 352 K. First order rate constant obtained was 4.6 $\pm$ 0.2 $\times$ $10^{-4}$ $s^{-1}$. Error estimation used Method A.

8. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of lutidine. A solution of $L^{tBu}$FeNPhNHPh (10.0 mg), lutidine (1.6 μL), and $C_6D_6$ (0.40 mL) was heated to 359 K. First order rate constant obtained was 6.5 $\pm$ 0.2 $\times$ $10^{-4}$ $s^{-1}$. Error estimation used Method A.

9. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of $Ph_3CH$. A solution of $L^{tBu}$FeNPhNHPh (3.0 mg), $Ph_3CH$ (34 mg), and $C_6D_6$ (0.30 mL) was heated to 358 K. First order rate constant obtained was 9.8 $\pm$ 0.3 $\times$ $10^{-4}$ $s^{-1}$. Error estimation used Method A.

10. Thermolysis of $L^{tBu}$FeNPhNHPh in the presence of DHA. A solution of $L^{tBu}$FeNPhNHPh (6.0 mg), DHA (19 mg), and $C_6D_6$ (0.30 mL) was heated to 358 K. First order rate constant obtained was $9.3 \pm 0.2 \times 10^{-4}$ $s^{-1}$. Error estimation used Method A.

**Trapping and Control Experiments Related to Scheme 3**

$L^{tBu}$FeNPhNHPh and 3-hexyne (attempt to trap LFeH). A J. Young resealable NMR tube was charged with $L^{tBu}$FeNPhNHPh (8.0 mg) and $C_6D_6$ (0.20 mL). To this was added 3-hexyne (0.12 mL). The contents of the NMR tube were mixed for 10 minutes at room temperature and the $^1$H NMR spectrum was recorded. The paramagnetic components of the mixture were identical to that of $L^{tBu}$FeNPhNHPh. The $^1$H NMR spectrum was recorded after heating the contents at 80 °C for 2 h and it showed the presence of $L^{tBu}$FeNHPh (83%) and $L^{tBu}$FeCEtCHEt (17%). This amount of vinyl complex was independent of [hexyne] (see Figure S-5 below).

$L^{tBu}$FeCEtCHEt and PhN=NPh (if trapping of LFeH was reversible, these would react). To test whether the formation of the vinyl complex is reversible, $L^{tBu}$FeCEtCHEt was prepared charging a J. Young resealable NMR tube with $[L^{tBu}FeH]_2$ (14.0 mg), $C_6D_6$ (0.3 mL), and 3-hexyne (3 μL). PhN=NPh (23 mg) was added to the NMR tube containing the vinyl compound. $^1$H NMR spectra were recorded after mixing the contents for 10 minutes at room temperature and after heating the contents at 80 °C for 2 h. The paramagnetic components of the mixture were identical to an experiment without PhN=NPh, showing that the vinyl complex does not revert to the hydride complex.

$L^{tBu}$FeNPhNHPh and $L^{tBu}$FeCEtCHEt (another attempt to see any potential reversibility of attempted trapping experiment). A J. Young resealable NMR tube was charged with $L^{tBu}$FeNPhNHPh (5.3 mg) and $C_6D_6$ (0.1 mL), A scintillation vial was charged with $L^{tBu}$FeCEtCHEt (4.6 mg) and $C_6D_6$ (0.2 mL). The solution of the vinyl complex was added to the NMR tube containing the hydrazido complex, the contents were mixed well for 10 minutes at room temperature, and the $^1$H NMR spectrum was recorded. The NMR spectra showed only the presence of $L^{tBu}$FeNPhNHPh and $L^{tBu}$FeCEtCHEt.

$L^{tBu}$FeNPhNHPh, 3-hexyne, and $[L^{tBu}FeH]_2$ (showing branching ratio in Scheme 3). A J. Young resealable NMR tube was charged with $[L^{tBu}FeH]_2$ (3.0 mg) and $C_6D_6$ (0.1 mL). A scintillation vial was charged with $L^{tBu}$FeNPhNHPh (8.0 mg), $C_6D_6$ (0.1 mL), and 3-hexyne (1.2 μL). This reaction mixture was added to the NMR tube, the contents were mixed well for 10 minutes at room temperature, and the $^1$H NMR spectrum was recorded. The $^1$H NMR spectrum showed the expected ratio of $L^{tBu}$FeNPhNHPh and $L^{tBu}$FeCEtCHEt if all hydride complex had reacted only with 3-hexyne. The resultant mixture was heated at 80 ˚C for 2 h and the $^1$H NMR spectrum showed the presence of $L^{tBu}$FeCEtCHEt and $L^{tBu}$FeNHPh.

**Table S1. Activation Parameters**

| T/ K | 1/T | k/ $s^{-1}$ | ln k | ln(k/T) |
|---|---|---|---|---|
| 363 | $2.75 \times 10^{-3}$ | $13.27 \times 10^{-4}$ | -6.62 | -12.52 |
| 352 | $2.84 \times 10^{-3}$ | $6.93 \times 10^{-4}$ | -7.27 | -13.14 |
| 344 | $2.90 \times 10^{-3}$ | $8.46 \times 10^{-4}$ | -7.07 | -12.92 |
| 338 | $2.95 \times 10^{-3}$ | $3.01 \times 10^{-4}$ | -8.11 | -13.93 |
| 329 | $3.04 \times 10^{-3}$ | $1.13 \times 10^{-4}$ | -9.09 | -14.88 |
| 315 | $3.18 \times 10^{-3}$ | $0.70 \times 10^{-4}$ | -9.57 | -15.32 |

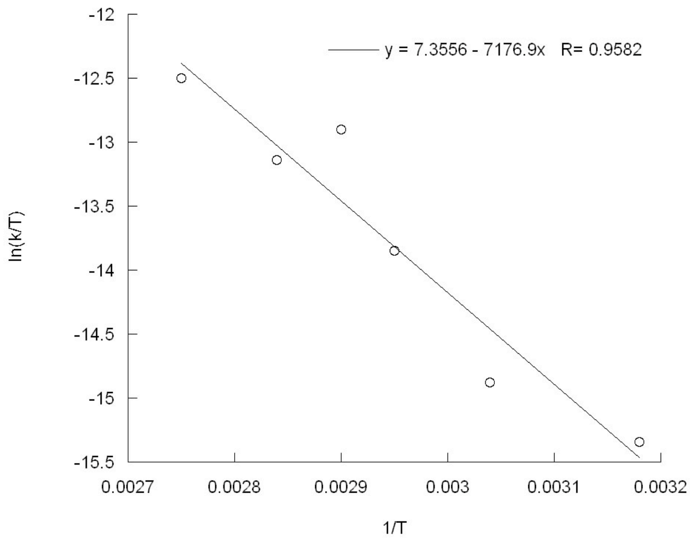


**Figure S-1.** Eyring plot for the reaction of $L^{tBu}FeNPhNHPh \rightarrow L^{tBu}FeNHPh$.

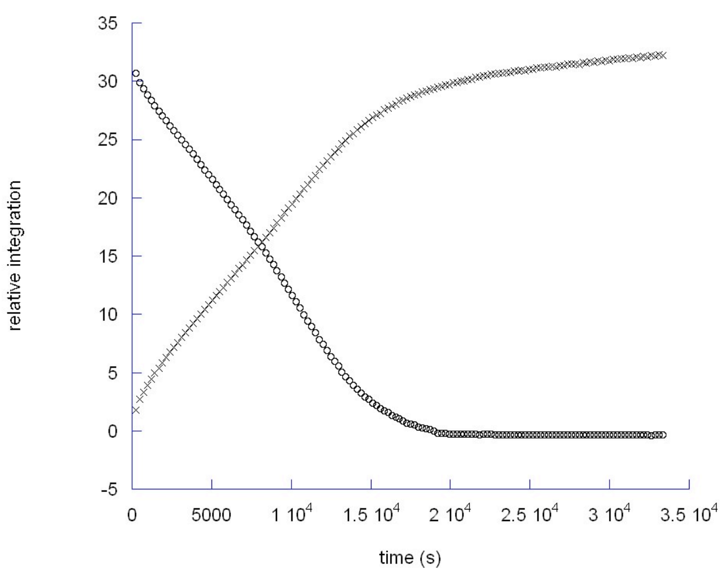


**Figure S-2.** Kinetic data for the conversion of $L^{tBu}FeNPhNHPh$ to $L^{tBu}FeNHPh$ in the presence of $L^{tBu}FeClK(solvent)_x$ at 315 K: (∘), [$L^{tBu}FeNPhNHPh$]; (×), [$L^{tBu}FeNHPh$] .

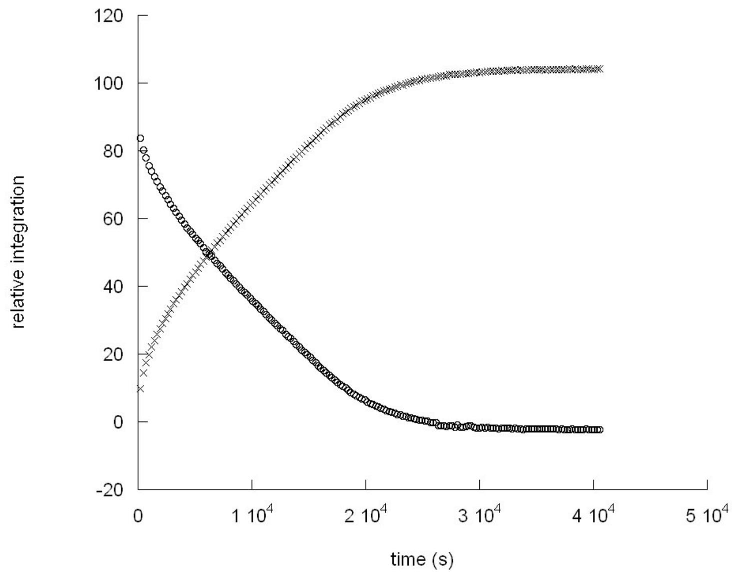


**Figure S-3.** Kinetic data for the conversion of L$^{tBu}$FeNPhNHPh to L$^{tBu}$FeNHPh in the presence of L$^{tBu}$FeNPhNPh at 315 K: ($\circ$), [L$^{tBu}$FeNPhNHPh]; ($\times$), [L$^{tBu}$FeNHPh] .

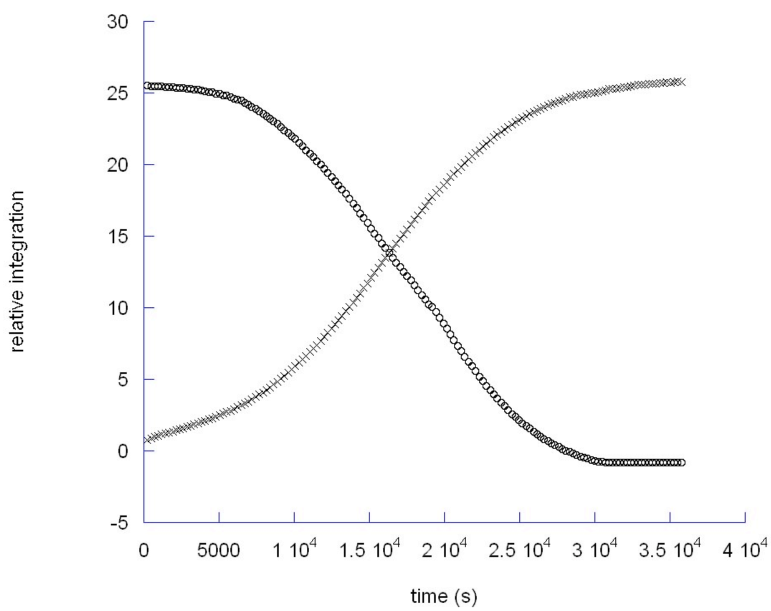


**Figure S-4.** Kinetic data for the conversion of L$^{tBu}$FeNPhNHPh to L$^{tBu}$FeNHPh in the presence of L$^{tBu}$FeCl at 315 K: ($\circ$), [L$^{tBu}$FeNPhNHPh]; ($\times$), [L$^{tBu}$FeNHPh].

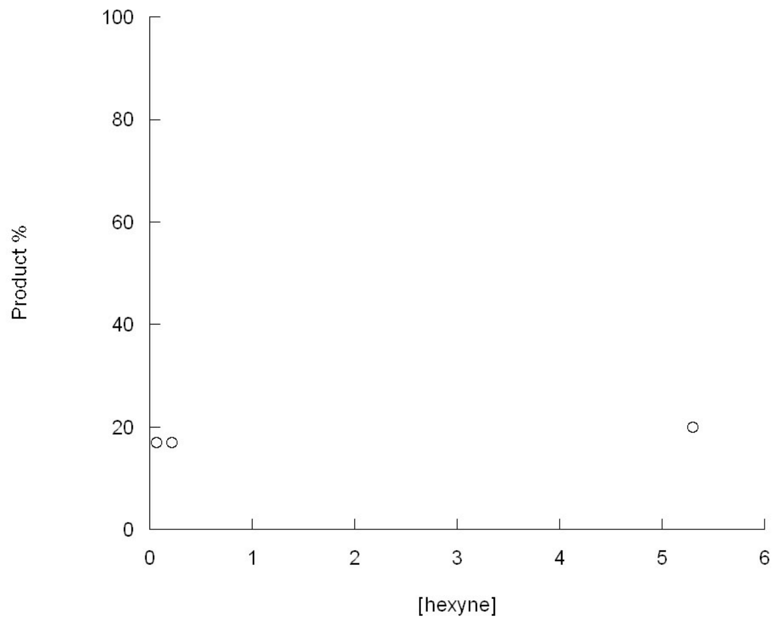


**Figure S-5.** In the decomposition of $L^{tBu}FeNPhNHPh$ with added 3-hexyne, a small amount of vinyl product is observed. This graph shows the amount of vinyl product vs the excess of [hexyne] (in M).

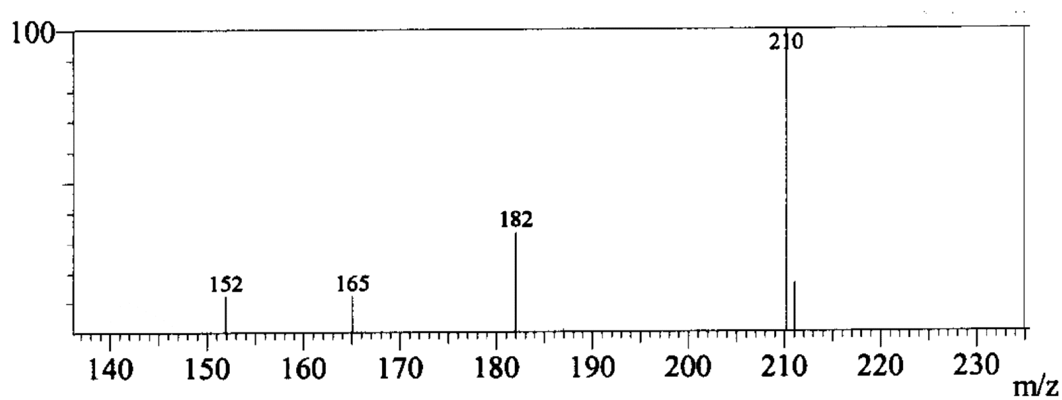


**Figure S-6a.** Mass spectrum of the organic byproducts from the crossover experiment.

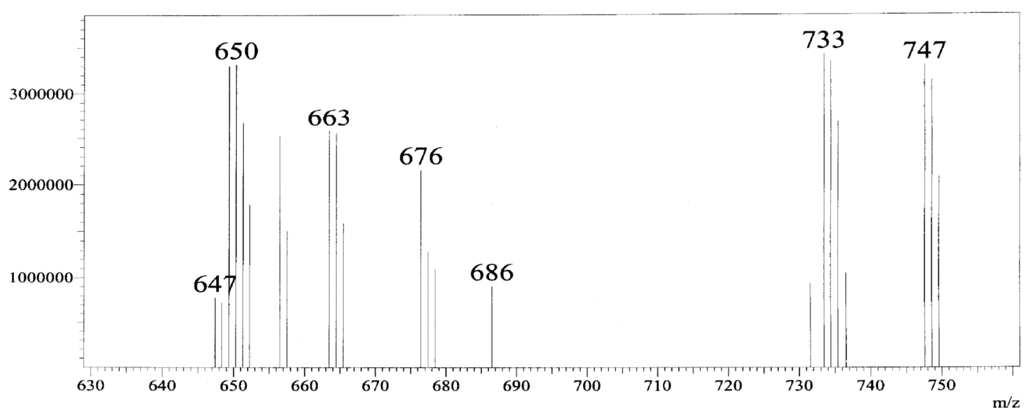


**Figure S-6b.** Mass spectrum of the products from the double crossover experiment.

**Table S2. Crystal data and structure refinement for $[L^{tBu'}FeH]_2$**

| | | |
|---|---|---|
| Identification code | holas09 | |
| Empirical formula | C96 H148 Fe2 N4 | |
| Formula weight | 1469.88 | |
| Temperature | 100.0(1) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | *C*2/*c* | |
| Unit cell dimensions | *a* = 50.910(3) Å | α = 90° |
| | *b* = 14.3387(9) Å | β = 123.668(1)° |
| | *c* = 28.6998(18) Å | γ = 90° |
| Volume | 17436.1(19) Å$^3$ | |
| *Z* | 8 | |
| Density (calculated) | 1.120 g/cm$^3$ | |
| Absorption coefficient | 0.379 mm$^{-1}$ | |
| *F*(000) | 6432 | |
| Crystal color, morphology | dark red, block | |
| Crystal size | 0.32 x 0.32 x 0.24 mm$^3$ | |
| Theta range for data collection | 1.71 to 30.51° | |
| Index ranges | $-72 \leq h \leq 71, -20 \leq k \leq 20, -40 \leq l \leq 40$ | |
| Reflections collected | 134195 | |
| Independent reflections | 26222 [*R*(int) = 0.0332] | |
| Observed reflections | 21241 | |
| Completeness to theta = 30.51° | 98.5% | |
| Absorption correction | Multi-scan | |
| Max. and min. transmission | 0.9146 and 0.8884 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 26222 / 15 / 978 | |
| Goodness-of-fit on $F^2$ | 1.017 | |
| Final *R* indices [*I*>2sigma(*I*)] | *R*1 = 0.0467, *wR*2 = 0.1235 | |
| *R* indices (all data) | *R*1 = 0.0607, *wR*2 = 0.1328 | |
| Largest diff. peak and hole | 2.696 and -1.040 e.Å$^{-3}$ | |

**Table S3. Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$ ) for[$L^{tBu'}$FeH]$_2$.**

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| Fe1 | 1440(1) | 9034(1) | 1037(1) | 16(1) |
| Fe2 | 1195(1) | 9961(1) | 140(1) | 16(1) |
| N11 | 1602(1) | 7732(1) | 1187(1) | 16(1) |
| N21 | 1395(1) | 9128(1) | 1677(1) | 16(1) |
| C11 | 1884(1) | 5692(1) | 1498(1) | 25(1) |
| C21 | 1396(1) | 5492(1) | 1476(1) | 29(1) |
| C31 | 1895(1) | 6093(1) | 2335(1) | 32(1) |
| C41 | 1685(1) | 6134(1) | 1689(1) | 21(1) |
| C51 | 1564(1) | 7165(1) | 1515(1) | 17(1) |
| C61 | 1408(1) | 7470(1) | 1769(1) | 18(1) |
| C71 | 1354(1) | 8359(1) | 1899(1) | 17(1) |
| C81 | 1226(1) | 8332(1) | 2288(1) | 23(1) |
| C91 | 1245(1) | 9223(1) | 2604(1) | 26(1) |
| C101 | 877(1) | 8056(2) | 1912(1) | 40(1) |
| C111 | 1402(1) | 7575(2) | 2747(1) | 48(1) |
| C12 | 1762(1) | 7420(1) | 927(1) | 17(1) |
| C22 | 2080(1) | 7659(1) | 1164(1) | 19(1) |
| C32 | 2237(1) | 7271(1) | 936(1) | 22(1) |
| C42 | 2086(1) | 6686(1) | 472(1) | 23(1) |
| C52 | 1765(1) | 6537(1) | 215(1) | 22(1) |
| C62 | 1599(1) | 6883(1) | 433(1) | 18(1) |
| C72 | 2259(1) | 8309(1) | 1664(1) | 20(1) |
| C82 | 2531(1) | 7804(1) | 2178(1) | 35(1) |
| C92 | 2379(1) | 9152(1) | 1514(1) | 39(1) |
| C102 | 1658(1) | 12595(1) | 2886(1) | 26(1) |
| C112 | 1474(1) | 12613(1) | 3161(1) | 38(1) |
| C122 | 1603(1) | 13473(1) | 2542(1) | 37(1) |
| C132 | 890(1) | 10584(1) | 1233(1) | 24(1) |

| | | | | |
|---|---|---|---|---|
| C142 | 639(1) | 10677(2) | 1369(1) | 35(1) |
| C152 | 816(1) | 11295(1) | 776(1) | 37(1) |
| C13 | 1454(1) | 10020(1) | 1950(1) | 17(1) |
| C23 | 1759(1) | 10193(1) | 2431(1) | 20(1) |
| C33 | 1817(1) | 11030(1) | 2720(1) | 22(1) |
| C43 | 1587(1) | 11711(1) | 2544(1) | 21(1) |
| C53 | 1294(1) | 11546(1) | 2053(1) | 20(1) |
| C63 | 1222(1) | 10717(1) | 1750(1) | 18(1) |
| C73 | 2030(1) | 9505(1) | 2647(1) | 26(1) |
| C83 | 2145(1) | 9137(2) | 3232(1) | 61(1) |
| C93 | 2304(1) | 9949(2) | 2657(1) | 49(1) |
| C103 | 2267(1) | 6209(1) | 260(1) | 29(1) |
| C113 | 2227(1) | 5149(1) | 246(1) | 37(1) |
| C123 | 2168(1) | 6570(2) | -318(1) | 38(1) |
| C133 | 1248(1) | 6670(1) | 130(1) | 20(1) |
| C143 | 1067(1) | 7295(1) | -388(1) | 26(1) |
| C153 | 1165(1) | 5650(1) | -52(1) | 28(1) |
| N14 | 1371(1) | 11048(1) | -67(1) | 17(1) |
| N24 | 748(1) | 10024(1) | -533(1) | 17(1) |
| C14 | 1596(1) | 12673(1) | -482(1) | 34(1) |
| C24 | 1071(1) | 12308(2) | -1319(1) | 37(1) |
| C34 | 1129(1) | 13435(1) | -598(1) | 36(1) |
| C44 | 1250(1) | 12509(1) | -685(1) | 24(1) |
| C54 | 1172(1) | 11677(1) | -428(1) | 19(1) |
| C64 | 842(1) | 11624(1) | -655(1) | 21(1) |
| C74 | 641(1) | 10892(1) | -739(1) | 19(1) |
| C84 | 283(1) | 11185(1) | -1098(1) | 25(1) |
| C94 | 240(1) | 12046(2) | -828(1) | 39(1) |
| C104 | 181(1) | 11445(2) | -1692(1) | 42(1) |
| C114 | 46(1) | 10459(2) | -1154(1) | 56(1) |
| C15 | 1709(1) | 11135(1) | 233(1) | 17(1) |
| C25 | 1867(1) | 11707(1) | 711(1) | 19(1) |
| C35 | 2194(1) | 11795(1) | 999(1) | 20(1) |
| C45 | 2369(1) | 11343(1) | 830(1) | 19(1) |
| C55 | 2208(1) | 10748(1) | 369(1) | 19(1) |
| C65 | 1881(1) | 10625(1) | 70(1) | 17(1) |

| | | | | |
|---|---|---|---|---|
| C75 | 1694(1) | 12224(1) | 927(1) | 29(1) |
| C85 | 1776(1) | 13266(1) | 1024(1) | 42(1) |
| C95 | 1769(1) | 11772(2) | 1470(1) | 46(1) |
| C105 | 2720(1) | 11541(1) | 1125(1) | 21(1) |
| C115 | 2775(1) | 12243(1) | 785(1) | 32(1) |
| C125 | 2921(1) | 10671(1) | 1252(1) | 31(1) |
| C135 | 1721(1) | 9958(1) | -425(1) | 19(1) |
| C145 | 1805(1) | 8948(1) | -223(1) | 25(1) |
| C155 | 1805(1) | 10161(1) | -853(1) | 28(1) |
| C16 | 558(1) | 9216(1) | -819(1) | 16(1) |
| C26 | 436(1) | 8660(1) | -576(1) | 16(1) |
| C36 | 245(1) | 7901(1) | -875(1) | 19(1) |
| C46 | 176(1) | 7655(1) | -1403(1) | 21(1) |
| C56 | 313(1) | 8184(1) | -1620(1) | 21(1) |
| C66 | 506(1) | 8956(1) | -1340(1) | 18(1) |
| C76 | 511(1) | 8842(1) | 9(1) | 18(1) |
| C86 | 745(1) | 8109(1) | 415(1) | 22(1) |
| C96 | 221(1) | 8842(1) | 43(1) | 27(1) |
| C106 | -38(1) | 6835(1) | -1723(1) | 26(1) |
| C116 | 70(1) | 5934(1) | -1379(1) | 33(1) |
| C126 | -381(1) | 7039(1) | -1923(1) | 36(1) |
| C136 | 671(1) | 9440(1) | -1583(1) | 21(1) |
| C146 | 966(1) | 8888(1) | -1429(1) | 30(1) |
| C156 | 465(1) | 9570(1) | -2219(1) | 30(1) |
| C17 | 288(1) | 6126(4) | 820(2) | 85(2) |
| C27 | 435(1) | 5333(3) | 699(2) | 58(1) |
| C37 | 601(1) | 4664(3) | 1084(2) | 69(1) |
| C47 | 740(2) | 3921(3) | 970(2) | 88(2) |
| C57 | 698(1) | 3879(3) | 451(2) | 71(1) |
| C67 | 530(1) | 4537(3) | 61(2) | 73(1) |
| C77 | 401(1) | 5256(4) | 188(2) | 69(1) |
| C17' | 757(4) | 3834(11) | 259(7) | 85(2) |
| C27' | 626(2) | 4511(7) | 538(4) | 58(1) |
| C37' | 482(4) | 5346(10) | 335(5) | 69(1) |
| C47' | 404(4) | 5949(10) | 640(5) | 88(2) |
| C57' | 485(3) | 5641(8) | 1162(5) | 71(1) |

| | | | | |
|---|---|---|---|---|
| C67' | 651(3) | 4846(9) | 1402(5) | 73(1) |
| C77' | 721(4) | 4274(11) | 1086(5) | 69(1) |
| C18 | 342(1) | 6419(2) | 2338(1) | 46(1) |
| C28 | 566(1) | 5648(1) | 2682(1) | 35(1) |
| C38 | 498(1) | 5022(2) | 2969(1) | 37(1) |
| C48 | 709(1) | 4318(2) | 3298(1) | 40(1) |
| C58 | 992(1) | 4239(2) | 3343(1) | 42(1) |
| C68 | 1062(1) | 4853(2) | 3054(1) | 48(1) |
| C78 | 851(1) | 5546(2) | 2727(1) | 45(1) |

**Table S4. Anisotropic displacement parameters ($Å^2$x $10^3$) for $[L^{tBu'}FeH]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12} ]$**

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Fe1 | 15(1) | 15(1) | 17(1) | -1(1) | 10(1) | -1(1) |
| Fe2 | 13(1) | 15(1) | 17(1) | -1(1) | 6(1) | -1(1) |
| N11 | 13(1) | 18(1) | 15(1) | -3(1) | 7(1) | -1(1) |
| N21 | 15(1) | 15(1) | 17(1) | -3(1) | 8(1) | -1(1) |
| C11 | 25(1) | 20(1) | 26(1) | 2(1) | 12(1) | 7(1) |
| C21 | 31(1) | 18(1) | 35(1) | -1(1) | 18(1) | -2(1) |
| C31 | 33(1) | 34(1) | 20(1) | 6(1) | 9(1) | 12(1) |
| C41 | 21(1) | 18(1) | 19(1) | 1(1) | 8(1) | 4(1) |
| C51 | 14(1) | 16(1) | 15(1) | -3(1) | 4(1) | -1(1) |
| C61 | 18(1) | 17(1) | 18(1) | 0(1) | 9(1) | -1(1) |
| C71 | 13(1) | 20(1) | 14(1) | -2(1) | 6(1) | -1(1) |
| C81 | 28(1) | 23(1) | 23(1) | -1(1) | 18(1) | 0(1) |
| C91 | 31(1) | 29(1) | 22(1) | -4(1) | 18(1) | -1(1) |
| C101 | 36(1) | 51(1) | 50(1) | -22(1) | 34(1) | -19(1) |
| C111 | 85(2) | 39(1) | 44(1) | 17(1) | 51(1) | 23(1) |
| C12 | 15(1) | 18(1) | 16(1) | -1(1) | 7(1) | 3(1) |
| C22 | 15(1) | 21(1) | 17(1) | -1(1) | 8(1) | 2(1) |
| C32 | 16(1) | 29(1) | 20(1) | -1(1) | 9(1) | 3(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C42 | 20(1) | 29(1) | 21(1) | -1(1) | 11(1) | 7(1) |
| C52 | 20(1) | 24(1) | 17(1) | -4(1) | 8(1) | 5(1) |
| C62 | 15(1) | 19(1) | 16(1) | -2(1) | 6(1) | 3(1) |
| C72 | 15(1) | 24(1) | 18(1) | -3(1) | 7(1) | -2(1) |
| C82 | 29(1) | 37(1) | 23(1) | -5(1) | 3(1) | 6(1) |
| C92 | 48(1) | 37(1) | 32(1) | -8(1) | 22(1) | -20(1) |
| C102 | 30(1) | 20(1) | 27(1) | -8(1) | 15(1) | -3(1) |
| C112 | 50(1) | 37(1) | 35(1) | -11(1) | 28(1) | -2(1) |
| C122 | 49(1) | 19(1) | 39(1) | -6(1) | 21(1) | -5(1) |
| C132 | 19(1) | 25(1) | 21(1) | -3(1) | 6(1) | 5(1) |
| C142 | 17(1) | 45(1) | 36(1) | -3(1) | 10(1) | 5(1) |
| C152 | 43(1) | 37(1) | 22(1) | 4(1) | 11(1) | 14(1) |
| C13 | 16(1) | 16(1) | 18(1) | -4(1) | 10(1) | -2(1) |
| C23 | 16(1) | 20(1) | 20(1) | -4(1) | 9(1) | -2(1) |
| C33 | 20(1) | 22(1) | 22(1) | -6(1) | 11(1) | -5(1) |
| C43 | 26(1) | 17(1) | 23(1) | -5(1) | 16(1) | -4(1) |
| C53 | 23(1) | 18(1) | 23(1) | -2(1) | 14(1) | 1(1) |
| C63 | 18(1) | 19(1) | 18(1) | -2(1) | 10(1) | 0(1) |
| C73 | 17(1) | 25(1) | 28(1) | -7(1) | 6(1) | 0(1) |
| C83 | 54(1) | 74(2) | 44(1) | 24(1) | 20(1) | 39(1) |
| C93 | 25(1) | 34(1) | 90(2) | -18(1) | 32(1) | -5(1) |
| C103 | 23(1) | 40(1) | 27(1) | -5(1) | 15(1) | 7(1) |
| C113 | 38(1) | 38(1) | 41(1) | 2(1) | 26(1) | 16(1) |
| C123 | 46(1) | 44(1) | 38(1) | 0(1) | 31(1) | 9(1) |
| C133 | 15(1) | 20(1) | 18(1) | -4(1) | 6(1) | 2(1) |
| C143 | 21(1) | 27(1) | 20(1) | -1(1) | 6(1) | 7(1) |
| C153 | 25(1) | 23(1) | 26(1) | -6(1) | 8(1) | -2(1) |
| N14 | 16(1) | 17(1) | 19(1) | -4(1) | 10(1) | -2(1) |
| N24 | 14(1) | 16(1) | 17(1) | -2(1) | 7(1) | -1(1) |
| C14 | 33(1) | 28(1) | 48(1) | 12(1) | 27(1) | 0(1) |
| C24 | 46(1) | 40(1) | 30(1) | 6(1) | 25(1) | 1(1) |
| C34 | 47(1) | 17(1) | 57(1) | 3(1) | 37(1) | 2(1) |
| C44 | 30(1) | 18(1) | 31(1) | 3(1) | 21(1) | 2(1) |
| C54 | 22(1) | 16(1) | 21(1) | -3(1) | 13(1) | -1(1) |
| C64 | 21(1) | 16(1) | 23(1) | 1(1) | 11(1) | 3(1) |
| C74 | 16(1) | 19(1) | 18(1) | -1(1) | 8(1) | 2(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C84 | 17(1) | 23(1) | 28(1) | 4(1) | 9(1) | 5(1) |
| C94 | 27(1) | 48(1) | 34(1) | -4(1) | 13(1) | 16(1) |
| C104 | 29(1) | 59(1) | 25(1) | 3(1) | 7(1) | 17(1) |
| C114 | 17(1) | 38(1) | 97(2) | 27(1) | 22(1) | 10(1) |
| C15 | 16(1) | 17(1) | 17(1) | -2(1) | 10(1) | -3(1) |
| C25 | 21(1) | 19(1) | 20(1) | -6(1) | 14(1) | -6(1) |
| C35 | 22(1) | 22(1) | 17(1) | -7(1) | 11(1) | -8(1) |
| C45 | 18(1) | 22(1) | 15(1) | -1(1) | 8(1) | -4(1) |
| C55 | 17(1) | 23(1) | 16(1) | -2(1) | 9(1) | -1(1) |
| C65 | 18(1) | 18(1) | 15(1) | -2(1) | 9(1) | -2(1) |
| C75 | 24(1) | 35(1) | 32(1) | -19(1) | 19(1) | -10(1) |
| C85 | 41(1) | 34(1) | 51(1) | -22(1) | 26(1) | -6(1) |
| C95 | 52(1) | 65(1) | 40(1) | -22(1) | 38(1) | -27(1) |
| C105 | 17(1) | 29(1) | 16(1) | -3(1) | 7(1) | -5(1) |
| C115 | 23(1) | 45(1) | 24(1) | 1(1) | 12(1) | -11(1) |
| C125 | 20(1) | 38(1) | 26(1) | -5(1) | 7(1) | 1(1) |
| C135 | 16(1) | 21(1) | 16(1) | -4(1) | 7(1) | 0(1) |
| C145 | 29(1) | 20(1) | 22(1) | -3(1) | 12(1) | -1(1) |
| C155 | 35(1) | 32(1) | 17(1) | -4(1) | 14(1) | -4(1) |
| C16 | 11(1) | 18(1) | 14(1) | -1(1) | 3(1) | 0(1) |
| C26 | 12(1) | 20(1) | 13(1) | -2(1) | 4(1) | 1(1) |
| C36 | 16(1) | 22(1) | 17(1) | -2(1) | 7(1) | -3(1) |
| C46 | 17(1) | 23(1) | 16(1) | -5(1) | 6(1) | -4(1) |
| C56 | 18(1) | 25(1) | 15(1) | -4(1) | 6(1) | -3(1) |
| C66 | 14(1) | 21(1) | 15(1) | 0(1) | 6(1) | 0(1) |
| C76 | 15(1) | 21(1) | 14(1) | -2(1) | 6(1) | 1(1) |
| C86 | 18(1) | 26(1) | 16(1) | 0(1) | 6(1) | 2(1) |
| C96 | 19(1) | 42(1) | 21(1) | -2(1) | 11(1) | 5(1) |
| C106 | 25(1) | 28(1) | 20(1) | -8(1) | 10(1) | -10(1) |
| C116 | 35(1) | 24(1) | 35(1) | -7(1) | 17(1) | -6(1) |
| C126 | 22(1) | 36(1) | 34(1) | -7(1) | 6(1) | -10(1) |
| C136 | 19(1) | 24(1) | 18(1) | -1(1) | 9(1) | -2(1) |
| C146 | 20(1) | 37(1) | 32(1) | 5(1) | 14(1) | 1(1) |
| C156 | 26(1) | 41(1) | 19(1) | 4(1) | 11(1) | 0(1) |
| C17 | 99(4) | 75(3) | 101(4) | -34(3) | 69(3) | -28(3) |
| C27 | 56(2) | 60(2) | 56(2) | -8(2) | 29(2) | -23(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C37 | 80(2) | 64(2) | 53(2) | 0(1) | 31(2) | -19(2) |
| C47 | 102(4) | 56(2) | 64(3) | 5(2) | 20(3) | -11(3) |
| C57 | 72(3) | 47(2) | 87(3) | -6(2) | 39(2) | -9(2) |
| C67 | 90(3) | 76(3) | 56(2) | 1(2) | 43(2) | -13(2) |
| C77 | 80(2) | 64(2) | 53(2) | 0(1) | 31(2) | -19(2) |
| C17' | 99(4) | 75(3) | 101(4) | -34(3) | 69(3) | -28(3) |
| C27' | 56(2) | 60(2) | 56(2) | -8(2) | 29(2) | -23(2) |
| C37' | 80(2) | 64(2) | 53(2) | 0(1) | 31(2) | -19(2) |
| C47' | 102(4) | 56(2) | 64(3) | 5(2) | 20(3) | -11(3) |
| C57' | 72(3) | 47(2) | 87(3) | -6(2) | 39(2) | -9(2) |
| C67' | 90(3) | 76(3) | 56(2) | 1(2) | 43(2) | -13(2) |
| C77' | 80(2) | 64(2) | 53(2) | 0(1) | 31(2) | -19(2) |
| C18 | 48(1) | 34(1) | 51(1) | 5(1) | 24(1) | 0(1) |
| C28 | 36(1) | 31(1) | 35(1) | -6(1) | 16(1) | -5(1) |
| C38 | 31(1) | 47(1) | 30(1) | 2(1) | 15(1) | 1(1) |
| C48 | 39(1) | 50(1) | 32(1) | 6(1) | 19(1) | 5(1) |
| C58 | 39(1) | 45(1) | 36(1) | -2(1) | 18(1) | 7(1) |
| C68 | 40(1) | 45(1) | 66(2) | -6(1) | 33(1) | -2(1) |
| C78 | 48(1) | 34(1) | 62(1) | -3(1) | 35(1) | -7(1) |

**Table S5. Bond lengths [Å] and angles [°] for [L$^{tBu'}$FeH]$_2$**

| | | | |
|---|---|---|---|
| Fe(1)-N(21) | 1.9780(12) | N(21)-C(13) | 1.4418(17) |
| Fe(1)-N(11) | 1.9885(12) | C(11)-C(41) | 1.535(2) |
| Fe(1)-Fe(2) | 2.5292(3) | C(11)-H(11A) | 0.9800 |
| Fe(1)-H(1) | 1.48(2) | C(11)-H(11B) | 0.9800 |
| Fe(1)-H(2) | 1.58(2) | C(11)-H(11C) | 0.9800 |
| Fe(2)-N(24) | 2.0097(12) | C(21)-C(41) | 1.545(2) |
| Fe(2)-N(14) | 2.0429(12) | C(21)-H(21A) | 0.9800 |
| Fe(2)-H(1) | 1.49(2) | C(21)-H(21B) | 0.9800 |
| Fe(2)-H(2) | 1.70(2) | C(21)-H(21C) | 0.9800 |
| N(11)-C(51) | 1.3369(18) | C(31)-C(41) | 1.545(2) |
| N(11)-C(12) | 1.4468(17) | C(31)-H(31A) | 0.9800 |
| N(21)-C(71) | 1.3455(18) | C(31)-H(31B) | 0.9800 |

| | | | |
|---|---|---|---|
| C(31)-H(31C) | 0.9800 | C(92)-H(92B) | 0.9800 |
| C(41)-C(51) | 1.572(2) | C(92)-H(92C) | 0.9800 |
| C(51)-C(61) | 1.416(2) | C(102)-C(43) | 1.519(2) |
| C(61)-C(71) | 1.3964(19) | C(102)-C(112) | 1.523(3) |
| C(61)-H(61) | 0.9500 | C(102)-C(122) | 1.527(3) |
| C(71)-C(81) | 1.573(2) | C(102)-H(102) | 1.0000 |
| C(81)-C(101) | 1.532(2) | C(112)-H(11J) | 0.9800 |
| C(81)-C(91) | 1.539(2) | C(112)-H(11K) | 0.9800 |
| C(81)-C(111) | 1.553(3) | C(112)-H(11L) | 0.9800 |
| C(91)-H(91A) | 0.9800 | C(122)-H(12G) | 0.9800 |
| C(91)-H(91B) | 0.9800 | C(122)-H(12H) | 0.9800 |
| C(91)-H(91C) | 0.9800 | C(122)-H(12I) | 0.9800 |
| C(101)-H(10A) | 0.9800 | C(132)-C(63) | 1.518(2) |
| C(101)-H(10B) | 0.9800 | C(132)-C(152) | 1.534(2) |
| C(101)-H(10C) | 0.9800 | C(132)-C(142) | 1.538(2) |
| C(111)-H(11P) | 0.9800 | C(132)-H(132) | 1.0000 |
| C(111)-H(11Q) | 0.9800 | C(142)-H(14M) | 0.9800 |
| C(111)-H(11R) | 0.9800 | C(142)-H(14N) | 0.9800 |
| C(12)-C(22) | 1.4045(19) | C(142)-H(14O) | 0.9800 |
| C(12)-C(62) | 1.4083(19) | C(152)-H(15J) | 0.9800 |
| C(22)-C(32) | 1.400(2) | C(152)-H(15K) | 0.9800 |
| C(22)-C(72) | 1.520(2) | C(152)-H(15L) | 0.9800 |
| C(32)-C(42) | 1.390(2) | C(13)-C(63) | 1.4074(19) |
| C(32)-H(32) | 0.9500 | C(13)-C(23) | 1.4134(19) |
| C(42)-C(52) | 1.390(2) | C(23)-C(33) | 1.393(2) |
| C(42)-C(103) | 1.518(2) | C(23)-C(73) | 1.521(2) |
| C(52)-C(62) | 1.392(2) | C(33)-C(43) | 1.385(2) |
| C(52)-H(52) | 0.9500 | C(33)-H(33) | 0.9500 |
| C(62)-C(133) | 1.5214(19) | C(43)-C(53) | 1.394(2) |
| C(72)-C(92) | 1.521(2) | C(53)-C(63) | 1.396(2) |
| C(72)-C(82) | 1.533(2) | C(53)-H(53) | 0.9500 |
| C(72)-H(72) | 1.0000 | C(73)-C(93) | 1.515(3) |
| C(82)-H(82A) | 0.9800 | C(73)-C(83) | 1.534(3) |
| C(82)-H(82B) | 0.9800 | C(73)-H(73) | 1.0000 |
| C(82)-H(82C) | 0.9800 | C(83)-H(83A) | 0.9800 |
| C(92)-H(92A) | 0.9800 | C(83)-H(83B) | 0.9800 |

| | | | |
|---|---|---|---|
| C(83)-H(83C) | 0.9800 | C(34)-H(34B) | 0.9800 |
| C(93)-H(93A) | 0.9800 | C(34)-H(34C) | 0.9800 |
| C(93)-H(93B) | 0.9800 | C(44)-C(54) | 1.565(2) |
| C(93)-H(93C) | 0.9800 | C(54)-C(64) | 1.427(2) |
| C(103)-C(113) | 1.531(3) | C(64)-C(74) | 1.392(2) |
| C(103)-C(123) | 1.532(3) | C(64)-H(64) | 0.9500 |
| C(103)-H(103) | 1.0000 | C(74)-C(84) | 1.574(2) |
| C(113)-H(11M) | 0.9800 | C(84)-C(104) | 1.528(3) |
| C(113)-H(11N) | 0.9800 | C(84)-C(114) | 1.531(3) |
| C(113)-H(11O) | 0.9800 | C(84)-C(94) | 1.536(2) |
| C(123)-H(12J) | 0.9800 | C(94)-H(94A) | 0.9800 |
| C(123)-H(12K) | 0.9800 | C(94)-H(94B) | 0.9800 |
| C(123)-H(12L) | 0.9800 | C(94)-H(94C) | 0.9800 |
| C(133)-C(143) | 1.530(2) | C(104)-H(10D) | 0.9800 |
| C(133)-C(153) | 1.531(2) | C(104)-H(10E) | 0.9800 |
| C(133)-H(133) | 1.0000 | C(104)-H(10F) | 0.9800 |
| C(143)-H(14D) | 0.9800 | C(114)-H(11S) | 0.9800 |
| C(143)-H(14E) | 0.9800 | C(114)-H(11T) | 0.9800 |
| C(143)-H(14F) | 0.9800 | C(114)-H(11U) | 0.9800 |
| C(153)-H(15D) | 0.9800 | C(15)-C(65) | 1.4061(19) |
| C(153)-H(15E) | 0.9800 | C(15)-C(25) | 1.4076(19) |
| C(153)-H(15F) | 0.9800 | C(25)-C(35) | 1.397(2) |
| N(14)-C(54) | 1.3235(19) | C(25)-C(75) | 1.520(2) |
| N(14)-C(15) | 1.4391(17) | C(35)-C(45) | 1.389(2) |
| N(24)-C(74) | 1.3571(18) | C(35)-H(35) | 0.9500 |
| N(24)-C(16) | 1.4392(17) | C(45)-C(55) | 1.3951(19) |
| C(14)-C(44) | 1.535(2) | C(45)-C(105) | 1.520(2) |
| C(14)-H(14J) | 0.9800 | C(55)-C(65) | 1.3952(19) |
| C(14)-H(14K) | 0.9800 | C(55)-H(55) | 0.9500 |
| C(14)-H(14L) | 0.9800 | C(65)-C(135) | 1.5216(19) |
| C(24)-C(44) | 1.543(2) | C(75)-C(95) | 1.529(3) |
| C(24)-H(24A) | 0.9800 | C(75)-C(85) | 1.535(3) |
| C(24)-H(24B) | 0.9800 | C(75)-H(75) | 1.0000 |
| C(24)-H(24C) | 0.9800 | C(85)-H(85A) | 0.9800 |
| C(34)-C(44) | 1.542(2) | C(85)-H(85B) | 0.9800 |
| C(34)-H(34A) | 0.9800 | C(85)-H(85C) | 0.9800 |

| | | | |
|---|---|---|---|
| C(95)-H(95A) | 0.9800 | C(86)-H(86B) | 0.9800 |
| C(95)-H(95B) | 0.9800 | C(86)-H(86C) | 0.9800 |
| C(95)-H(95C) | 0.9800 | C(96)-H(96A) | 0.9800 |
| C(105)-C(125) | 1.524(2) | C(96)-H(96B) | 0.9800 |
| C(105)-C(115) | 1.533(2) | C(96)-H(96C) | 0.9800 |
| C(105)-H(105) | 1.0000 | C(106)-C(116) | 1.530(3) |
| C(115)-H(11D) | 0.9800 | C(106)-C(126) | 1.534(2) |
| C(115)-H(11E) | 0.9800 | C(106)-H(106) | 1.0000 |
| C(115)-H(11F) | 0.9800 | C(116)-H(11G) | 0.9800 |
| C(125)-H(12D) | 0.9800 | C(116)-H(11H) | 0.9800 |
| C(125)-H(12E) | 0.9800 | C(116)-H(11I) | 0.9800 |
| C(125)-H(12F) | 0.9800 | C(126)-H(12A) | 0.9800 |
| C(135)-C(145) | 1.530(2) | C(126)-H(12B) | 0.9800 |
| C(135)-C(155) | 1.533(2) | C(126)-H(12C) | 0.9800 |
| C(135)-H(135) | 1.0000 | C(136)-C(156) | 1.530(2) |
| C(145)-H(14A) | 0.9800 | C(136)-C(146) | 1.530(2) |
| C(145)-H(14B) | 0.9800 | C(136)-H(136) | 1.0000 |
| C(145)-H(14C) | 0.9800 | C(146)-H(14G) | 0.9800 |
| C(155)-H(15A) | 0.9800 | C(146)-H(14H) | 0.9800 |
| C(155)-H(15B) | 0.9800 | C(146)-H(14I) | 0.9800 |
| C(155)-H(15C) | 0.9800 | C(156)-H(15G) | 0.9800 |
| C(16)-C(26) | 1.410(2) | C(156)-H(15H) | 0.9800 |
| C(16)-C(66) | 1.4162(19) | C(156)-H(15I) | 0.9800 |
| C(26)-C(36) | 1.3923(19) | C(17)-C(27) | 1.504(6) |
| C(26)-C(76) | 1.5232(19) | C(17)-H(17A) | 0.9800 |
| C(36)-C(46) | 1.397(2) | C(17)-H(17B) | 0.9800 |
| C(36)-H(36) | 0.9500 | C(17)-H(17C) | 0.9800 |
| C(46)-C(56) | 1.390(2) | C(27)-C(37) | 1.348(6) |
| C(46)-C(106) | 1.520(2) | C(27)-C(77) | 1.384(6) |
| C(56)-C(66) | 1.399(2) | C(37)-C(47) | 1.412(8) |
| C(56)-H(56) | 0.9500 | C(37)-H(37) | 0.9500 |
| C(66)-C(136) | 1.526(2) | C(47)-C(57) | 1.383(8) |
| C(76)-C(86) | 1.531(2) | C(47)-H(47) | 0.9500 |
| C(76)-C(96) | 1.536(2) | C(57)-C(67) | 1.346(6) |
| C(76)-H(76) | 1.0000 | C(57)-H(57) | 0.9500 |
| C(86)-H(86A) | 0.9800 | C(67)-C(77) | 1.375(7) |

| | |
|---|---|
| C(67)-H(67) | 0.9500 |
| C(77)-H(77) | 0.9500 |
| C(17')-C(27') | 1.620(13) |
| C(17')-H(17D) | 0.9800 |
| C(17')-H(17E) | 0.9800 |
| C(17')-H(17F) | 0.9800 |
| C(27')-C(37') | 1.355(15) |
| C(27')-C(77') | 1.404(14) |
| C(37')-C(47') | 1.432(16) |
| C(37')-H(37') | 0.9500 |
| C(47')-C(57') | 1.388(15) |
| C(47')-H(47') | 0.9500 |
| C(57')-C(67') | 1.356(14) |
| C(57')-H(57') | 0.9500 |
| C(67')-C(77') | 1.411(15) |
| C(67')-H(67') | 0.9500 |
| C(77')-H(77') | 0.9500 |
| C(18)-C(28) | 1.502(3) |
| C(18)-H(18A) | 0.9800 |
| C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 |
| C(28)-C(38) | 1.387(3) |
| C(28)-C(78) | 1.389(3) |
| C(38)-C(48) | 1.392(3) |
| C(38)-H(38A) | 0.9500 |
| C(48)-C(58) | 1.377(3) |
| C(48)-H(48A) | 0.9500 |
| C(58)-C(68) | 1.385(3) |
| C(58)-H(58A) | 0.9500 |
| C(68)-C(78) | 1.382(3) |
| C(68)-H(68A) | 0.9500 |
| C(78)-H(78A) | 0.9500 |
| N(21)-Fe(1)-N(11) | 96.41(5) |
| N(21)-Fe(1)-Fe(2) | 131.62(4) |
| N(11)-Fe(1)-Fe(2) | 128.63(3) |
| N(21)-Fe(1)-H(1) | 157.1(8) |
| N(11)-Fe(1)-H(1) | 105.7(8) |
| Fe(2)-Fe(1)-H(1) | 31.7(8) |
| N(21)-Fe(1)-H(2) | 91.2(7) |
| N(11)-Fe(1)-H(2) | 166.7(7) |
| Fe(2)-Fe(1)-H(2) | 41.2(7) |
| H(1)-Fe(1)-H(2) | 68.3(11) |
| N(24)-Fe(2)-N(14) | 97.60(5) |
| N(24)-Fe(2)-Fe(1) | 131.17(4) |
| N(14)-Fe(2)-Fe(1) | 130.43(4) |
| N(24)-Fe(2)-H(1) | 147.5(8) |
| N(14)-Fe(2)-H(1) | 109.6(8) |
| Fe(1)-Fe(2)-H(1) | 31.5(8) |
| N(24)-Fe(2)-H(2) | 117.5(7) |
| N(14)-Fe(2)-H(2) | 117.9(7) |
| Fe(1)-Fe(2)-H(2) | 37.8(7) |
| H(1)-Fe(2)-H(2) | 65.0(10) |
| C(51)-N(11)-C(12) | 121.14(12) |
| C(51)-N(11)-Fe(1) | 121.19(9) |
| C(12)-N(11)-Fe(1) | 117.68(9) |
| C(71)-N(21)-C(13) | 120.71(12) |
| C(71)-N(21)-Fe(1) | 120.77(9) |
| C(13)-N(21)-Fe(1) | 117.89(9) |
| C(41)-C(11)-H(11A) | 109.5 |
| C(41)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 |
| C(41)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| C(41)-C(21)-H(21A) | 109.5 |
| C(41)-C(21)-H(21B) | 109.5 |
| H(21A)-C(21)-H(21B) | 109.5 |
| C(41)-C(21)-H(21C) | 109.5 |
| H(21A)-C(21)-H(21C) | 109.5 |
| H(21B)-C(21)-H(21C) | 109.5 |
| C(41)-C(31)-H(31A) | 109.5 |
| C(41)-C(31)-H(31B) | 109.5 |

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| H(31A)-C(31)-H(31B) | 109.5 |
| C(41)-C(31)-H(31C) | 109.5 |
| H(31A)-C(31)-H(31C) | 109.5 |
| H(31B)-C(31)-H(31C) | 109.5 |
| C(11)-C(41)-C(21) | 106.72(13) |
| C(11)-C(41)-C(31) | 104.90(13) |
| C(21)-C(41)-C(31) | 109.01(14) |
| C(11)-C(41)-C(51) | 119.58(13) |
| C(21)-C(41)-C(51) | 108.48(12) |
| C(31)-C(41)-C(51) | 107.79(12) |
| N(11)-C(51)-C(61) | 121.17(13) |
| N(11)-C(51)-C(41) | 127.80(13) |
| C(61)-C(51)-C(41) | 111.00(12) |
| C(71)-C(61)-C(51) | 132.02(13) |
| C(71)-C(61)-H(61) | 114.0 |
| C(51)-C(61)-H(61) | 114.0 |
| N(21)-C(71)-C(61) | 121.07(13) |
| N(21)-C(71)-C(81) | 126.13(12) |
| C(61)-C(71)-C(81) | 112.71(12) |
| C(101)-C(81)-C(91) | 107.33(14) |
| C(101)-C(81)-C(111) | 108.30(17) |
| C(91)-C(81)-C(111) | 105.12(14) |
| C(101)-C(81)-C(71) | 106.30(13) |
| C(91)-C(81)-C(71) | 118.85(13) |
| C(111)-C(81)-C(71) | 110.56(13) |
| C(81)-C(91)-H(91A) | 109.5 |
| C(81)-C(91)-H(91B) | 109.5 |
| H(91A)-C(91)-H(91B) | 109.5 |
| C(81)-C(91)-H(91C) | 109.5 |
| H(91A)-C(91)-H(91C) | 109.5 |
| H(91B)-C(91)-H(91C) | 109.5 |
| C(81)-C(101)-H(10A) | 109.5 |
| C(81)-C(101)-H(10B) | 109.5 |
| H(10A)-C(101)-H(10B) | 109.5 |
| C(81)-C(101)-H(10C) | 109.5 |
| H(10A)-C(101)-H(10C) | 109.5 |
| H(10B)-C(101)-H(10C) | 109.5 |
| C(81)-C(111)-H(11P) | 109.5 |
| C(81)-C(111)-H(11Q) | 109.5 |
| H(11P)-C(111)-H(11Q) | 109.5 |
| C(81)-C(111)-H(11R) | 109.5 |
| H(11P)-C(111)-H(11R) | 109.5 |
| H(11Q)-C(111)-H(11R) | 109.5 |
| C(22)-C(12)-C(62) | 119.96(13) |
| C(22)-C(12)-N(11) | 119.96(12) |
| C(62)-C(12)-N(11) | 120.08(12) |
| C(32)-C(22)-C(12) | 118.61(13) |
| C(32)-C(22)-C(72) | 119.03(13) |
| C(12)-C(22)-C(72) | 122.35(12) |
| C(42)-C(32)-C(22) | 122.26(14) |
| C(42)-C(32)-H(32) | 118.9 |
| C(22)-C(32)-H(32) | 118.9 |
| C(32)-C(42)-C(52) | 117.54(13) |
| C(32)-C(42)-C(103) | 121.42(14) |
| C(52)-C(42)-C(103) | 121.03(14) |
| C(42)-C(52)-C(62) | 122.40(13) |
| C(42)-C(52)-H(52) | 118.8 |
| C(62)-C(52)-H(52) | 118.8 |
| C(52)-C(62)-C(12) | 118.74(13) |
| C(52)-C(62)-C(133) | 118.81(12) |
| C(12)-C(62)-C(133) | 122.45(12) |
| C(22)-C(72)-C(92) | 110.14(13) |
| C(22)-C(72)-C(82) | 111.65(13) |
| C(92)-C(72)-C(82) | 110.96(15) |
| C(22)-C(72)-H(72) | 108.0 |
| C(92)-C(72)-H(72) | 108.0 |
| C(82)-C(72)-H(72) | 108.0 |
| C(72)-C(82)-H(82A) | 109.5 |
| C(72)-C(82)-H(82B) | 109.5 |
| H(82A)-C(82)-H(82B) | 109.5 |
| C(72)-C(82)-H(82C) | 109.5 |
| H(82A)-C(82)-H(82C) | 109.5 |

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| H(82B)-C(82)-H(82C) | 109.5 | H(14N)-C(142)-H(14O) | 109.5 |
| C(72)-C(92)-H(92A) | 109.5 | C(132)-C(152)-H(15J) | 109.5 |
| C(72)-C(92)-H(92B) | 109.5 | C(132)-C(152)-H(15K) | 109.5 |
| H(92A)-C(92)-H(92B) | 109.5 | H(15J)-C(152)-H(15K) | 109.5 |
| C(72)-C(92)-H(92C) | 109.5 | C(132)-C(152)-H(15L) | 109.5 |
| H(92A)-C(92)-H(92C) | 109.5 | H(15J)-C(152)-H(15L) | 109.5 |
| H(92B)-C(92)-H(92C) | 109.5 | H(15K)-C(152)-H(15L) | 109.5 |
| C(43)-C(102)-C(112) | 110.72(14) | C(63)-C(13)-C(23) | 119.59(13) |
| C(43)-C(102)-C(122) | 112.19(14) | C(63)-C(13)-N(21) | 122.21(12) |
| C(112)-C(102)-C(122) | 112.08(16) | C(23)-C(13)-N(21) | 118.19(12) |
| C(43)-C(102)-H(102) | 107.2 | C(33)-C(23)-C(13) | 119.16(13) |
| C(112)-C(102)-H(102) | 107.2 | C(33)-C(23)-C(73) | 118.18(13) |
| C(122)-C(102)-H(102) | 107.2 | C(13)-C(23)-C(73) | 122.66(13) |
| C(102)-C(112)-H(11J) | 109.5 | C(43)-C(33)-C(23) | 122.25(14) |
| C(102)-C(112)-H(11K) | 109.5 | C(43)-C(33)-H(33) | 118.9 |
| H(11J)-C(112)-H(11K) | 109.5 | C(23)-C(33)-H(33) | 118.9 |
| C(102)-C(112)-H(11L) | 109.5 | C(33)-C(43)-C(53) | 117.61(13) |
| H(11J)-C(112)-H(11L) | 109.5 | C(33)-C(43)-C(102) | 120.19(14) |
| H(11K)-C(112)-H(11L) | 109.5 | C(53)-C(43)-C(102) | 122.19(14) |
| C(102)-C(122)-H(12G) | 109.5 | C(43)-C(53)-C(63) | 122.60(14) |
| C(102)-C(122)-H(12H) | 109.5 | C(43)-C(53)-H(53) | 118.7 |
| H(12G)-C(122)-H(12H) | 109.5 | C(63)-C(53)-H(53) | 118.7 |
| C(102)-C(122)-H(12I) | 109.5 | C(53)-C(63)-C(13) | 118.64(13) |
| H(12G)-C(122)-H(12I) | 109.5 | C(53)-C(63)-C(132) | 118.75(13) |
| H(12H)-C(122)-H(12I) | 109.5 | C(13)-C(63)-C(132) | 122.54(13) |
| C(63)-C(132)-C(152) | 111.54(14) | C(93)-C(73)-C(23) | 110.65(15) |
| C(63)-C(132)-C(142) | 111.85(13) | C(93)-C(73)-C(83) | 109.53(19) |
| C(152)-C(132)-C(142) | 108.22(14) | C(23)-C(73)-C(83) | 112.09(15) |
| C(63)-C(132)-H(132) | 108.4 | C(93)-C(73)-H(73) | 108.2 |
| C(152)-C(132)-H(132) | 108.4 | C(23)-C(73)-H(73) | 108.2 |
| C(142)-C(132)-H(132) | 108.4 | C(83)-C(73)-H(73) | 108.2 |
| C(132)-C(142)-H(14M) | 109.5 | C(73)-C(83)-H(83A) | 109.5 |
| C(132)-C(142)-H(14N) | 109.5 | C(73)-C(83)-H(83B) | 109.5 |
| H(14M)-C(142)-H(14N) | 109.5 | H(83A)-C(83)-H(83B) | 109.5 |
| C(132)-C(142)-H(14O) | 109.5 | C(73)-C(83)-H(83C) | 109.5 |
| H(14M)-C(142)-H(14O) | 109.5 | H(83A)-C(83)-H(83C) | 109.5 |

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| H(83B)-C(83)-H(83C) | 109.5 |
| C(73)-C(93)-H(93A) | 109.5 |
| C(73)-C(93)-H(93B) | 109.5 |
| H(93A)-C(93)-H(93B) | 109.5 |
| C(73)-C(93)-H(93C) | 109.5 |
| H(93A)-C(93)-H(93C) | 109.5 |
| H(93B)-C(93)-H(93C) | 109.5 |
| C(42)-C(103)-C(113) | 110.88(15) |
| C(42)-C(103)-C(123) | 111.81(14) |
| C(113)-C(103)-C(123) | 110.35(15) |
| C(42)-C(103)-H(103) | 107.9 |
| C(113)-C(103)-H(103) | 107.9 |
| C(123)-C(103)-H(103) | 107.9 |
| C(103)-C(113)-H(11M) | 109.5 |
| C(103)-C(113)-H(11N) | 109.5 |
| H(11M)-C(113)-H(11N) | 109.5 |
| C(103)-C(113)-H(11O) | 109.5 |
| H(11M)-C(113)-H(11O) | 109.5 |
| H(11N)-C(113)-H(11O) | 109.5 |
| C(103)-C(123)-H(12J) | 109.5 |
| C(103)-C(123)-H(12K) | 109.5 |
| H(12J)-C(123)-H(12K) | 109.5 |
| C(103)-C(123)-H(12L) | 109.5 |
| H(12J)-C(123)-H(12L) | 109.5 |
| H(12K)-C(123)-H(12L) | 109.5 |
| C(62)-C(133)-C(143) | 108.87(13) |
| C(62)-C(133)-C(153) | 113.80(12) |
| C(143)-C(133)-C(153) | 109.01(12) |
| C(62)-C(133)-H(133) | 108.3 |
| C(143)-C(133)-H(133) | 108.3 |
| C(153)-C(133)-H(133) | 108.3 |
| C(133)-C(143)-H(14D) | 109.5 |
| C(133)-C(143)-H(14E) | 109.5 |
| H(14D)-C(143)-H(14E) | 109.5 |
| C(133)-C(143)-H(14F) | 109.5 |
| H(14D)-C(143)-H(14F) | 109.5 |
| H(14E)-C(143)-H(14F) | 109.5 |
| C(133)-C(153)-H(15D) | 109.5 |
| C(133)-C(153)-H(15E) | 109.5 |
| H(15D)-C(153)-H(15E) | 109.5 |
| C(133)-C(153)-H(15F) | 109.5 |
| H(15D)-C(153)-H(15F) | 109.5 |
| H(15E)-C(153)-H(15F) | 109.5 |
| C(54)-N(14)-C(15) | 123.47(12) |
| C(54)-N(14)-Fe(2) | 118.61(10) |
| C(15)-N(14)-Fe(2) | 117.62(9) |
| C(74)-N(24)-C(16) | 120.53(12) |
| C(74)-N(24)-Fe(2) | 115.37(9) |
| C(16)-N(24)-Fe(2) | 123.87(9) |
| C(44)-C(14)-H(14J) | 109.5 |
| C(44)-C(14)-H(14K) | 109.5 |
| H(14J)-C(14)-H(14K) | 109.5 |
| C(44)-C(14)-H(14L) | 109.5 |
| H(14J)-C(14)-H(14L) | 109.5 |
| H(14K)-C(14)-H(14L) | 109.5 |
| C(44)-C(24)-H(24A) | 109.5 |
| C(44)-C(24)-H(24B) | 109.5 |
| H(24A)-C(24)-H(24B) | 109.5 |
| C(44)-C(24)-H(24C) | 109.5 |
| H(24A)-C(24)-H(24C) | 109.5 |
| H(24B)-C(24)-H(24C) | 109.5 |
| C(44)-C(34)-H(34A) | 109.5 |
| C(44)-C(34)-H(34B) | 109.5 |
| H(34A)-C(34)-H(34B) | 109.5 |
| C(44)-C(34)-H(34C) | 109.5 |
| H(34A)-C(34)-H(34C) | 109.5 |
| H(34B)-C(34)-H(34C) | 109.5 |
| C(14)-C(44)-C(34) | 106.52(14) |
| C(14)-C(44)-C(24) | 106.19(15) |
| C(34)-C(44)-C(24) | 108.95(15) |
| C(14)-C(44)-C(54) | 118.35(13) |
| C(34)-C(44)-C(54) | 110.57(13) |

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| C(24)-C(44)-C(54) | 105.93(13) | C(25)-C(15)-N(14) | 118.68(12) |
| N(14)-C(54)-C(64) | 121.14(13) | C(35)-C(25)-C(15) | 118.54(13) |
| N(14)-C(54)-C(44) | 127.20(13) | C(35)-C(25)-C(75) | 119.07(13) |
| C(64)-C(54)-C(44) | 111.57(13) | C(15)-C(25)-C(75) | 122.39(13) |
| C(74)-C(64)-C(54) | 133.47(13) | C(45)-C(35)-C(25) | 122.54(13) |
| C(74)-C(64)-H(64) | 113.3 | C(45)-C(35)-H(35) | 118.7 |
| C(54)-C(64)-H(64) | 113.3 | C(25)-C(35)-H(35) | 118.7 |
| N(24)-C(74)-C(64) | 122.34(13) | C(35)-C(45)-C(55) | 117.51(13) |
| N(24)-C(74)-C(84) | 124.86(13) | C(35)-C(45)-C(105) | 119.99(13) |
| C(64)-C(74)-C(84) | 112.80(13) | C(55)-C(45)-C(105) | 122.42(13) |
| C(104)-C(84)-C(114) | 106.78(18) | C(45)-C(55)-C(65) | 122.30(13) |
| C(104)-C(84)-C(94) | 108.14(15) | C(45)-C(55)-H(55) | 118.9 |
| C(114)-C(84)-C(94) | 106.00(17) | C(65)-C(55)-H(55) | 118.9 |
| C(104)-C(84)-C(74) | 110.47(14) | C(55)-C(65)-C(15) | 118.74(13) |
| C(114)-C(84)-C(74) | 116.42(13) | C(55)-C(65)-C(135) | 119.46(12) |
| C(94)-C(84)-C(74) | 108.67(13) | C(15)-C(65)-C(135) | 121.80(12) |
| C(84)-C(94)-H(94A) | 109.5 | C(25)-C(75)-C(95) | 109.55(16) |
| C(84)-C(94)-H(94B) | 109.5 | C(25)-C(75)-C(85) | 112.91(14) |
| H(94A)-C(94)-H(94B) | 109.5 | C(95)-C(75)-C(85) | 109.73(15) |
| C(84)-C(94)-H(94C) | 109.5 | C(25)-C(75)-H(75) | 108.2 |
| H(94A)-C(94)-H(94C) | 109.5 | C(95)-C(75)-H(75) | 108.2 |
| H(94B)-C(94)-H(94C) | 109.5 | C(85)-C(75)-H(75) | 108.2 |
| C(84)-C(104)-H(10D) | 109.5 | C(75)-C(85)-H(85A) | 109.5 |
| C(84)-C(104)-H(10E) | 109.5 | C(75)-C(85)-H(85B) | 109.5 |
| H(10D)-C(104)-H(10E) | 109.5 | H(85A)-C(85)-H(85B) | 109.5 |
| C(84)-C(104)-H(10F) | 109.5 | C(75)-C(85)-H(85C) | 109.5 |
| H(10D)-C(104)-H(10F) | 109.5 | H(85A)-C(85)-H(85C) | 109.5 |
| H(10E)-C(104)-H(10F) | 109.5 | H(85B)-C(85)-H(85C) | 109.5 |
| C(84)-C(114)-H(11S) | 109.5 | C(75)-C(95)-H(95A) | 109.5 |
| C(84)-C(114)-H(11T) | 109.5 | C(75)-C(95)-H(95B) | 109.5 |
| H(11S)-C(114)-H(11T) | 109.5 | H(95A)-C(95)-H(95B) | 109.5 |
| C(84)-C(114)-H(11U) | 109.5 | C(75)-C(95)-H(95C) | 109.5 |
| H(11S)-C(114)-H(11U) | 109.5 | H(95A)-C(95)-H(95C) | 109.5 |
| H(11T)-C(114)-H(11U) | 109.5 | H(95B)-C(95)-H(95C) | 109.5 |
| C(65)-C(15)-C(25) | 120.19(13) | C(45)-C(105)-C(125) | 113.91(13) |
| C(65)-C(15)-N(14) | 121.06(12) | C(45)-C(105)-C(115) | 109.93(12) |

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| C(125)-C(105)-C(115) | 110.69(14) | C(66)-C(16)-N(24) | 119.24(12) |
| C(45)-C(105)-H(105) | 107.3 | C(36)-C(26)-C(16) | 119.03(12) |
| C(125)-C(105)-H(105) | 107.3 | C(36)-C(26)-C(76) | 118.43(13) |
| C(115)-C(105)-H(105) | 107.3 | C(16)-C(26)-C(76) | 122.52(12) |
| C(105)-C(115)-H(11D) | 109.5 | C(26)-C(36)-C(46) | 122.38(14) |
| C(105)-C(115)-H(11E) | 109.5 | C(26)-C(36)-H(36) | 118.8 |
| H(11D)-C(115)-H(11E) | 109.5 | C(46)-C(36)-H(36) | 118.8 |
| C(105)-C(115)-H(11F) | 109.5 | C(56)-C(46)-C(36) | 117.48(13) |
| H(11D)-C(115)-H(11F) | 109.5 | C(56)-C(46)-C(106) | 121.50(13) |
| H(11E)-C(115)-H(11F) | 109.5 | C(36)-C(46)-C(106) | 121.02(14) |
| C(105)-C(125)-H(12D) | 109.5 | C(46)-C(56)-C(66) | 122.69(13) |
| C(105)-C(125)-H(12E) | 109.5 | C(46)-C(56)-H(56) | 118.7 |
| H(12D)-C(125)-H(12E) | 109.5 | C(66)-C(56)-H(56) | 118.7 |
| C(105)-C(125)-H(12F) | 109.5 | C(56)-C(66)-C(16) | 118.47(13) |
| H(12D)-C(125)-H(12F) | 109.5 | C(56)-C(66)-C(136) | 119.06(13) |
| H(12E)-C(125)-H(12F) | 109.5 | C(16)-C(66)-C(136) | 122.30(12) |
| C(65)-C(135)-C(145) | 110.39(12) | C(26)-C(76)-C(86) | 109.64(11) |
| C(65)-C(135)-C(155) | 112.71(12) | C(26)-C(76)-C(96) | 114.05(12) |
| C(145)-C(135)-C(155) | 109.82(13) | C(86)-C(76)-C(96) | 108.80(13) |
| C(65)-C(135)-H(135) | 107.9 | C(26)-C(76)-H(76) | 108.1 |
| C(145)-C(135)-H(135) | 107.9 | C(86)-C(76)-H(76) | 108.1 |
| C(155)-C(135)-H(135) | 107.9 | C(96)-C(76)-H(76) | 108.1 |
| C(135)-C(145)-H(14A) | 109.5 | C(76)-C(86)-H(86A) | 109.5 |
| C(135)-C(145)-H(14B) | 109.5 | C(76)-C(86)-H(86B) | 109.5 |
| H(14A)-C(145)-H(14B) | 109.5 | H(86A)-C(86)-H(86B) | 109.5 |
| C(135)-C(145)-H(14C) | 109.5 | C(76)-C(86)-H(86C) | 109.5 |
| H(14A)-C(145)-H(14C) | 109.5 | H(86A)-C(86)-H(86C) | 109.5 |
| H(14B)-C(145)-H(14C) | 109.5 | H(86B)-C(86)-H(86C) | 109.5 |
| C(135)-C(155)-H(15A) | 109.5 | C(76)-C(96)-H(96A) | 109.5 |
| C(135)-C(155)-H(15B) | 109.5 | C(76)-C(96)-H(96B) | 109.5 |
| H(15A)-C(155)-H(15B) | 109.5 | H(96A)-C(96)-H(96B) | 109.5 |
| C(135)-C(155)-H(15C) | 109.5 | C(76)-C(96)-H(96C) | 109.5 |
| H(15A)-C(155)-H(15C) | 109.5 | H(96A)-C(96)-H(96C) | 109.5 |
| H(15B)-C(155)-H(15C) | 109.5 | H(96B)-C(96)-H(96C) | 109.5 |
| C(26)-C(16)-C(66) | 119.76(12) | C(46)-C(106)-C(116) | 112.45(13) |
| C(26)-C(16)-N(24) | 120.94(12) | C(46)-C(106)-C(126) | 111.49(14) |

| | | | |
|---|---|---|---|
| C(116)-C(106)-C(126) | 109.43(15) | H(17A)-C(17)-H(17B) | 109.5 |
| C(46)-C(106)-H(106) | 107.8 | C(27)-C(17)-H(17C) | 109.5 |
| C(116)-C(106)-H(106) | 107.8 | H(17A)-C(17)-H(17C) | 109.5 |
| C(126)-C(106)-H(106) | 107.8 | H(17B)-C(17)-H(17C) | 109.5 |
| C(106)-C(116)-H(11G) | 109.5 | C(37)-C(27)-C(77) | 117.7(5) |
| C(106)-C(116)-H(11H) | 109.5 | C(37)-C(27)-C(17) | 121.0(4) |
| H(11G)-C(116)-H(11H) | 109.5 | C(77)-C(27)-C(17) | 121.3(5) |
| C(106)-C(116)-H(11I) | 109.5 | C(27)-C(37)-C(47) | 120.9(4) |
| H(11G)-C(116)-H(11I) | 109.5 | C(27)-C(37)-H(37) | 119.5 |
| H(11H)-C(116)-H(11I) | 109.5 | C(47)-C(37)-H(37) | 119.5 |
| C(106)-C(126)-H(12A) | 109.5 | C(57)-C(47)-C(37) | 118.9(4) |
| C(106)-C(126)-H(12B) | 109.5 | C(57)-C(47)-H(47) | 120.5 |
| H(12A)-C(126)-H(12B) | 109.5 | C(37)-C(47)-H(47) | 120.5 |
| C(106)-C(126)-H(12C) | 109.5 | C(67)-C(57)-C(47) | 120.8(5) |
| H(12A)-C(126)-H(12C) | 109.5 | C(67)-C(57)-H(57) | 119.6 |
| H(12B)-C(126)-H(12C) | 109.5 | C(47)-C(57)-H(57) | 119.6 |
| C(66)-C(136)-C(156) | 114.37(12) | C(57)-C(67)-C(77) | 118.8(4) |
| C(66)-C(136)-C(146) | 109.52(13) | C(57)-C(67)-H(67) | 120.6 |
| C(156)-C(136)-C(146) | 108.90(13) | C(77)-C(67)-H(67) | 120.6 |
| C(66)-C(136)-H(136) | 108.0 | C(67)-C(77)-C(27) | 122.8(5) |
| C(156)-C(136)-H(136) | 108.0 | C(67)-C(77)-H(77) | 118.6 |
| C(146)-C(136)-H(136) | 108.0 | C(27)-C(77)-H(77) | 118.6 |
| C(136)-C(146)-H(14G) | 109.5 | C(27')-C(17')-H(17D) | 109.5 |
| C(136)-C(146)-H(14H) | 109.5 | C(27')-C(17')-H(17E) | 109.5 |
| H(14G)-C(146)-H(14H) | 109.5 | H(17D)-C(17')-H(17E) | 109.5 |
| C(136)-C(146)-H(14I) | 109.5 | C(27')-C(17')-H(17F) | 109.5 |
| H(14G)-C(146)-H(14I) | 109.5 | H(17D)-C(17')-H(17F) | 109.5 |
| H(14H)-C(146)-H(14I) | 109.5 | H(17E)-C(17')-H(17F) | 109.5 |
| C(136)-C(156)-H(15G) | 109.5 | C(37')-C(27')-C(77') | 117.7(11) |
| C(136)-C(156)-H(15H) | 109.5 | C(37')-C(27')-C(17') | 126.1(11) |
| H(15G)-C(156)-H(15H) | 109.5 | C(77')-C(27')-C(17') | 115.3(11) |
| C(136)-C(156)-H(15I) | 109.5 | C(27')-C(37')-C(47') | 122.5(12) |
| H(15G)-C(156)-H(15I) | 109.5 | C(27')-C(37')-H(37') | 118.7 |
| H(15H)-C(156)-H(15I) | 109.5 | C(47')-C(37')-H(37') | 118.7 |
| C(27)-C(17)-H(17A) | 109.5 | C(57')-C(47')-C(37') | 116.7(12) |
| C(27)-C(17)-H(17B) | 109.5 | C(57')-C(47')-H(47') | 121.7 |

| | |
|---|---|
| C(37')-C(47')-H(47') | 121.7 |
| C(67')-C(57')-C(47') | 123.1(12) |
| C(67')-C(57')-H(57') | 118.4 |
| C(47')-C(57')-H(57') | 118.4 |
| C(57')-C(67')-C(77') | 117.9(12) |
| C(57')-C(67')-H(67') | 121.0 |
| C(77')-C(67')-H(67') | 121.0 |
| C(27')-C(77')-C(67') | 121.7(14) |
| C(27')-C(77')-H(77') | 119.1 |
| C(67')-C(77')-H(77') | 119.1 |
| C(28)-C(18)-H(18A) | 109.5 |
| C(28)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| C(28)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| C(38)-C(28)-C(78) | 118.01(19) |
| C(38)-C(28)-C(18) | 121.15(19) |
| C(78)-C(28)-C(18) | 120.8(2) |
| C(28)-C(38)-C(48) | 121.24(19) |
| C(28)-C(38)-H(38A) | 119.4 |
| C(48)-C(38)-H(38A) | 119.4 |
| C(58)-C(48)-C(38) | 119.8(2) |
| C(58)-C(48)-H(48A) | 120.1 |
| C(38)-C(48)-H(48A) | 120.1 |
| C(48)-C(58)-C(68) | 119.7(2) |
| C(48)-C(58)-H(58A) | 120.2 |
| C(68)-C(58)-H(58A) | 120.2 |
| C(78)-C(68)-C(58) | 120.1(2) |
| C(78)-C(68)-H(68A) | 119.9 |
| C(58)-C(68)-H(68A) | 119.9 |
| C(68)-C(78)-C(28) | 121.2(2) |
| C(68)-C(78)-H(78A) | 119.4 |
| C(28)-C(78)-H(78A) | 119.4 |

**Table S6. Crystal data and structure refinement for $L^{tBu}$FeNPhNPh**

| | | |
|---|---|---|
| Identification code | holas19 | |
| Empirical formula | C47 H63 Fe N4 | |
| Formula weight | 739.86 | |
| Temperature | 100.0(1) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | *C*2/*c* | |
| Unit cell dimensions | *a* = 22.938(4) Å | α = 90° |
| | *b* = 10.2673(17) Å | β = 115.543(2)° |
| | *c* = 19.629(3) Å | γ = 90° |
| Volume | 4170.9(12) $Å^3$ | |
| *Z* | 4 | |
| Density (calculated) | 1.178 $g/cm^3$ | |
| Absorption coefficient | 0.398 $mm^{-1}$ | |
| *F*(000) | 1596 | |
| Crystal color, morphology | red-black, block | |
| Crystal size | 0.32 x 0.28 x 0.12 $mm^3$ | |
| Theta range for data collection | 1.97 to 32.03° | |
| Index ranges | $-33 \leq h \leq 34, -13 \leq k \leq 15, -29 \leq l \leq 29$ | |
| Reflections collected | 27124 | |
| Independent reflections | 7230 [*R*(int) = 0.0331] | |
| Observed reflections | 5927 | |
| Completeness to theta = 32.03° | 99.6% | |
| Absorption correction | Multi-scan | |
| Max. and min. transmission | 0.9538 and 0.8833 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 7230 / 0 / 243 | |
| Goodness-of-fit on *F*2 | 1.054 | |
| Final *R* indices [*I*>2sigma(*I*)] | *R*1 = 0.0384, *wR*2 = 0.0965 | |
| *R* indices (all data) | *R*1 = 0.0512, *wR*2 = 0.1035 | |
| Largest diff. peak and hole | 1.008 and -0.228 e•$Å^{-3}$ | |

**Table S7. Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$ ) for $L^{tBu}$FeNPhNPh.**

| | x | y | z | Ueq |
|---|---|---|---|---|
| Fe | 0 | 4752(1) | 2500 | 13(1) |
| N1 | 317(1) | 2976(1) | 2783(1) | 16(1) |
| C1 | 358(1) | 2558(1) | 3492(1) | 17(1) |
| C2 | 952(1) | 2704(1) | 4124(1) | 21(1) |
| C3 | 1026(1) | 2264(1) | 4826(1) | 26(1) |
| C4 | 524(1) | 1636(1) | 4906(1) | 30(1) |
| C5 | -56(1) | 1448(1) | 4276(1) | 28(1) |
| C6 | -145(1) | 1911(1) | 3572(1) | 21(1) |
| N11 | 720(1) | 6028(1) | 2917(1) | 13(1) |
| C11 | 1161(1) | 8364(1) | 2944(1) | 15(1) |
| C21 | 622(1) | 7318(1) | 2806(1) | 14(1) |
| C31 | 0 | 7863(2) | 2500 | 16(1) |
| C41 | 1872(1) | 7943(1) | 3365(1) | 19(1) |
| C51 | 1056(1) | 8809(1) | 2146(1) | 22(1) |
| C61 | 1084(1) | 9562(1) | 3376(1) | 23(1) |
| C12 | 1319(1) | 5524(1) | 3481(1) | 13(1) |
| C22 | 1713(1) | 4704(1) | 3279(1) | 16(1) |
| C32 | 2285(1) | 4239(1) | 3856(1) | 21(1) |
| C42 | 2453(1) | 4523(1) | 4608(1) | 23(1) |
| C52 | 2043(1) | 5275(1) | 4798(1) | 20(1) |
| C62 | 1473(1) | 5794(1) | 4245(1) | 15(1) |
| C72 | 1533(1) | 4310(1) | 2464(1) | 18(1) |
| C82 | 1766(1) | 2933(1) | 2408(1) | 23(1) |
| C92 | 1795(1) | 5268(1) | 2062(1) | 32(1) |
| C102 | 1036(1) | 6610(1) | 4482(1) | 18(1) |
| C112 | 1415(1) | 7467(1) | 5169(1) | 26(1) |
| C122 | 556(1) | 5748(1) | 4628(1) | 31(1) |

**Table S8. Hydrogen coordinates (x 10 $^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for $L^{tBu}$FeNPhNPh.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H2A | 1304 | 3104 | 4072 | 25 |
| H3A | 1426 | 2394 | 5256 | 32 |
| H4A | 577 | 1337 | 5387 | 36 |
| H5A | -398 | 998 | 4326 | 33 |
| H6A | -547 | 1787 | 3145 | 25 |
| H31A | 0 | 8789 | 2500 | 19 |
| H41A | 1945 | 7160 | 3127 | 28 |

| | | | | |
|---|---|---|---|---|
| H41B | 1971 | 7753 | 3893 | 28 |
| H41C | 2153 | 8646 | 3345 | 28 |
| H51A | 1105 | 8061 | 1865 | 33 |
| H51B | 1376 | 9476 | 2190 | 33 |
| H51C | 620 | 9172 | 1878 | 33 |
| H61A | 1079 | 9277 | 3850 | 34 |
| H61B | 677 | 10008 | 3065 | 34 |
| H61C | 1446 | 10161 | 3486 | 34 |
| H32A | 2565 | 3715 | 3730 | 26 |
| H42A | 2847 | 4204 | 4991 | 28 |
| H52A | 2153 | 5441 | 5315 | 24 |
| H72A | 1051 | 4315 | 2187 | 22 |
| H82A | 1643 | 2335 | 2713 | 35 |
| H82B | 2237 | 2935 | 2596 | 35 |
| H82C | 1567 | 2648 | 1880 | 35 |
| H92A | 1600 | 6127 | 2036 | 48 |
| H92B | 1686 | 4954 | 1550 | 48 |
| H92C | 2265 | 5333 | 2344 | 48 |
| H10A | 779 | 7201 | 4051 | 21 |
| H11A | 1753 | 7939 | 5090 | 39 |
| H11B | 1615 | 6920 | 5620 | 39 |
| H11C | 1122 | 8092 | 5237 | 39 |
| H12A | 288 | 5269 | 4166 | 46 |
| H12B | 280 | 6294 | 4776 | 46 |
| H12C | 794 | 5130 | 5034 | 46 |

**Table S9. Bond lengths [Å] and angles [°] for $L^{tBu}$FeNPhNPh**

| | | | |
|---|---|---|---|
| Fe-N(1)#1 | 1.9527(10) | C(11)-C(51) | 1.5471(15) |
| Fe-N(1) | 1.9527(10) | C(11)-C(21) | 1.5701(15) |
| Fe-N(11) | 1.9871(9) | C(21)-C(31) | 1.4045(12) |
| Fe-N(11)#1 | 1.9871(9) | C(31)-C(21)#1 | 1.4045(12) |
| N(1)-N(1)#1 | 1.3976(18) | C(31)-H(31A) | 0.9500 |
| N(1)-C(1) | 1.4203(14) | C(41)-H(41A) | 0.9800 |
| C(1)-C(6) | 1.3974(16) | C(41)-H(41B) | 0.9800 |
| C(1)-C(2) | 1.3998(16) | C(41)-H(41C) | 0.9800 |
| C(2)-C(3) | 1.3894(17) | C(51)-H(51A) | 0.9800 |
| C(2)-H(2A) | 0.9500 | C(51)-H(51B) | 0.9800 |
| C(3)-C(4) | 1.388(2) | C(51)-H(51C) | 0.9800 |
| C(3)-H(3A) | 0.9500 | C(61)-H(61A) | 0.9800 |
| C(4)-C(5) | 1.384(2) | C(61)-H(61B) | 0.9800 |
| C(4)-H(4A) | 0.9500 | C(61)-H(61C) | 0.9800 |
| C(5)-C(6) | 1.3912(17) | C(12)-C(22) | 1.4115(14) |

| | | | |
|---|---|---|---|
| C(5)-H(5A) | 0.9500 | C(12)-C(62) | 1.4121(14) |
| C(6)-H(6A) | 0.9500 | C(22)-C(32) | 1.3962(15) |
| N(11)-C(21) | 1.3451(14) | C(22)-C(72) | 1.5250(15) |
| N(11)-C(12) | 1.4372(13) | C(32)-C(42) | 1.3866(17) |
| C(11)-C(41) | 1.5398(15) | C(32)-H(32A) | 0.9500 |
| C(11)-C(61) | 1.5466(16) | C(42)-C(52) | 1.3860(17) |
| C(42)-H(42A) | 0.9500 | N(1)#1-Fe-N(1) | 41.94(5) |
| C(52)-C(62) | 1.3966(15) | N(1)#1-Fe-N(11) | 150.93(4) |
| C(52)-H(52A) | 0.9500 | N(1)-Fe-N(11) | 110.92(4) |
| C(62)-C(102) | 1.5247(15) | N(1)#1-Fe-N(11)#1 | 110.92(4) |
| C(72)-C(82) | 1.5322(17) | N(1)-Fe-N(11)#1 | 150.93(4) |
| C(72)-C(92) | 1.5345(18) | N(11)-Fe-N(11)#1 | 97.52(5) |
| C(72)-H(72A) | 1.0000 | N(1)#1-N(1)-C(1) | 112.70(10) |
| C(82)-H(82A) | 0.9800 | N(1)#1-N(1)-Fe | 69.03(3) |
| C(82)-H(82B) | 0.9800 | C(6)-C(1)-C(2) | 119.15(10) |
| C(82)-H(82C) | 0.9800 | C(6)-C(1)-N(1) | 122.98(10) |
| C(92)-H(92A) | 0.9800 | C(2)-C(1)-N(1) | 117.61(10) |
| C(92)-H(92B) | 0.9800 | C(3)-C(2)-C(1) | 119.99(12) |
| C(92)-H(92C) | 0.9800 | C(1)-N(1)-Fe | 114.85(7) |
| C(102)-C(112) | 1.5291(16) | C(1)-C(2)-H(2A) | 120.0 |
| C(102)-C(122) | 1.5323(17) | C(3)-C(2)-H(2A) | 120.0 |
| C(102)-H(10A) | 1.0000 | C(4)-C(3)-C(2) | 120.71(12) |
| C(112)-H(11A) | 0.9800 | C(4)-C(3)-H(3A) | 119.6 |
| C(112)-H(11B) | 0.9800 | C(2)-C(3)-H(3A) | 119.6 |
| C(112)-H(11C) | 0.9800 | C(5)-C(4)-C(3) | 119.31(12) |
| C(122)-H(12A) | 0.9800 | C(5)-C(4)-H(4A) | 120.3 |
| C(122)-H(12B) | 0.9800 | C(3)-C(4)-H(4A) | 120.3 |
| C(122)-H(12C) | 0.9800 | C(4)-C(5)-C(6) | 120.78(12) |

| | | | |
|---|---|---|---|
| C(4)-C(5)-H(5A) | 119.6 | C(11)-C(41)-H(41C) | 109.5 |
| C(6)-C(5)-H(5A) | 119.6 | H(41A)-C(41)-H(41C) | 109.5 |
| C(5)-C(6)-C(1) | 119.99(12) | H(41B)-C(41)-H(41C) | 109.5 |
| C(5)-C(6)-H(6A) | 120.0 | C(11)-C(51)-H(51A) | 109.5 |
| C(1)-C(6)-H(6A) | 120.0 | C(11)-C(51)-H(51B) | 109.5 |
| C(21)-N(11)-C(12) | 121.11(9) | H(51A)-C(51)-H(51B) | 109.5 |
| C(21)-N(11)-Fe | 122.08(7) | C(11)-C(51)-H(51C) | 109.5 |
| C(12)-N(11)-Fe | 115.35(7) | H(51A)-C(51)-H(51C) | 109.5 |
| C(41)-C(11)-C(61) | 105.89(9) | H(51B)-C(51)-H(51C) | 109.5 |
| C(41)-C(11)-C(51) | 107.05(9) | C(11)-C(61)-H(61A) | 109.5 |
| C(61)-C(11)-C(51) | 108.38(10) | C(11)-C(61)-H(61B) | 109.5 |
| C(41)-C(11)-C(21) | 118.21(9) | H(61A)-C(61)-H(61B) | 109.5 |
| C(61)-C(11)-C(21) | 111.82(9) | C(11)-C(61)-H(61C) | 109.5 |
| C(51)-C(11)-C(21) | 105.09(8) | H(61A)-C(61)-H(61C) | 109.5 |

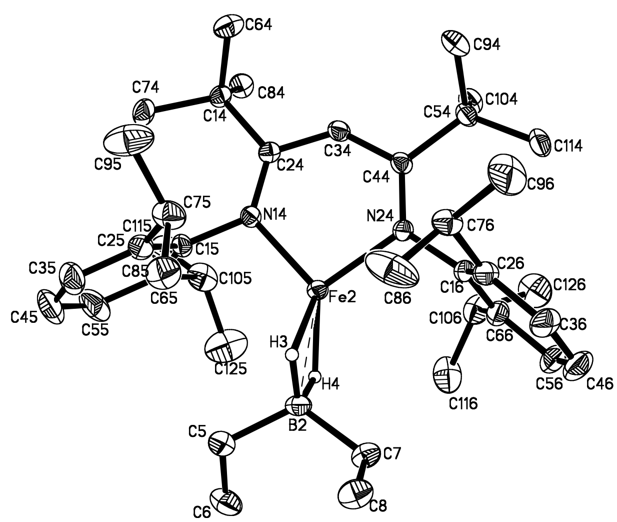
| | | | |
|---|---|---|---|
| N(11)-C(21)-C(31) | 121.99(10) | H(61B)-C(61)-H(61C) | 109.5 |
| N(11)-C(21)-C(11) | 125.59(9) | C(22)-C(12)-C(62) | 121.17(10) |
| C(22)-C(12)-N(11) | 120.91(9) | C(72)-C(82)-H(82A) | 109.5 |
| C(62)-C(12)-N(11) | 117.74(9) | C(72)-C(82)-H(82B) | 109.5 |
| C(32)-C(22)-C(12) | 117.90(10) | H(82A)-C(82)-H(82B) | 109.5 |
| C(32)-C(22)-C(72) | 119.64(10) | C(72)-C(82)-H(82C) | 109.5 |
| C(12)-C(22)-C(72) | 122.46(10) | H(82A)-C(82)-H(82C) | 109.5 |
| C(42)-C(32)-C(22) | 121.65(10) | H(82B)-C(82)-H(82C) | 109.5 |
| C(42)-C(32)-H(32A) | 119.2 | C(72)-C(92)-H(92A) | 109.5 |
| C(22)-C(32)-H(32A) | 119.2 | C(72)-C(92)-H(92B) | 109.5 |
| C(52)-C(42)-C(32) | 119.59(11) | H(92A)-C(92)-H(92B) | 109.5 |
| C(52)-C(42)-H(42A) | 120.2 | C(72)-C(92)-H(92C) | 109.5 |
| C(32)-C(42)-H(42A) | 120.2 | H(92A)-C(92)-H(92C) | 109.5 |
| C(42)-C(52)-C(62) | 121.33(10) | H(92B)-C(92)-H(92C) | 109.5 |
| C(42)-C(52)-H(52A) | 119.3 | C(62)-C(102)-C(112) | 112.70(9) |
| C(62)-C(52)-H(52A) | 119.3 | C(62)-C(102)-C(122) | 111.03(10) |
| C(52)-C(62)-C(12) | 118.21(10) | C(112)-C(102)-C(122) | 110.47(10) |
| C(52)-C(62)-C(102) | 119.41(9) | C(62)-C(102)-H(10A) | 107.5 |
| C(12)-C(62)-C(102) | 122.37(9) | C(112)-C(102)-H(10A) | 107.5 |
| C(22)-C(72)-C(82) | 112.04(10) | C(122)-C(102)-H(10A) | 107.5 |
| C(22)-C(72)-C(92) | 112.37(10) | C(102)-C(112)-H(11A) | 109.5 |
| C(82)-C(72)-C(92) | 109.20(10) | C(102)-C(112)-H(11B) | 109.5 |
| C(22)-C(72)-H(72A) | 107.7 | H(11A)-C(112)-H(11B) | 109.5 |
| C(82)-C(72)-H(72A) | 107.7 | C(102)-C(112)-H(11C) | 109.5 |
| C(92)-C(72)-H(72A) | 107.7 | H(11A)-C(112)-H(11C) | 109.5 |
| H(11B)-C(112)-H(11C) | 109.5 | C(31)-C(21)-C(11) | 112.31(10) |
| C(102)-C(122)-H(12A) | 109.5 | C(21)#1-C(31)-C(21) | 132.99(14) |
| C(102)-C(122)-H(12B) | 109.5 | C(21)#1-C(31)-H(31A) | 113.5 |
| H(12A)-C(122)-H(12B) | 109.5 | C(21)-C(31)-H(31A) | 113.5 |
| C(102)-C(122)-H(12C) | 109.5 | C(11)-C(41)-H(41A) | 109.5 |
| H(12A)-C(122)-H(12C) | 109.5 | C(11)-C(41)-H(41B) | 109.5 |
| H(12B)-C(122)-H(12C) | 109.5 | H(41A)-C(41)-H(41B) | 109.5 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

**Details on Reaction of $[L^{tBu}FeH]_2$ with $BEt_3$.**

The iron(II) hydride dimer $[L^{tBu}Fe(\mu\text{-}H)_2FeL^{tBu}]$ abstracts hydrocarbyl groups from $BEt_3$ to give $L^{Me}FeEt$ and $L^{tBu}Fe(\mu\text{-}H)_2BEt_2$. The most convenient synthesis of the dihydridoborate complex is the same as the synthesis of $[L^{tBu}FeH]_2$, but with a longer reaction time. An ORTEP diagram is given below, and details of the reaction will be reported separately.[3]

**$L^{tBu}Fe(\mu\text{-}H)_2BEt_2$.** A Schlenk flask was loaded with a mixture of $L^{tBu}FeCl$ (722 mg, 1.21 mmol) and $KHBEt_3$ (167 mg, 1.21 mmol) in toluene (50 mL). The mixture was stirred at 80 °C for 18 h. Volatile materials were removed under vacuum and the residue was extracted with pentane (50 mL), filtered and concentrated to 10 mL. Crystallization at -26 ºC gave dark red blocks (224 mg, 59%). $^1H$ NMR (500 MHz, $C_6D_6$): 71 (6H, $BEt_2$ $CH_3$), 42 (1H, backbone), 35 (18H, backbone $CH_3$), 16 (4H), -13 (12H, *i*Pr $CH_3$), -61 (12H, *i*Pr $CH_3$), -66 (4H), -89 (2H, p-H), -313 (4H) ppm. UV-vis (pentane): 333 ($\varepsilon$ = 9.42 $mM^{-1}cm^{-1}$), 414 ($\varepsilon$ = 6.82 $mM^{-1}cm^{-1}$), 597 ($\varepsilon$ = 1.27 $mM^{-1}cm^{-1}$) nm. $\mu_{eff}$ ($C_6D_6$, 25 °C): 5.7(1) $\mu_B$. Elem. Anal. Calcd for $C_{39}H_{65}N_2BFe$: C, 74.52; H, 10.42; N, 4.46. Found: C, 74.60; H 10.20, ; N, 4.34.




**References**

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