

Supporting Information for

Chemistry of Nitrosyl Iron Complexes Supported by a β - Diketiminato Ligand

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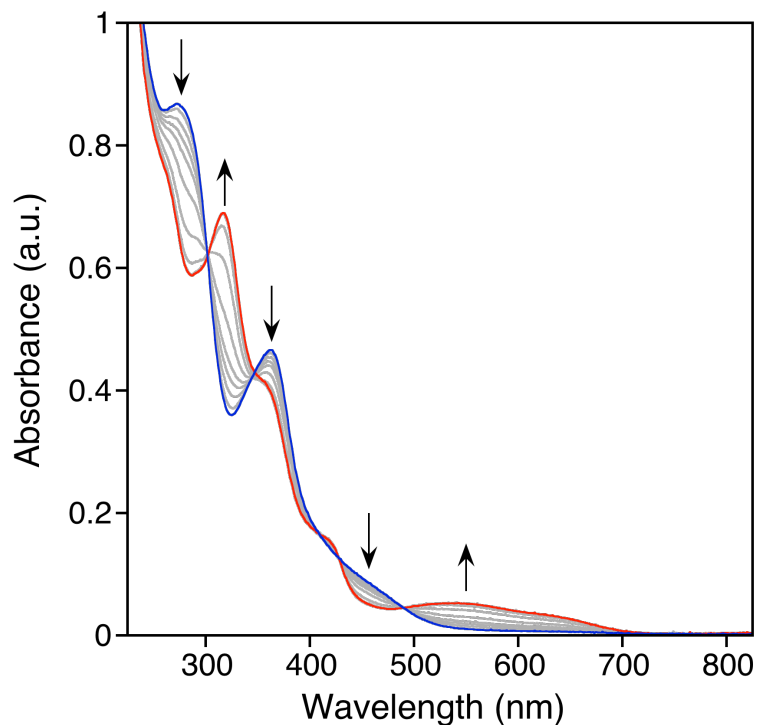


Figure S1. UV-vis spectroscopic changes associated with oxidation of **2** to **1** by air in THF at 25 °C.

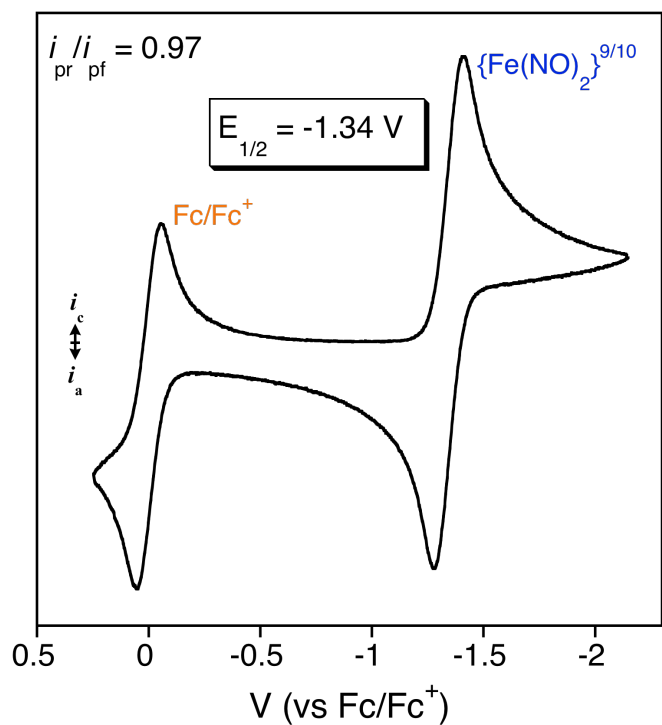


Figure S2. Cyclic voltammogram of compound **1** in THF at a glassy carbon electrode (0.1 M Bu₄NBAr₄^F supporting electrolyte).

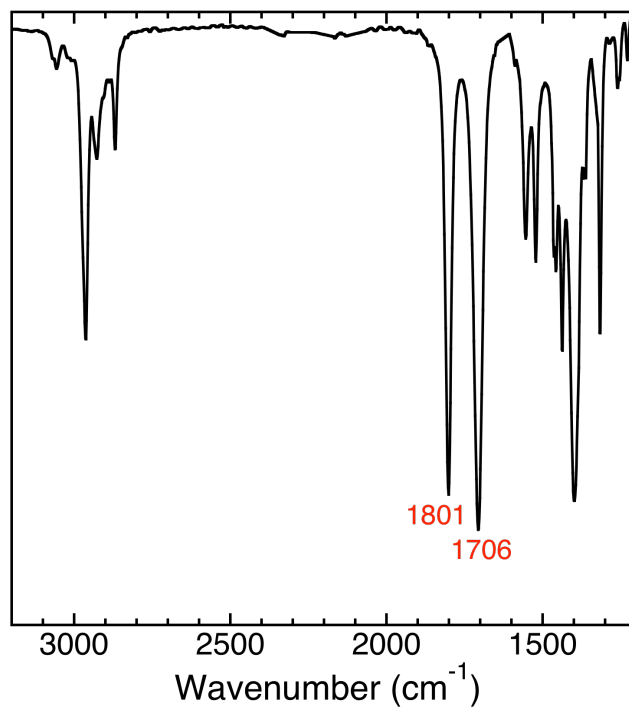


Figure S3. IR spectrum of compound **3** in benzene-*d*₆.

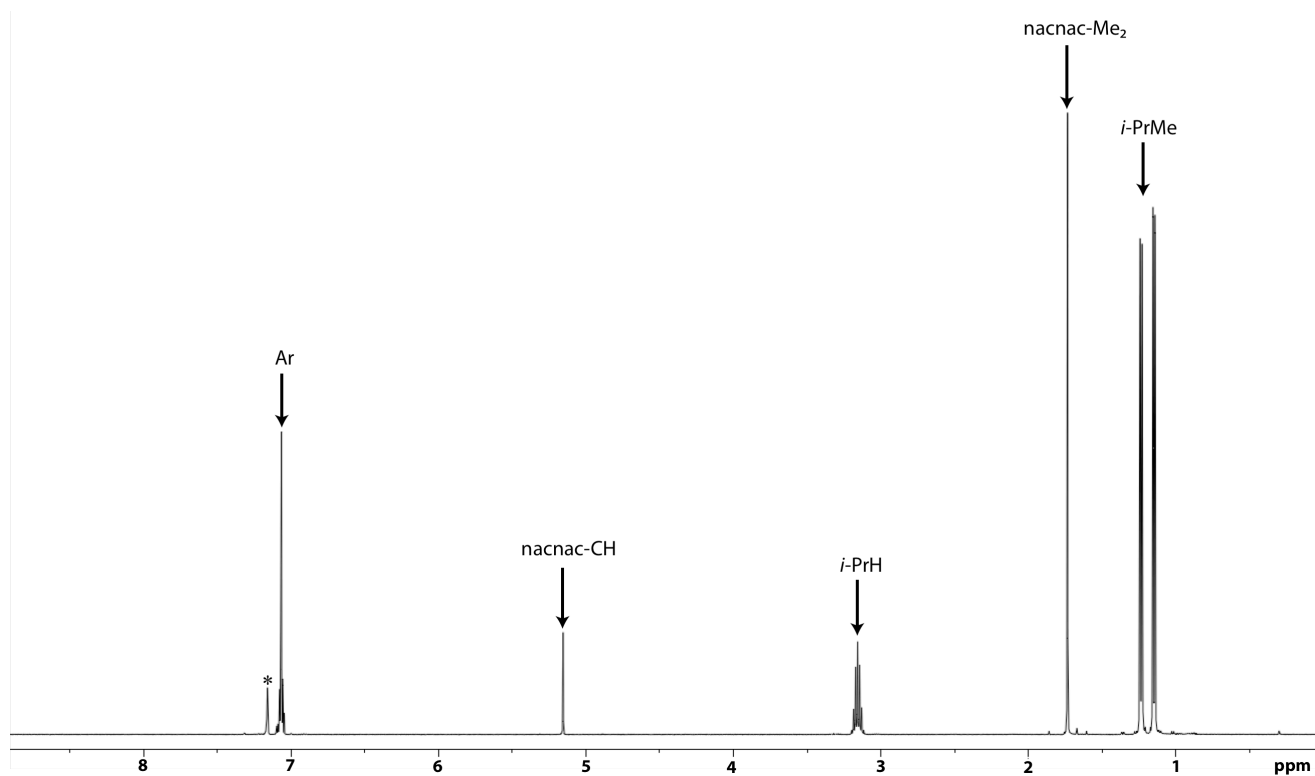


Figure S4. 500 MHz ¹H NMR spectrum of compound **3** in benzene-*d*₆. The asterisk denotes a peak due to the NMR solvent.

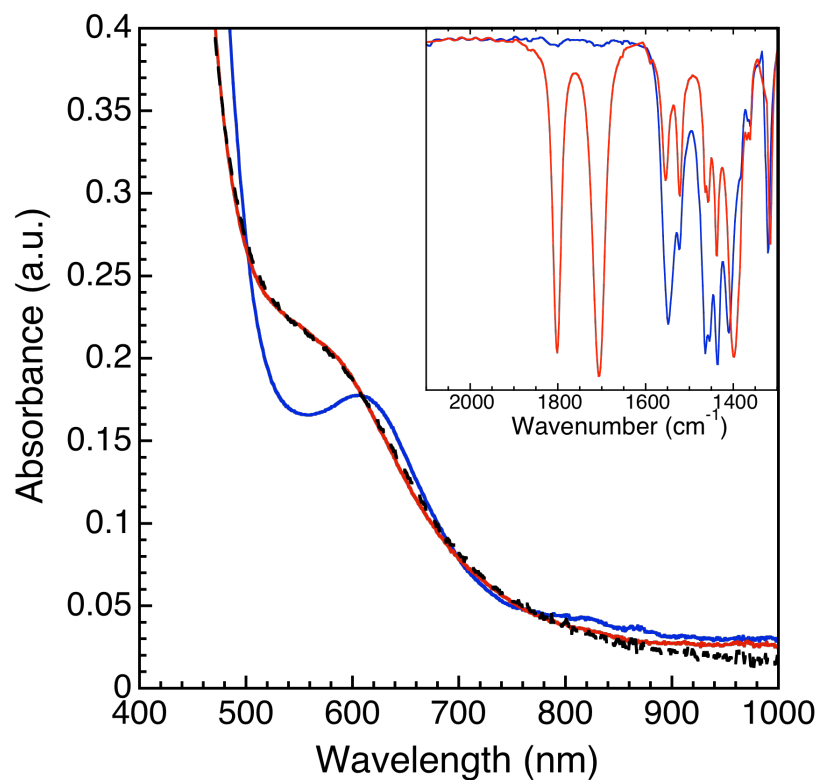


Figure S5. Electronic absorption spectrum of the reaction product of compound **3** and KC_8 in benzene- d_6 (—); same product after exposure to air (—); authentic **3** (---). Inset displays the IR spectrum of compound **3** before (—) and after (—) treatment with KC_8 in benzene- d_6 .

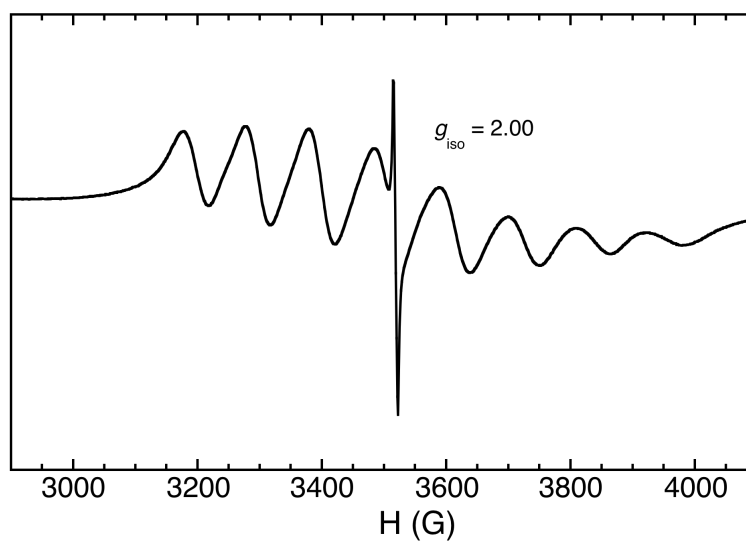


Figure S6. X-Band EPR spectrum (295 K) of the reaction product of compound **3** and KC_8 in benzene- d_6 . The sharp peak corresponds to an unknown organic impurity. $A_{\text{iso}}(^{59}\text{Co}) = 100 \text{ G}$.

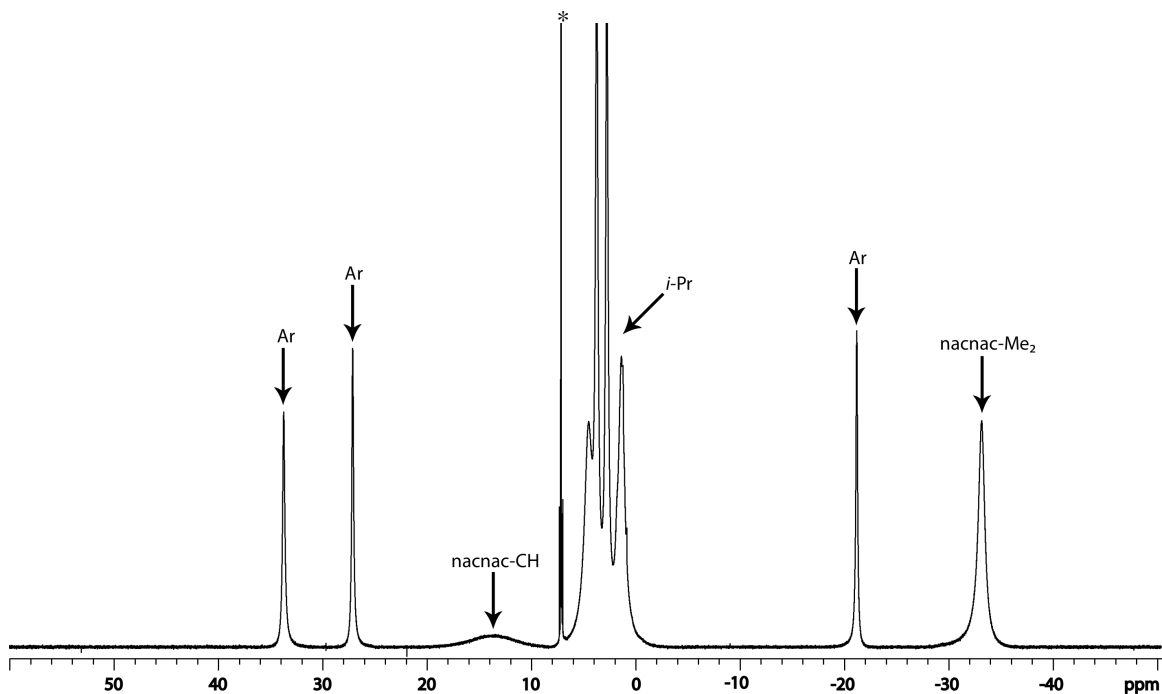


Figure S7. 500 ^1H NMR spectrum of compound **4** in benzene- d_6 . The asterisk denotes a peak due to the NMR solvent.

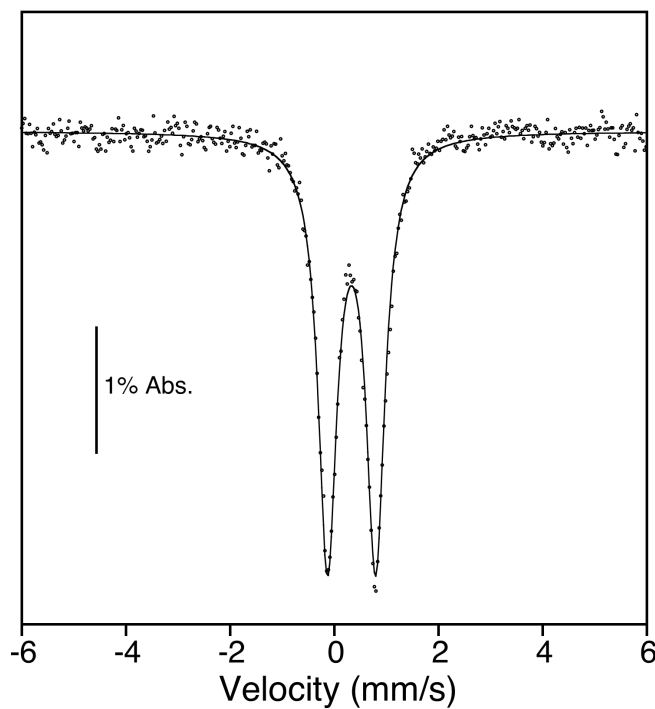


Figure S8. Zero-field ^{57}Fe Mössbauer spectrum of polycrystalline **4** recorded at 90 K; $\delta = 0.33(2)$ mm/s, $\Delta E_Q = 0.92(2)$ mm/s, $\Gamma = 0.44(2)$ mm/s.

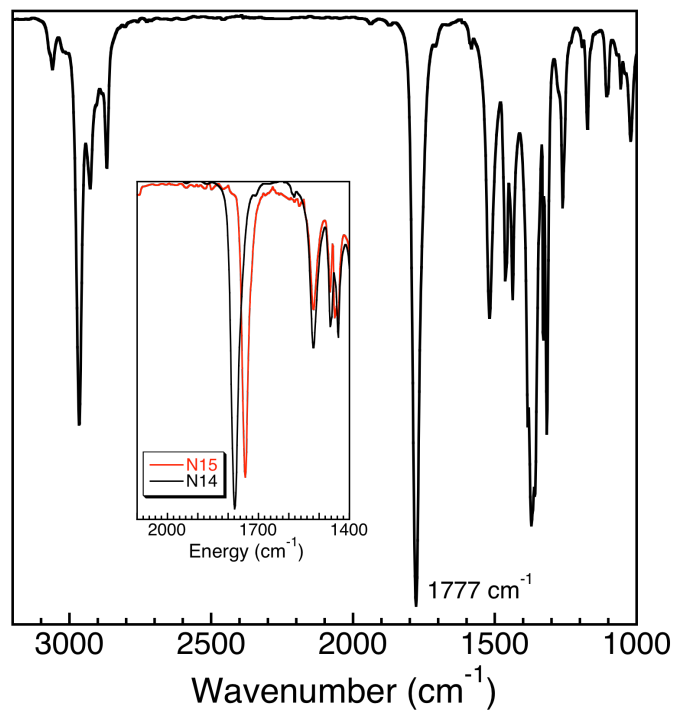


Figure S9. IR spectrum of compound **4** in benzene- d_6 . Inset shows an overlay of ν_{NO} for the ^{14}N and ^{15}N isotopomers.

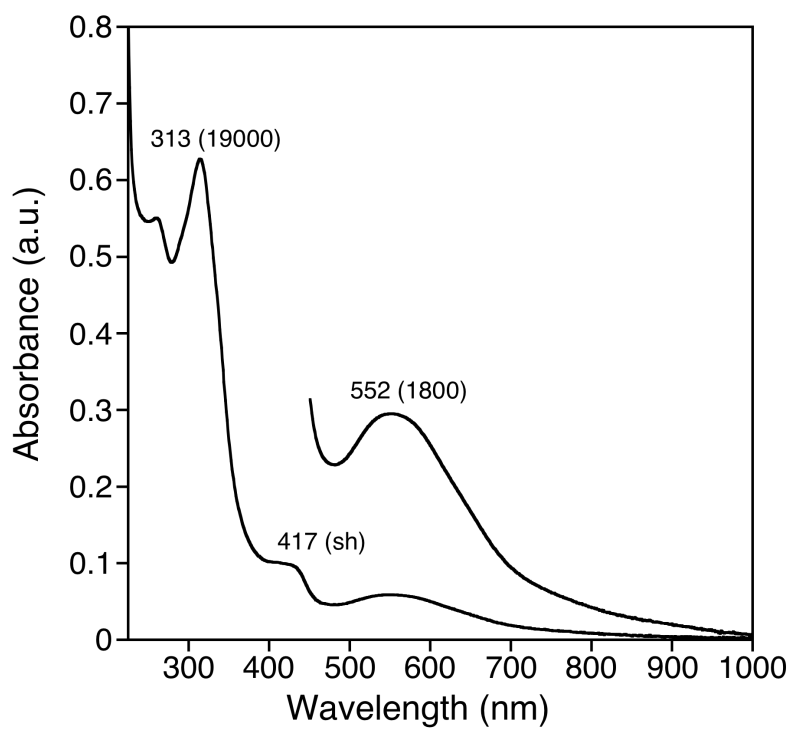


Figure S10. Electronic absorption spectrum of compound **4** in THF.

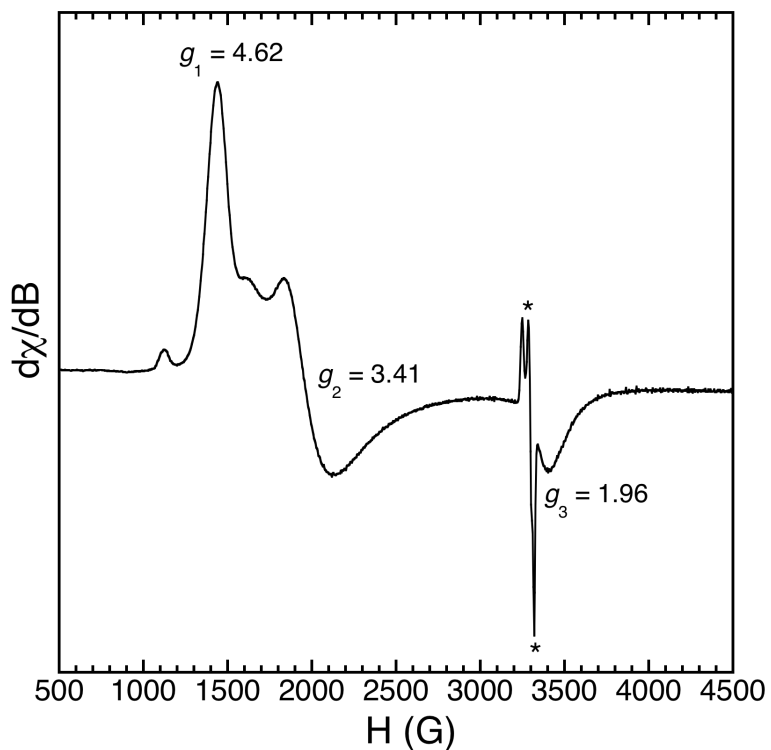


Figure S11. X-band EPR spectrum of compound **4** recorded in a 2-MeTHF glass at 77 K. Asterisks denote an impurity due to compound **1** (DNIC).

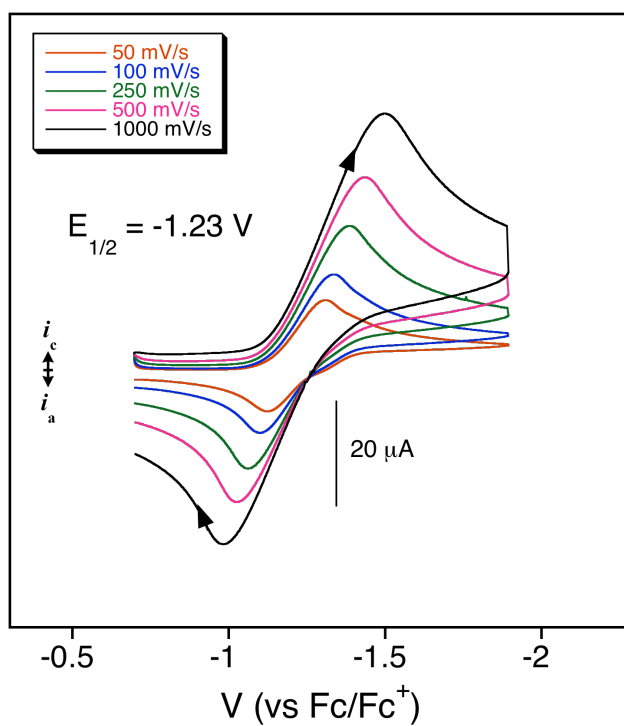


Figure S12. Cyclic voltammogram at various scan rates of compound **4** in THF at a glassy carbon electrode (0.1 M Bu_4NPF_6 supporting electrolyte).

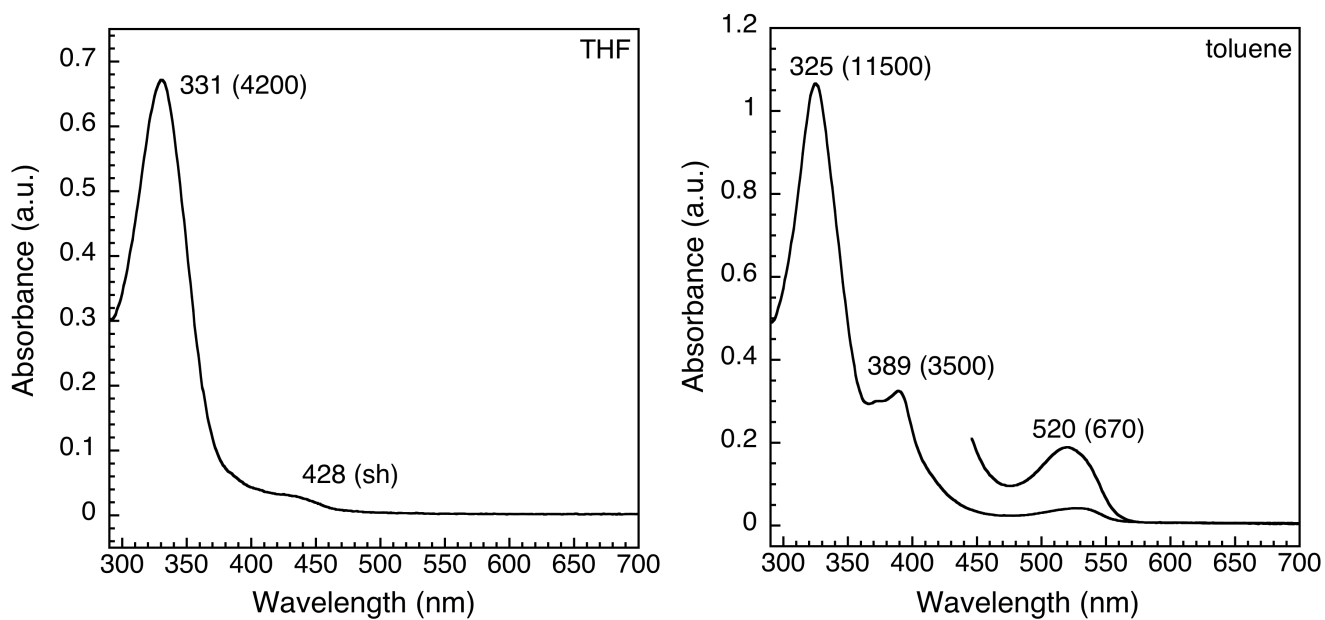


Figure S13. Electronic absorption spectra of compound **5** in THF (monomer) and toluene (dimer).

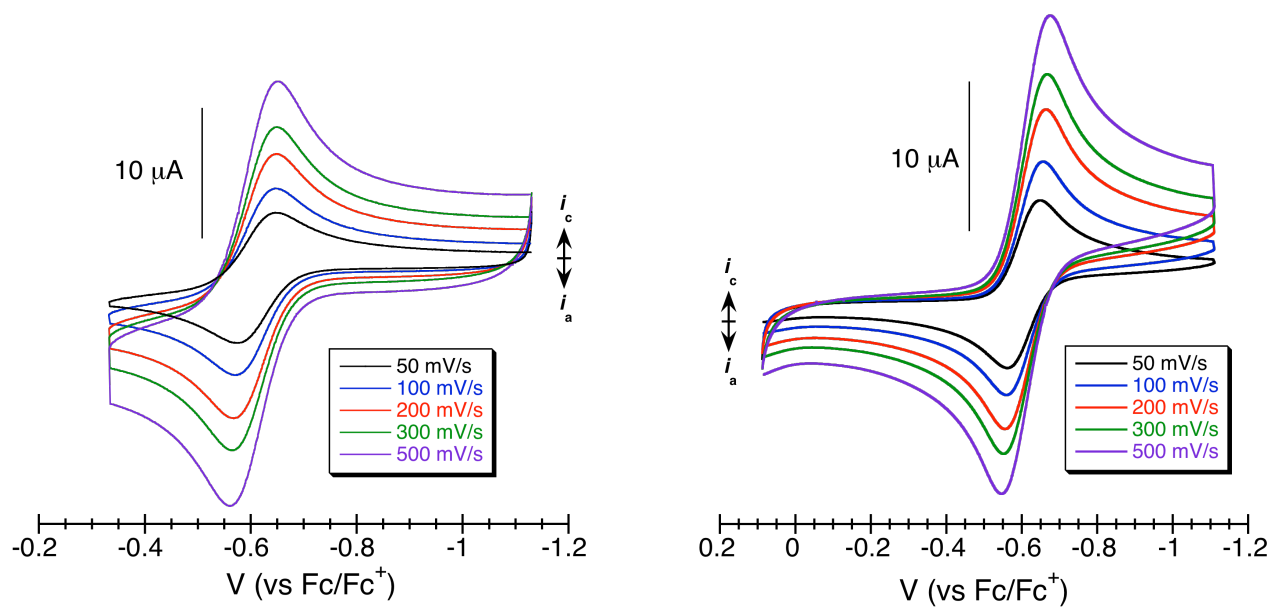


Figure S14. Cyclic voltammograms of compounds **5** (left) and **6** (right) in THF at a glassy carbon electrode (0.1 M $\text{Bu}_4\text{NBAR}_4^{\text{F}}$ supporting electrolyte).

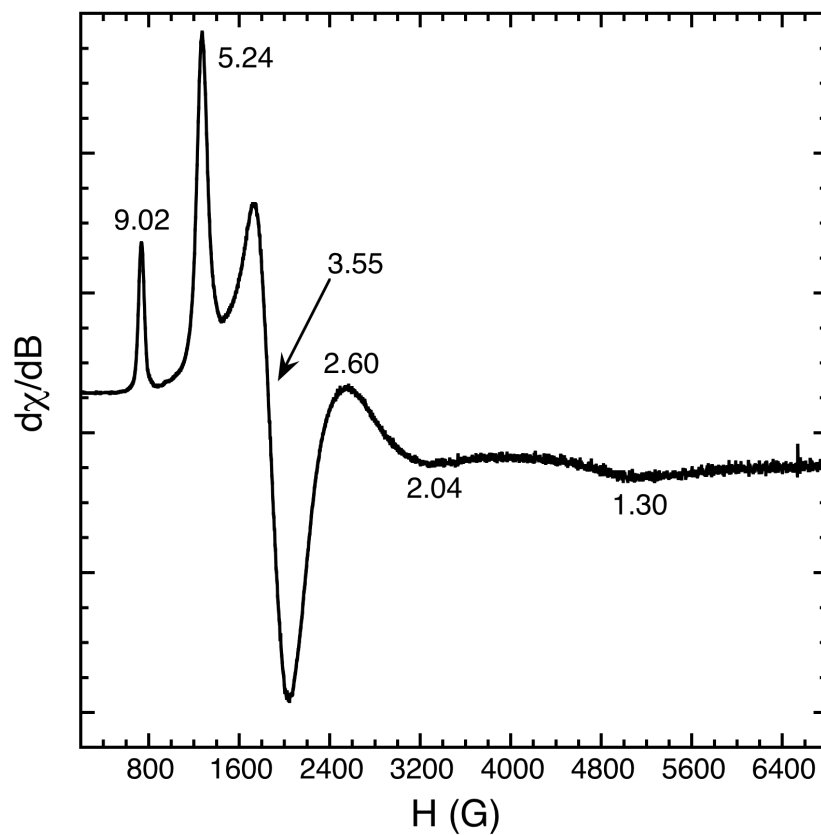


Figure S15. X-band EPR spectrum of compound **6** recorded in a 2-MeTHF glass at 77 K.

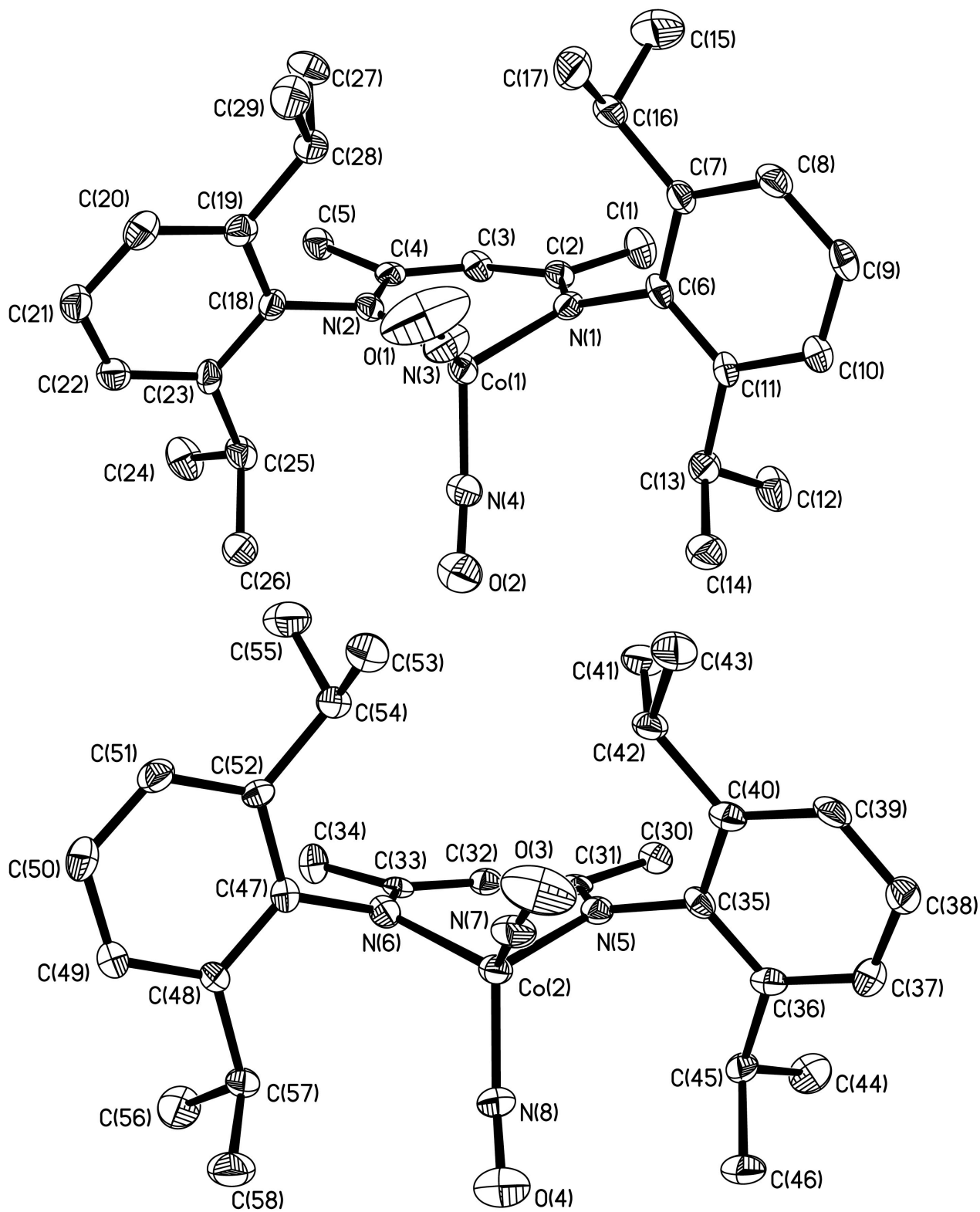


Figure S16. Fully labeled thermal ellipsoid (50%) drawings of the solid-state structure of compound **3** showing both crystallographically independent molecules from the asymmetric unit. Hydrogen atoms omitted for clarity.

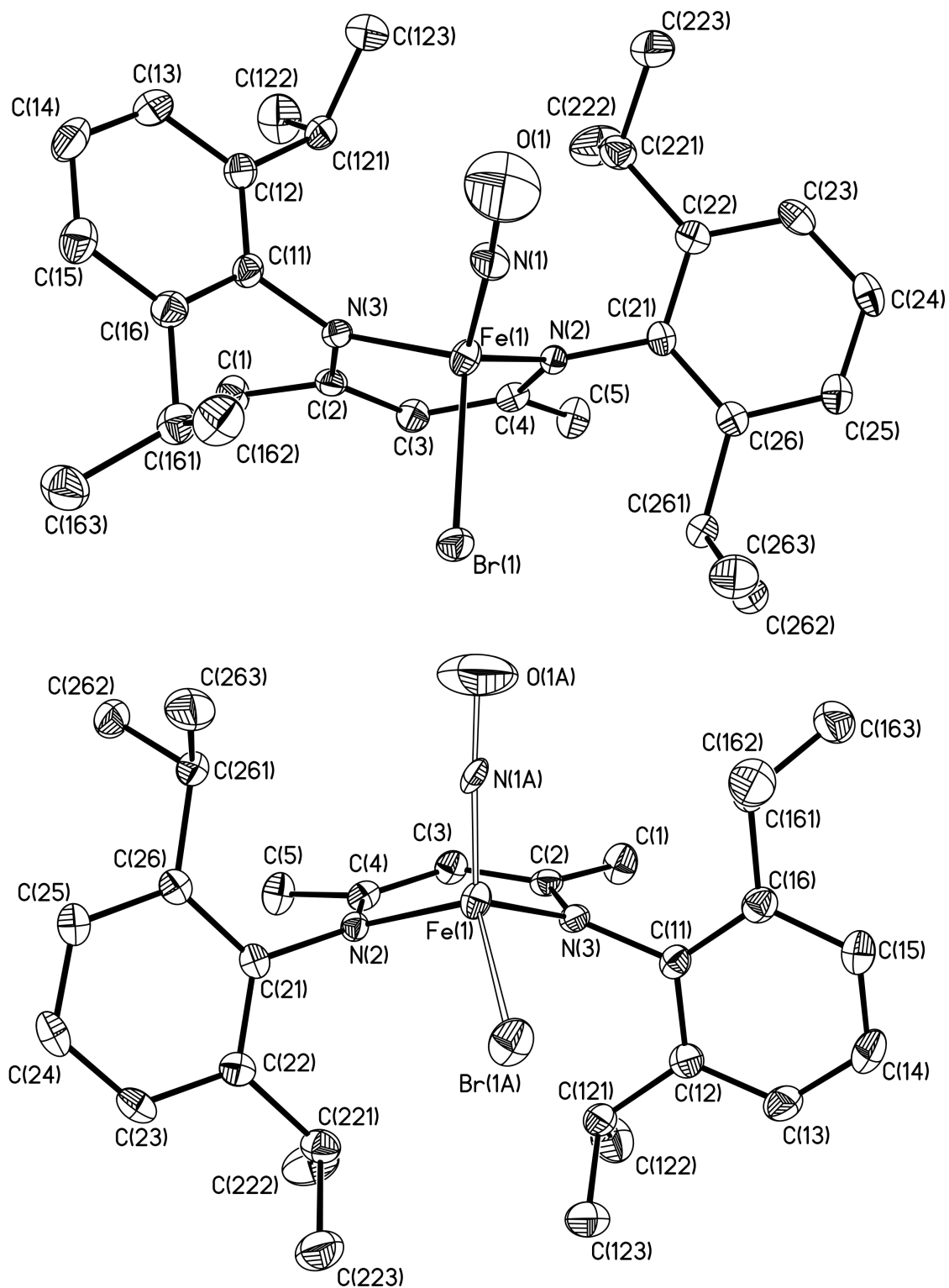


Figure S17. Fully labeled thermal ellipsoid (50%) drawing of the solid-state structure of compound **4** displaying both components of the disorder (major = upper; minor = lower). Hydrogen atoms omitted for clarity.

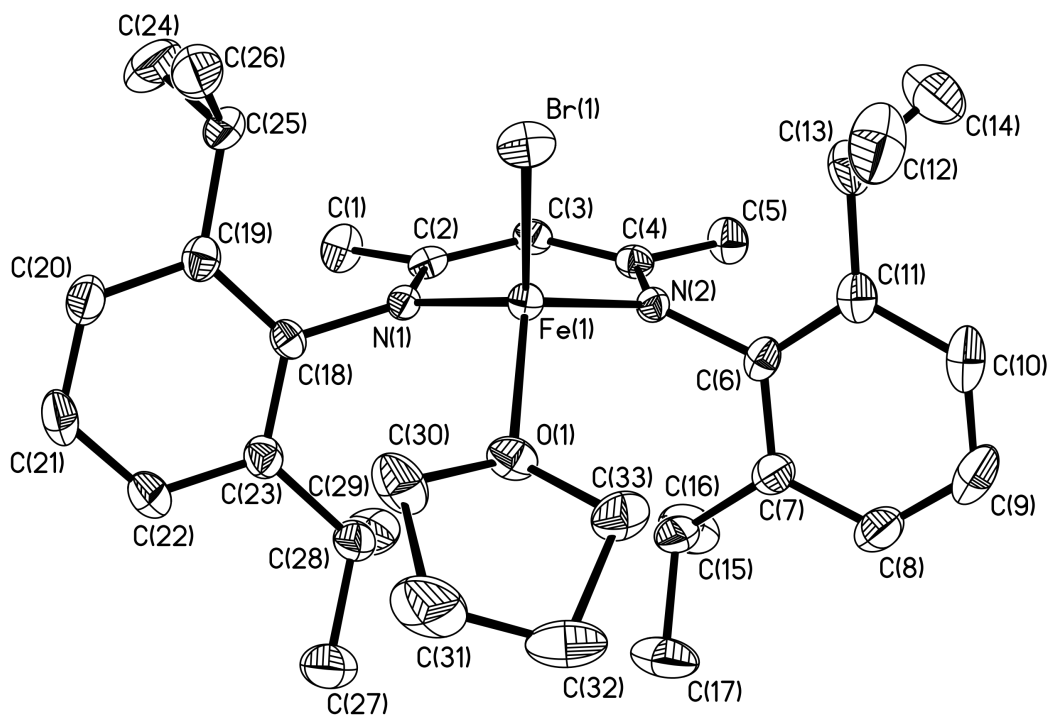


Figure S18. Fully labeled thermal ellipsoid (50%) drawing of the solid-state structure of compound **5**.
Hydrogen atoms omitted for clarity.

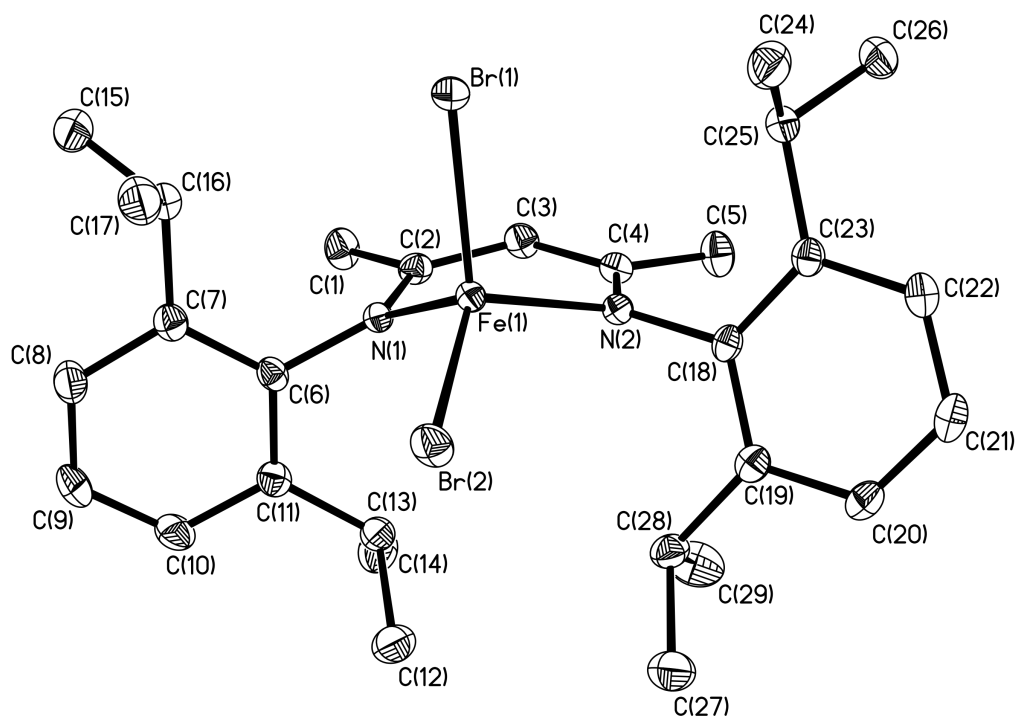


Figure S19. Fully labeled thermal ellipsoid (50%) drawing of the solid-state structure of compound **6**.
Hydrogen atoms omitted for clarity.

Table S1. Bond lengths (Å) and angles (deg) for [Co(NO)₂(Ar-nacnac)], **3**.

Co(1)-N(3)	1.633(4)	C(11)-C(13)	1.512(6)
Co(1)-N(4)	1.695(4)	C(12)-C(13)	1.534(6)
Co(1)-N(1)	1.955(4)	C(13)-C(14)	1.529(6)
Co(1)-N(2)	1.957(4)	C(15)-C(16)	1.530(7)
O(1)-N(3)	1.165(5)	C(16)-C(17)	1.527(7)
N(1)-C(2)	1.333(5)	C(18)-C(19)	1.401(6)
N(1)-C(6)	1.442(5)	C(18)-C(23)	1.416(6)
C(1)-C(2)	1.501(6)	C(19)-C(20)	1.379(6)
C(2)-C(3)	1.397(6)	C(19)-C(28)	1.520(6)
N(2)-C(4)	1.317(5)	C(20)-C(21)	1.392(6)
N(2)-C(18)	1.437(5)	C(21)-C(22)	1.373(6)
O(2)-N(4)	1.166(5)	C(22)-C(23)	1.382(6)
Co(2)-N(7)	1.650(4)	C(23)-C(25)	1.509(6)
Co(2)-N(8)	1.707(4)	C(24)-C(25)	1.528(6)
Co(2)-N(5)	1.952(4)	C(25)-C(26)	1.536(6)
Co(2)-N(6)	1.954(4)	C(27)-C(28)	1.524(7)
C(3)-C(4)	1.400(6)	C(28)-C(29)	1.532(6)
O(3)-N(7)	1.159(5)	C(30)-C(31)	1.517(6)
C(4)-C(5)	1.516(6)	C(31)-C(32)	1.392(6)
O(4)-N(8)	1.166(5)	C(32)-C(33)	1.388(6)
N(5)-C(31)	1.323(5)	C(33)-C(34)	1.505(6)
N(5)-C(35)	1.436(5)	C(35)-C(40)	1.402(6)
C(6)-C(11)	1.407(6)	C(35)-C(36)	1.408(6)
C(6)-C(7)	1.409(6)	C(36)-C(37)	1.386(6)
N(6)-C(33)	1.331(5)	C(36)-C(45)	1.510(6)
N(6)-C(47)	1.438(5)	C(37)-C(38)	1.374(6)
C(7)-C(8)	1.389(6)	C(38)-C(39)	1.376(6)
C(7)-C(16)	1.522(6)	C(39)-C(40)	1.387(6)
C(8)-C(9)	1.381(6)	C(40)-C(42)	1.528(6)
C(9)-C(10)	1.374(6)	C(41)-C(42)	1.541(6)
C(10)-C(11)	1.392(6)	C(42)-C(43)	1.523(6)

C(44)-C(45)	1.532(6)	N(7)-Co(2)-N(6)	119.42(17)
C(45)-C(46)	1.533(6)	N(8)-Co(2)-N(6)	110.84(17)
C(47)-C(48)	1.396(6)	N(5)-Co(2)-N(6)	93.02(15)
C(47)-C(52)	1.412(6)	O(1)-N(3)-Co(1)	173.0(4)
C(48)-C(49)	1.392(6)	C(2)-C(3)-C(4)	127.2(4)
C(48)-C(57)	1.518(6)	O(2)-N(4)-Co(1)	150.1(4)
C(49)-C(50)	1.375(6)	N(2)-C(4)-C(3)	123.2(4)
C(50)-C(51)	1.374(6)	N(2)-C(4)-C(5)	120.2(4)
C(51)-C(52)	1.388(6)	C(3)-C(4)-C(5)	116.7(4)
C(52)-C(54)	1.523(6)	C(31)-N(5)-C(35)	120.6(4)
C(53)-C(54)	1.530(7)	C(31)-N(5)-Co(2)	124.3(3)
C(54)-C(55)	1.529(6)	C(35)-N(5)-Co(2)	115.1(3)
C(56)-C(57)	1.533(6)	C(11)-C(6)-C(7)	120.4(4)
C(57)-C(58)	1.528(6)	C(11)-C(6)-N(1)	120.7(4)
		C(7)-C(6)-N(1)	118.7(4)
N(3)-Co(1)-N(4)	110.5(2)	C(33)-N(6)-C(47)	119.1(4)
N(3)-Co(1)-N(1)	117.00(18)	C(33)-N(6)-Co(2)	123.0(3)
N(4)-Co(1)-N(1)	111.65(17)	C(47)-N(6)-Co(2)	117.9(3)
N(3)-Co(1)-N(2)	112.47(17)	C(8)-C(7)-C(6)	118.7(4)
N(4)-Co(1)-N(2)	111.17(16)	C(8)-C(7)-C(16)	118.7(4)
N(1)-Co(1)-N(2)	93.03(15)	C(6)-C(7)-C(16)	122.6(4)
C(2)-N(1)-C(6)	119.1(4)	O(3)-N(7)-Co(2)	170.0(4)
C(2)-N(1)-Co(1)	123.5(3)	C(9)-C(8)-C(7)	121.2(4)
C(6)-N(1)-Co(1)	117.4(3)	O(4)-N(8)-Co(2)	148.0(4)
N(1)-C(2)-C(3)	123.3(4)	C(10)-C(9)-C(8)	119.7(4)
N(1)-C(2)-C(1)	119.6(4)	C(9)-C(10)-C(11)	121.7(4)
C(3)-C(2)-C(1)	117.1(4)	C(10)-C(11)-C(6)	118.2(4)
C(4)-N(2)-C(18)	120.3(4)	C(10)-C(11)-C(13)	119.4(4)
C(4)-N(2)-Co(1)	124.3(3)	C(6)-C(11)-C(13)	122.4(4)
C(18)-N(2)-Co(1)	115.3(3)	C(11)-C(13)-C(14)	110.8(4)
N(7)-Co(2)-N(8)	110.23(19)	C(11)-C(13)-C(12)	111.8(4)
N(7)-Co(2)-N(5)	111.35(17)	C(14)-C(13)-C(12)	110.4(4)
N(8)-Co(2)-N(5)	110.80(17)	C(7)-C(16)-C(17)	110.2(4)

C(7)-C(16)-C(15)	111.7(4)	C(35)-C(36)-C(45)	123.4(4)
C(17)-C(16)-C(15)	109.2(4)	C(38)-C(37)-C(36)	121.4(4)
C(19)-C(18)-C(23)	120.8(4)	C(37)-C(38)-C(39)	120.1(4)
C(19)-C(18)-N(2)	118.8(4)	C(38)-C(39)-C(40)	121.1(4)
C(23)-C(18)-N(2)	120.3(4)	C(39)-C(40)-C(35)	118.1(4)
C(20)-C(19)-C(18)	118.4(4)	C(39)-C(40)-C(42)	120.5(4)
C(20)-C(19)-C(28)	120.5(4)	C(35)-C(40)-C(42)	121.4(4)
C(18)-C(19)-C(28)	121.1(4)	C(43)-C(42)-C(40)	113.6(4)
C(19)-C(20)-C(21)	121.8(4)	C(43)-C(42)-C(41)	110.0(4)
C(22)-C(21)-C(20)	118.9(4)	C(40)-C(42)-C(41)	111.9(4)
C(21)-C(22)-C(23)	122.1(4)	C(36)-C(45)-C(44)	111.9(4)
C(22)-C(23)-C(18)	118.0(4)	C(36)-C(45)-C(46)	110.2(4)
C(22)-C(23)-C(25)	119.5(4)	C(44)-C(45)-C(46)	109.7(4)
C(18)-C(23)-C(25)	122.5(4)	C(48)-C(47)-C(52)	120.7(4)
C(23)-C(25)-C(24)	113.0(4)	C(48)-C(47)-N(6)	120.4(4)
C(23)-C(25)-C(26)	109.8(4)	C(52)-C(47)-N(6)	118.9(4)
C(24)-C(25)-C(26)	109.6(4)	C(49)-C(48)-C(47)	118.9(4)
C(19)-C(28)-C(27)	111.3(4)	C(49)-C(48)-C(57)	119.4(4)
C(19)-C(28)-C(29)	113.1(4)	C(47)-C(48)-C(57)	121.7(4)
C(27)-C(28)-C(29)	109.9(4)	C(50)-C(49)-C(48)	120.6(4)
N(5)-C(31)-C(32)	122.9(4)	C(51)-C(50)-C(49)	120.5(4)
N(5)-C(31)-C(30)	119.9(4)	C(50)-C(51)-C(52)	121.1(4)
C(32)-C(31)-C(30)	117.2(4)	C(51)-C(52)-C(47)	118.3(4)
C(33)-C(32)-C(31)	127.3(4)	C(51)-C(52)-C(54)	119.2(4)
N(6)-C(33)-C(32)	123.8(4)	C(47)-C(52)-C(54)	122.5(4)
N(6)-C(33)-C(34)	118.9(4)	C(52)-C(54)-C(55)	111.6(4)
C(32)-C(33)-C(34)	117.3(4)	C(52)-C(54)-C(53)	110.6(4)
C(40)-C(35)-C(36)	121.3(4)	C(55)-C(54)-C(53)	109.6(4)
C(40)-C(35)-N(5)	118.3(4)	C(48)-C(57)-C(58)	110.3(4)
C(36)-C(35)-N(5)	120.2(4)	C(48)-C(57)-C(56)	111.3(4)
C(37)-C(36)-C(35)	117.9(4)	C(58)-C(57)-C(56)	110.7(4)
C(37)-C(36)-C(45)	118.8(4)		

Table S2. Bond lengths (Å) and angles (deg) for [Fe(NO)Br(Ar-nacnac)], **4**.

Fe(1)-N(1A)	1.613(8)	C(25)-C(26)	1.394(4)
Fe(1)-N(1)	1.644(5)	C(26)-C(261)	1.516(4)
Fe(1)-N(3)	1.938(2)	C(121)-C(122)	1.527(5)
Fe(1)-N(2)	1.971(2)	C(121)-C(123)	1.532(5)
Fe(1)-Br(1)	2.4136(9)	C(161)-C(163)	1.528(5)
Fe(1)-Br(1A)	2.4544(17)	C(161)-C(162)	1.533(4)
N(1)-O(1)	1.217(6)	C(221)-C(223)	1.520(4)
N(1A)-O(1A)	1.238(9)	C(221)-C(222)	1.530(5)
N(2)-C(4)	1.327(4)	C(261)-C(262)	1.534(4)
N(2)-C(21)	1.449(3)	C(261)-C(263)	1.538(4)
N(3)-C(2)	1.342(4)		
N(3)-C(11)	1.450(3)	N(1A)-Fe(1)-N(1)	110.5(3)
C(1)-C(2)	1.507(4)	N(1A)-Fe(1)-N(3)	110.3(3)
C(2)-C(3)	1.397(4)	N(1)-Fe(1)-N(3)	112.24(16)
C(3)-C(4)	1.407(4)	N(1A)-Fe(1)-N(2)	109.1(3)
C(4)-C(5)	1.512(4)	N(1)-Fe(1)-N(2)	117.38(15)
C(11)-C(16)	1.402(4)	N(3)-Fe(1)-N(2)	96.49(10)
C(11)-C(12)	1.408(4)	N(1A)-Fe(1)-Br(1)	5.0(3)
C(12)-C(13)	1.395(4)	N(1)-Fe(1)-Br(1)	115.22(15)
C(12)-C(121)	1.520(4)	N(3)-Fe(1)-Br(1)	106.11(7)
C(13)-C(14)	1.382(5)	N(2)-Fe(1)-Br(1)	107.35(7)
C(14)-C(15)	1.383(5)	N(1A)-Fe(1)-Br(1A)	115.6(3)
C(15)-C(16)	1.397(4)	N(1)-Fe(1)-Br(1A)	5.17(15)
C(16)-C(161)	1.515(4)	N(3)-Fe(1)-Br(1A)	108.77(8)
C(21)-C(22)	1.405(4)	N(2)-Fe(1)-Br(1A)	114.85(8)
C(21)-C(26)	1.406(4)	Br(1)-Fe(1)-Br(1A)	120.31(4)
C(22)-C(23)	1.389(4)	O(1)-N(1)-Fe(1)	175.5(6)
C(22)-C(221)	1.520(4)	O(1A)-N(1A)-Fe(1)	162.4(12)
C(23)-C(24)	1.383(4)	C(4)-N(2)-C(21)	120.6(2)
C(24)-C(25)	1.376(4)	C(4)-N(2)-Fe(1)	116.76(19)

C(21)-N(2)-Fe(1)	121.57(17)	C(22)-C(21)-N(2)	118.5(2)
C(2)-N(3)-C(11)	118.7(2)	C(26)-C(21)-N(2)	119.9(2)
C(2)-N(3)-Fe(1)	116.36(18)	C(23)-C(22)-C(21)	118.1(3)
C(11)-N(3)-Fe(1)	124.80(18)	C(23)-C(22)-C(221)	119.9(3)
N(3)-C(2)-C(3)	122.9(3)	C(21)-C(22)-C(221)	121.9(3)
N(3)-C(2)-C(1)	119.2(3)	C(24)-C(23)-C(22)	121.1(3)
C(3)-C(2)-C(1)	117.9(3)	C(25)-C(24)-C(23)	120.0(3)
C(2)-C(3)-C(4)	129.1(3)	C(24)-C(25)-C(26)	121.5(3)
N(2)-C(4)-C(3)	123.4(3)	C(25)-C(26)-C(21)	117.7(3)
N(2)-C(4)-C(5)	120.4(3)	C(25)-C(26)-C(261)	118.6(3)
C(3)-C(4)-C(5)	116.1(2)	C(21)-C(26)-C(261)	123.6(2)
C(16)-C(11)-C(12)	121.5(3)	C(12)-C(121)-C(122)	112.4(3)
C(16)-C(11)-N(3)	120.8(2)	C(12)-C(121)-C(123)	109.9(3)
C(12)-C(11)-N(3)	117.6(2)	C(122)-C(121)-C(123)	110.0(3)
C(13)-C(12)-C(11)	118.1(3)	C(16)-C(161)-C(163)	112.2(3)
C(13)-C(12)-C(121)	119.7(3)	C(16)-C(161)-C(162)	110.6(3)
C(11)-C(12)-C(121)	122.2(3)	C(163)-C(161)-C(162)	109.9(3)
C(14)-C(13)-C(12)	121.1(3)	C(223)-C(221)-C(22)	113.3(3)
C(13)-C(14)-C(15)	120.0(3)	C(223)-C(221)-C(222)	111.0(3)
C(14)-C(15)-C(16)	121.2(3)	C(22)-C(221)-C(222)	110.1(3)
C(15)-C(16)-C(11)	118.0(30)	C(26)-C(261)-C(262)	112.6(2)
C(15)-C(16)-C(161)	119.6(3)	C(26)-C(261)-C(263)	110.0(2)
C(11)-C(16)-C(161)	122.4(3)	C(262)-C(261)-C(263)	109.4(3)
C(22)-C(21)-C(26)	121.5(2)		

Table S3. Bond lengths (Å) and angles (deg) for [Fe(THF)Br(Ar-nacnac)], **5**.

Br(1)-Fe(1)	2.4114(6)	C(7)-C(16)	1.528(6)
Fe(1)-N(2)	1.998(3)	C(22)-C(21)	1.388(6)
Fe(1)-N(1)	2.009(3)	C(13)-C(12)	1.532(6)
Fe(1)-O(1)	2.061(2)	C(13)-C(14)	1.541(6)
N(2)-C(4)	1.337(4)	C(16)-C(15)	1.521(7)
N(2)-C(6)	1.444(4)	C(16)-C(17)	1.532(6)
O(1)-C(33)	1.453(4)	C(32)-C(31)	1.522(7)
O(1)-C(30)	1.460(5)	C(8)-C(9)	1.379(7)
C(19)-C(20)	1.401(5)	C(21)-C(20)	1.369(6)
C(19)-C(18)	1.405(5)	C(10)-C(9)	1.376(6)
C(19)-C(25)	1.514(5)	C(30)-C(31)	1.515(6)
C(4)-C(3)	1.397(5)		
C(4)-C(5)	1.515(5)	N(2)-Fe(1)-N(1)	94.01(11)
N(1)-C(2)	1.331(4)	N(2)-Fe(1)-O(1)	114.51(11)
N(1)-C(18)	1.444(4)	N(1)-Fe(1)-O(1)	109.99(11)
C(18)-C(23)	1.410(5)	N(2)-Fe(1)-Br(1)	119.67(8)
C(2)-C(3)	1.408(5)	N(1)-Fe(1)-Br(1)	121.06(8)
C(2)-C(1)	1.512(5)	O(1)-Fe(1)-Br(1)	98.45(7)
C(11)-C(10)	1.406(5)	C(4)-N(2)-C(6)	118.7(3)
C(11)-C(6)	1.408(5)	C(4)-N(2)-Fe(1)	120.6(2)
C(11)-C(13)	1.506(6)	C(6)-N(2)-Fe(1)	120.7(2)
C(23)-C(22)	1.395(5)	C(33)-O(1)-C(30)	106.7(3)
C(23)-C(28)	1.526(5)	C(33)-O(1)-Fe(1)	122.5(2)
C(33)-C(32)	1.519(6)	C(30)-O(1)-Fe(1)	120.4(2)
C(28)-C(29)	1.527(6)	C(20)-C(19)-C(18)	118.2(3)
C(28)-C(27)	1.537(6)	C(20)-C(19)-C(25)	118.9(3)
C(25)-C(26)	1.530(6)	C(18)-C(19)-C(25)	122.8(3)
C(25)-C(24)	1.536(6)	N(2)-C(4)-C(3)	123.6(3)
C(6)-C(7)	1.412(5)	N(2)-C(4)-C(5)	119.9(3)
C(7)-C(8)	1.390(5)	C(3)-C(4)-C(5)	116.5(3)

C(2)-N(1)-C(18)	119.8(3)	C(26)-C(25)-C(24)	109.4(3)
C(2)-N(1)-Fe(1)	120.5(2)	C(11)-C(6)-C(7)	121.1(3)
C(18)-N(1)-Fe(1)	119.4(2)	C(11)-C(6)-N(2)	120.8(3)
C(19)-C(18)-C(23)	121.0(3)	C(7)-C(6)-N(2)	118.0(3)
C(19)-C(18)-N(1)	120.5(3)	C(8)-C(7)-C(6)	118.6(4)
C(23)-C(18)-N(1)	118.4(3)	C(8)-C(7)-C(16)	120.0(4)
N(1)-C(2)-C(3)	123.8(3)	C(6)-C(7)-C(16)	121.4(3)
N(1)-C(2)-C(1)	120.5(3)	C(21)-C(22)-C(23)	121.3(4)
C(3)-C(2)-C(1)	115.7(3)	C(11)-C(13)-C(12)	110.8(4)
C(10)-C(11)-C(6)	117.6(4)	C(11)-C(13)-C(14)	111.8(3)
C(10)-C(11)-C(13)	119.7(3)	C(12)-C(13)-C(14)	109.8(4)
C(6)-C(11)-C(13)	122.8(3)	C(15)-C(16)-C(7)	112.1(4)
C(4)-C(3)-C(2)	128.9(3)	C(15)-C(16)-C(17)	110.0(4)
C(22)-C(23)-C(18)	118.1(3)	C(7)-C(16)-C(17)	112.1(4)
C(22)-C(23)-C(28)	120.3(3)	C(33)-C(32)-C(31)	102.8(4)
C(18)-C(23)-C(28)	121.6(3)	C(9)-C(8)-C(7)	121.1(4)
O(1)-C(33)-C(32)	102.7(3)	C(20)-C(21)-C(22)	119.9(4)
C(23)-C(28)-C(29)	111.7(3)	C(9)-C(10)-C(11)	121.5(4)
C(23)-C(28)-C(27)	113.7(3)	O(1)-C(30)-C(31)	106.2(4)
C(29)-C(28)-C(27)	108.9(4)	C(21)-C(20)-C(19)	121.5(4)
C(19)-C(25)-C(26)	111.1(3)	C(10)-C(9)-C(8)	120.2(4)
C(19)-C(25)-C(24)	112.0(3)	C(30)-C(31)-C(32)	105.2(4)

Table S4. Bond lengths (Å) and angles (deg) for [FeBr₂(Ar-nacnac)], **6**.

Br(1)-Fe(1)	2.3446(3)	C(22)-C(23)	1.396(2)
Fe(1)-N(1)	1.9459(13)	C(23)-C(25)	1.520(2)
Fe(1)-N(2)	1.9730(13)	C(24)-C(25)	1.528(2)
Fe(1)-Br(2)	2.3188(3)	C(25)-C(26)	1.538(2)
N(1)-C(2)	1.342(2)	C(27)-C(28)	1.529(2)
N(1)-C(6)	1.4466(19)	C(28)-C(29)	1.528(2)
C(1)-C(2)	1.507(2)		
N(2)-C(4)	1.333(2)	N(1)-Fe(1)-N(2)	96.36(5)
N(2)-C(18)	1.450(2)	N(1)-Fe(1)-Br(2)	112.39(4)
C(2)-C(3)	1.401(2)	N(2)-Fe(1)-Br(2)	116.18(4)
C(3)-C(4)	1.412(2)	N(1)-Fe(1)-Br(1)	107.08(4)
C(4)-C(5)	1.508(2)	N(2)-Fe(1)-Br(1)	106.70(4)
C(6)-C(7)	1.406(2)	Br(2)-Fe(1)-Br(1)	116.068(11)
C(6)-C(11)	1.406(2)	C(2)-N(1)-C(6)	118.67(13)
C(7)-C(8)	1.396(2)	C(2)-N(1)-Fe(1)	116.01(10)
C(7)-C(16)	1.523(2)	C(6)-N(1)-Fe(1)	125.14(10)
C(8)-C(9)	1.381(3)	C(4)-N(2)-C(18)	120.25(13)
C(9)-C(10)	1.384(3)	C(4)-N(2)-Fe(1)	116.77(10)
C(10)-C(11)	1.396(2)	C(18)-N(2)-Fe(1)	121.96(10)
C(11)-C(13)	1.520(2)	N(1)-C(2)-C(3)	122.92(14)
C(12)-C(13)	1.532(2)	N(1)-C(2)-C(1)	119.48(14)
C(13)-C(14)	1.529(3)	C(3)-C(2)-C(1)	117.57(15)
C(15)-C(16)	1.530(2)	C(2)-C(3)-C(4)	129.09(15)
C(16)-C(17)	1.539(3)	N(2)-C(4)-C(3)	123.06(15)
C(18)-C(23)	1.407(2)	N(2)-C(4)-C(5)	120.73(14)
C(18)-C(19)	1.411(2)	C(3)-C(4)-C(5)	116.20(14)
C(19)-C(20)	1.395(2)	C(7)-C(6)-C(11)	121.62(15)
C(19)-C(28)	1.520(2)	C(7)-C(6)-N(1)	120.86(14)
C(20)-C(21)	1.380(2)	C(11)-C(6)-N(1)	117.52(14)
C(21)-C(22)	1.378(2)	C(8)-C(7)-C(6)	117.95(15)

C(8)-C(7)-C(16)	119.49(15)	C(19)-C(18)-N(2)	118.30(14)
C(6)-C(7)-C(16)	122.55(14)	C(20)-C(19)-C(18)	117.80(15)
C(9)-C(8)-C(7)	121.18(16)	C(20)-C(19)-C(28)	119.98(14)
C(8)-C(9)-C(10)	120.20(16)	C(18)-C(19)-C(28)	122.16(14)
C(9)-C(10)-C(11)	120.97(16)	C(21)-C(20)-C(19)	121.34(15)
C(10)-C(11)-C(6)	118.06(15)	C(22)-C(21)-C(20)	120.09(15)
C(10)-C(11)-C(13)	119.30(15)	C(21)-C(22)-C(23)	121.39(15)
C(6)-C(11)-C(13)	122.63(14)	C(22)-C(23)-C(18)	117.84(14)
C(11)-C(13)-C(14)	112.35(14)	C(22)-C(23)-C(25)	118.14(14)
C(11)-C(13)-C(12)	110.16(15)	C(18)-C(23)-C(25)	123.98(14)
C(14)-C(13)-C(12)	110.24(15)	C(23)-C(25)-C(24)	110.39(14)
C(7)-C(16)-C(15)	111.87(14)	C(23)-C(25)-C(26)	112.31(14)
C(7)-C(16)-C(17)	110.64(14)	C(24)-C(25)-C(26)	109.36(14)
C(15)-C(16)-C(17)	109.99(15)	C(19)-C(28)-C(29)	110.23(15)
C(23)-C(18)-C(19)	121.51(14)	C(19)-C(28)-C(27)	112.69(14)
C(23)-C(18)-N(2)	120.16(14)	C(29)-C(28)-C(27)	110.66(15)