Supporting Information for

Masked Radicals: Iron Complexes of Trityl, Benzophenone, and Phenylacetylene

K. Cory MacLeod,‡ Ida M. DiMucci,‡ Edward P. Zovinka,‡ Sean F. McWilliams, Brandon Q. Mercado, Kyle M. Lancaster, and Patrick L. Holland**

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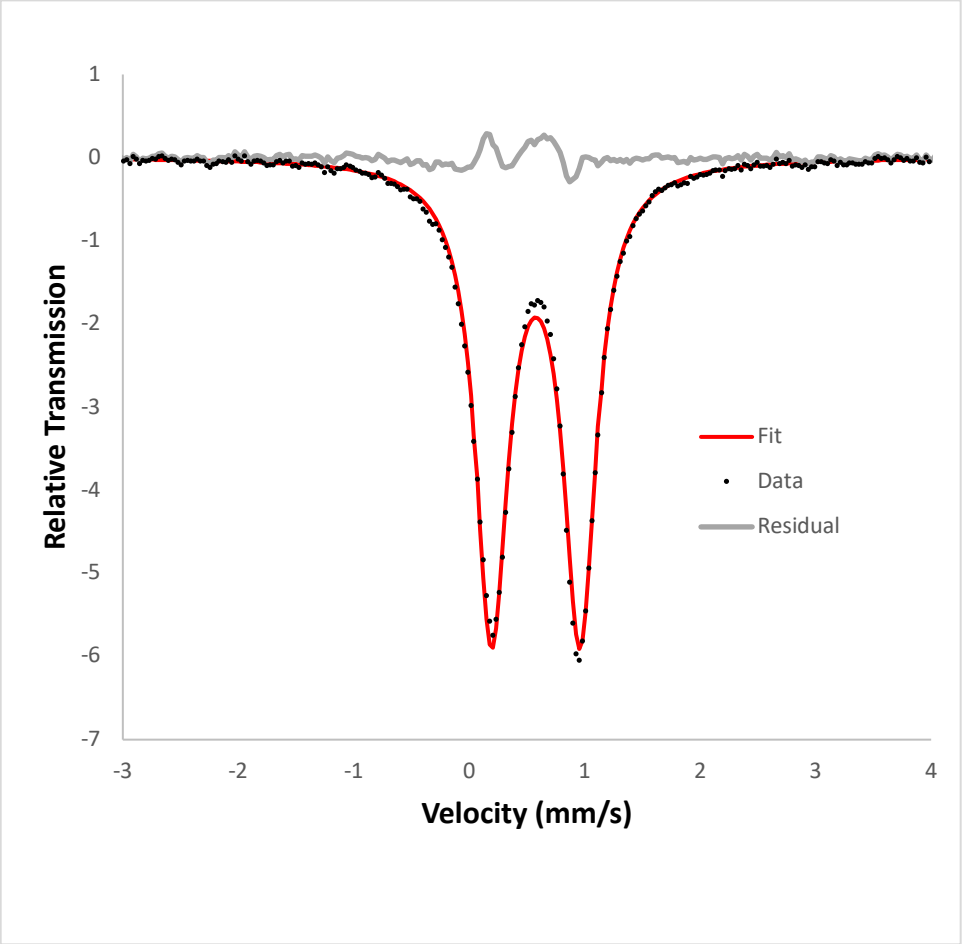


Figure S-1. Zero-field Mössbauer spectrum of $L^{Me}Fe(CPh_3)$ **(1)** recorded at 80 K. The black circles are the data, the red line is a one-component simulation of the data (δ = 0.58 mm/s, $|\Delta E_Q|$ = 0.76 mm/s, Γ = 0.35 mm s^{-1}), and the gray line is the residual.

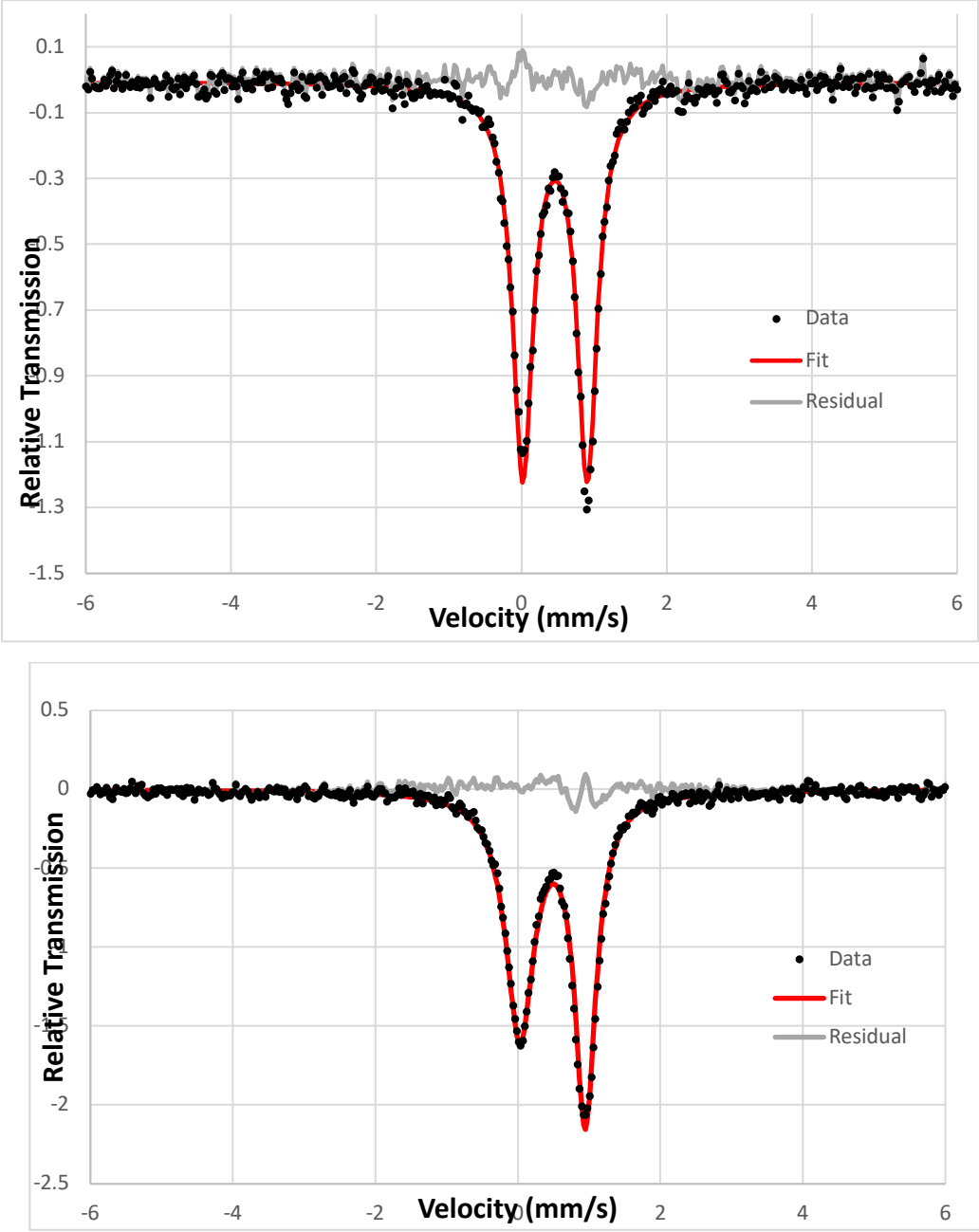


Figure S-2. Zero-field Mössbauer spectrum of $L^{Me}Fe(Ph_2CO)$ **(2)** recorded at (a) 223 K and (b) 173 K. The black circles are the data, the red lines are one-component simulations of the data and the gray lines are the residuals. Fit parameters: (a, 223 K) δ = 0.46 mm/s, $|\Delta E_Q|$ = 0.89 mm/s, Γ = 0.34 mm/s; (b, 173 K) δ = 0.49 mm/s, $|\Delta E_Q|$ = 0.92 mm/s, Γ_L = 0.48 mm/s, Γ_R = 0.36 mm/s.

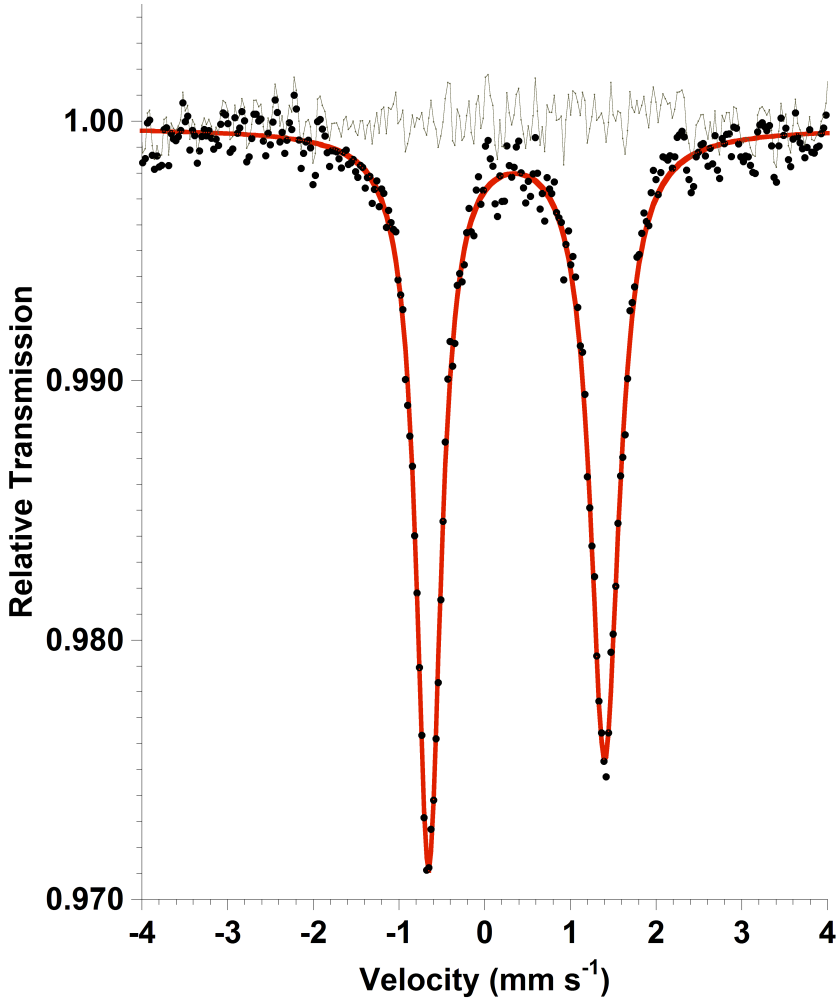


Figure S-3. Zero-field Mössbauer spectrum of [K(2.2.2-cryptand)][$L^{Me}FeCH_3$] **(3)** recorded at 80 K. The black circles are the data, the red line is a one-component simulation of the data (δ = 0.38 mm/s, $|\Delta E_Q|$ = 2.06 mm/s, Γ_L = 0.35 mm/s, Γ_R = 0.42 mm/s.), and the gray line is the residual.

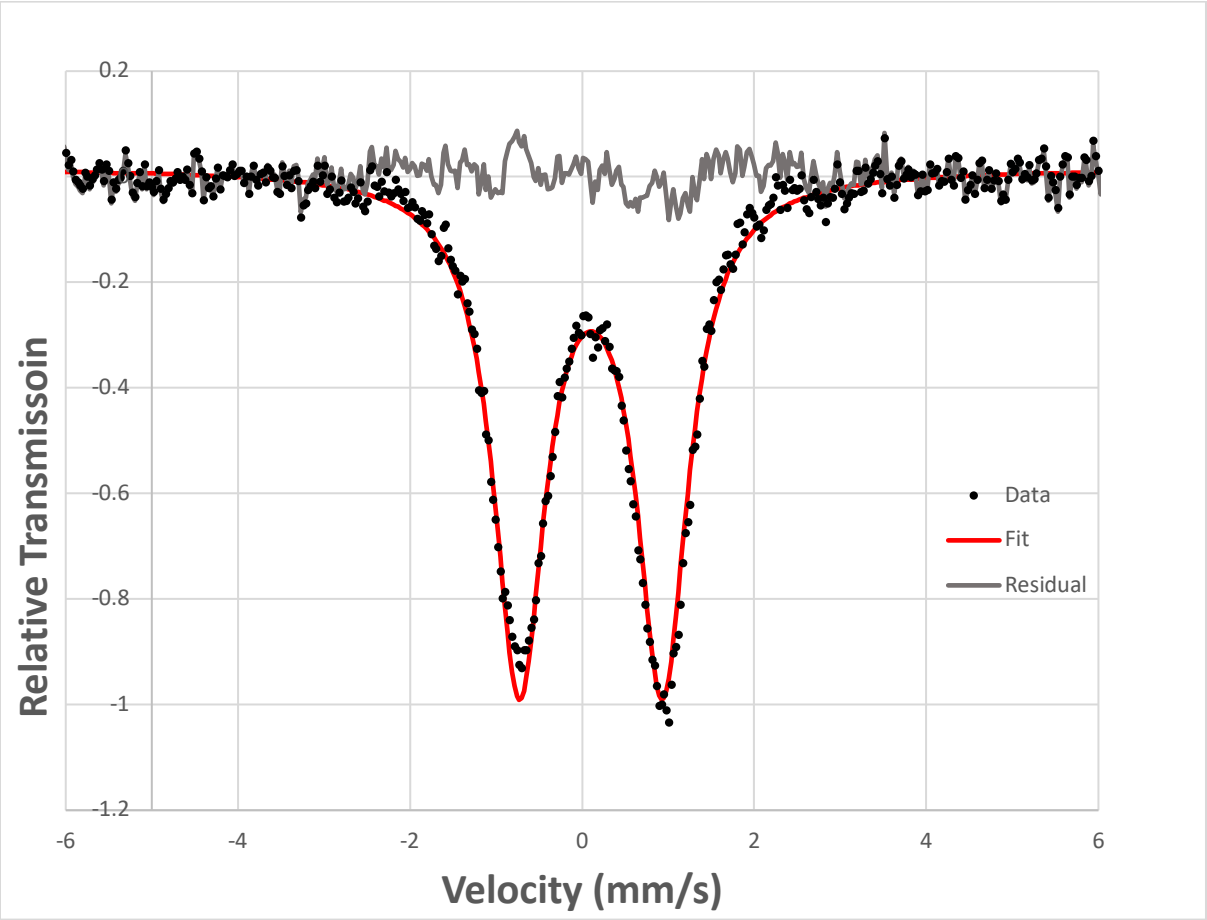


Figure S-4. Zero-field Mössbauer spectrum of $L^{Me}Fe(OCPh_2CHCPh)$ **(6)** recorded at 173 K. The black circles are the data, the red line is a one-component simulation of the data (δ = 0.10 mm/s, $|\Delta E_Q|$ = 1.66 mm/s, Γ = 0.73 mm/s), and the gray line is the residual.

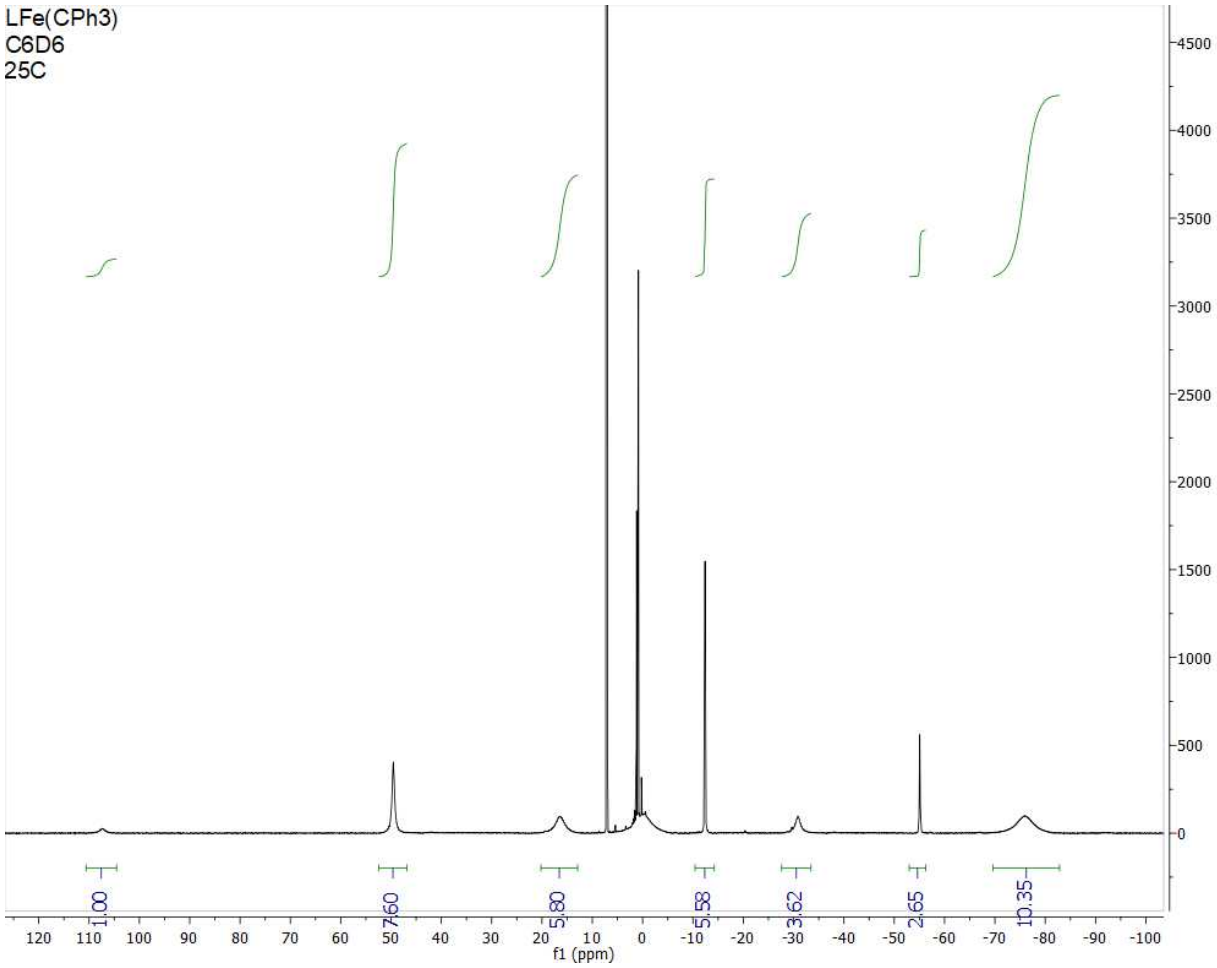


Figure S-5: ^{1}H NMR spectrum of $L^{Me}Fe(CPh_3)$ **(1)** in C_6D_6.

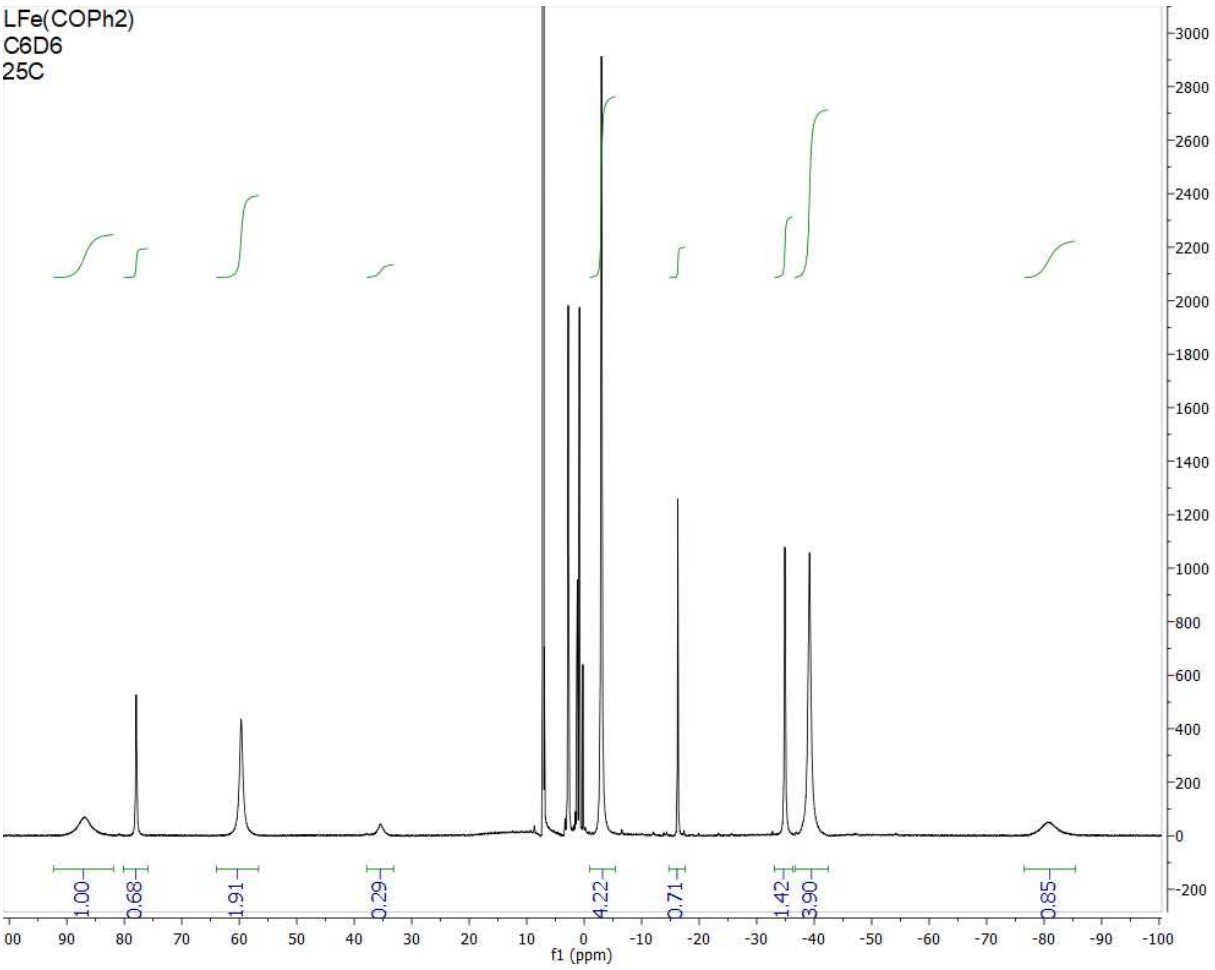


Figure S-6: ^{1}H NMR spectrum of $L^{Me}Fe(Ph_2CO)$ **(2)** in C_6D_6.

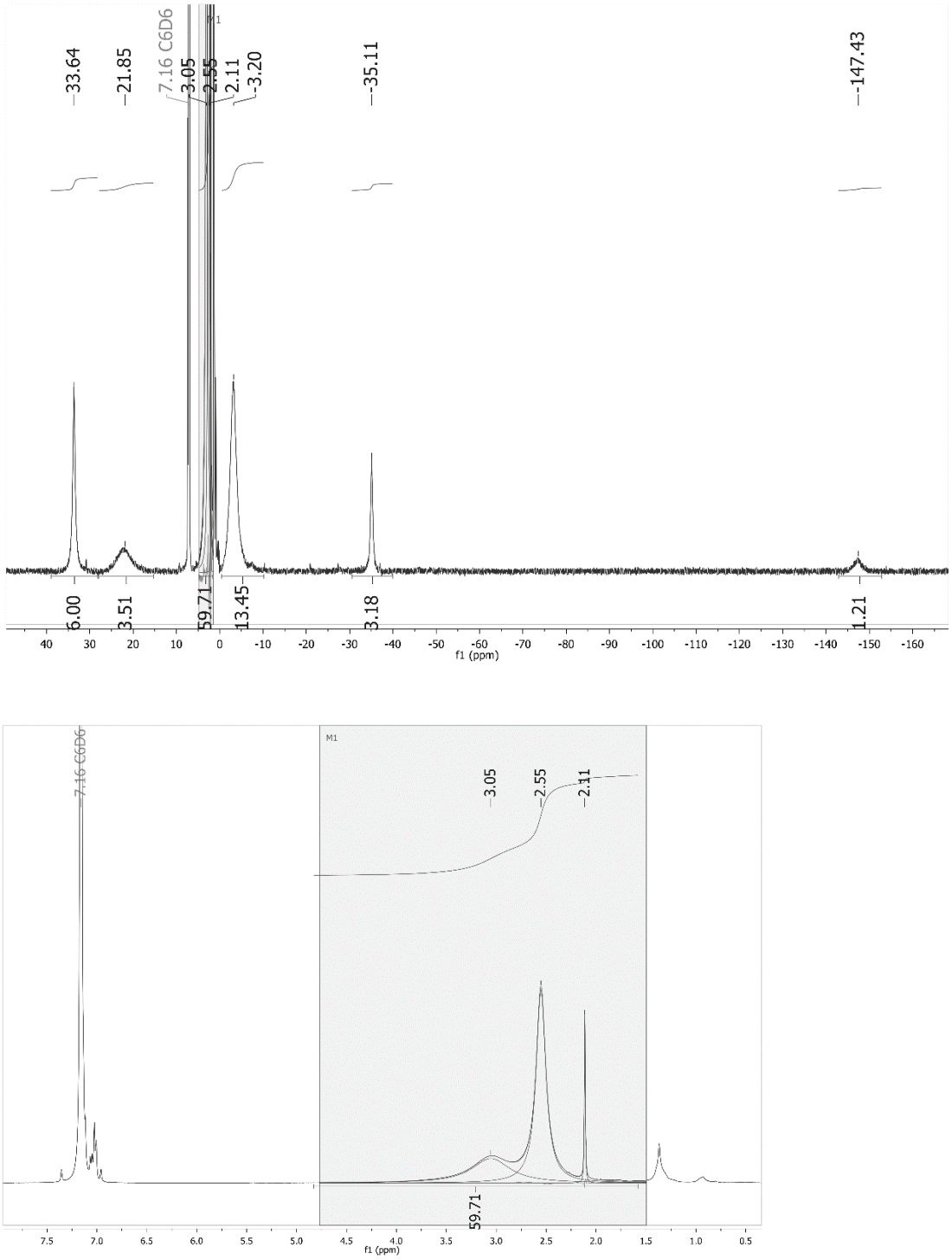


Figure S-7: ^{1}H NMR spectrum of [K(18-crown-6)][L^{Me}FeCH$_3$] **(3)** in C_6D_6: (top) full spectrum, (bottom) closeup of the region from 0 to 8 ppm.

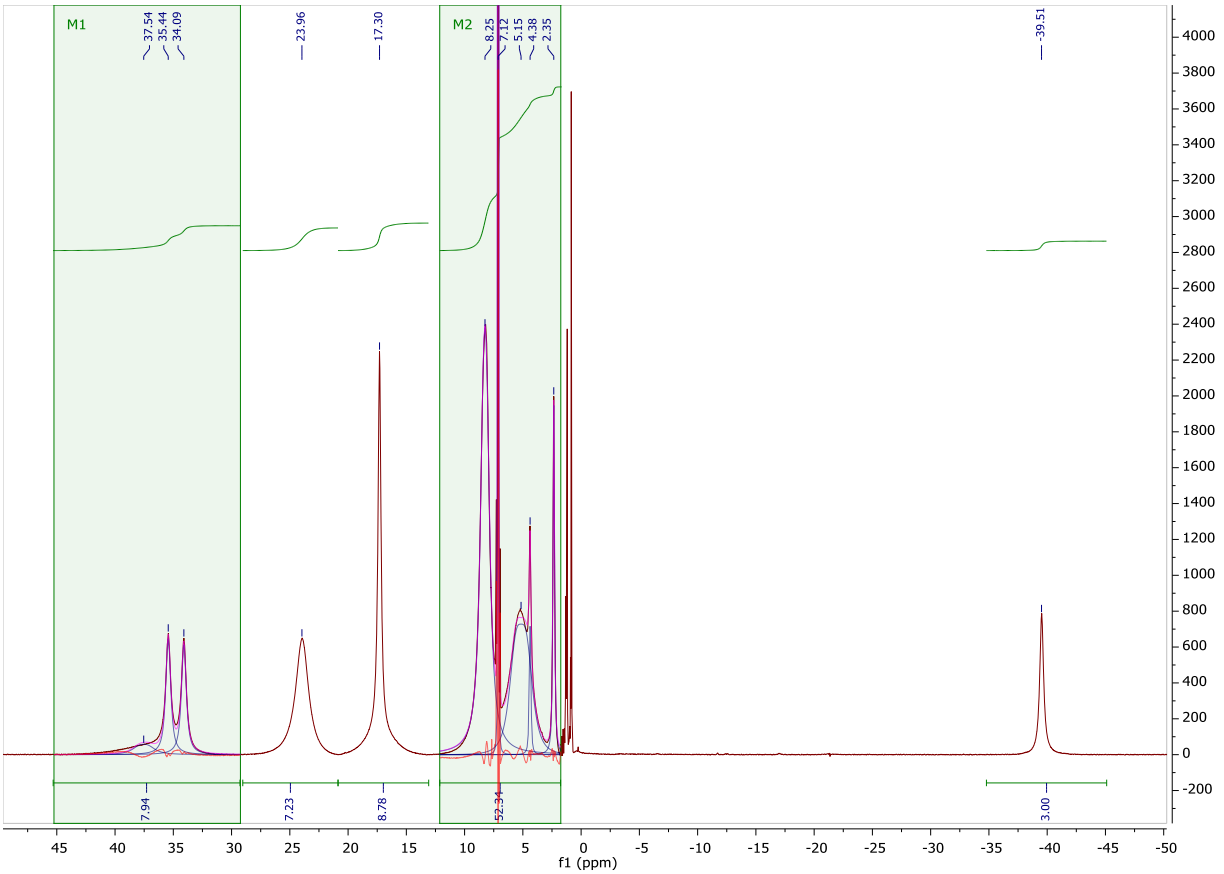
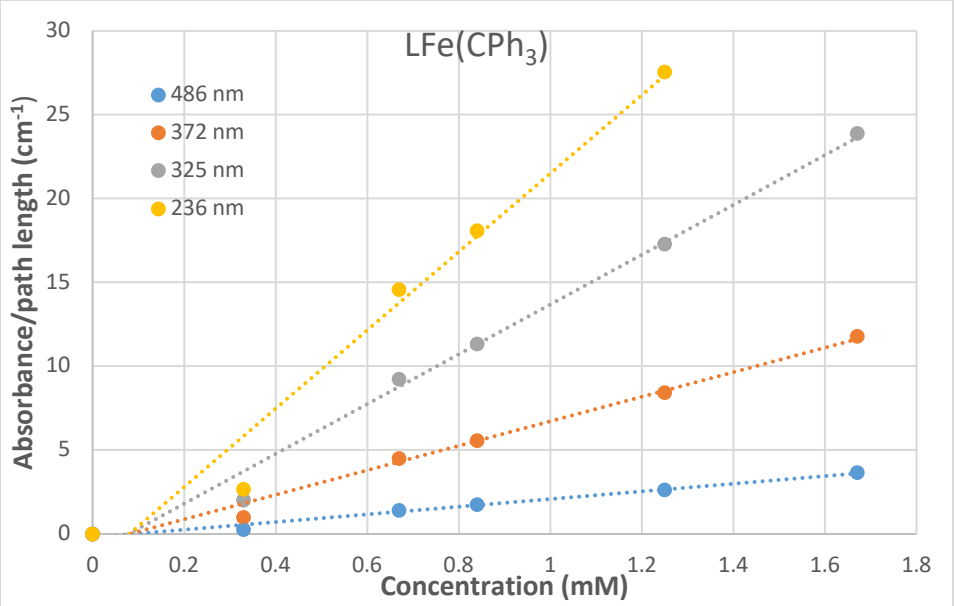
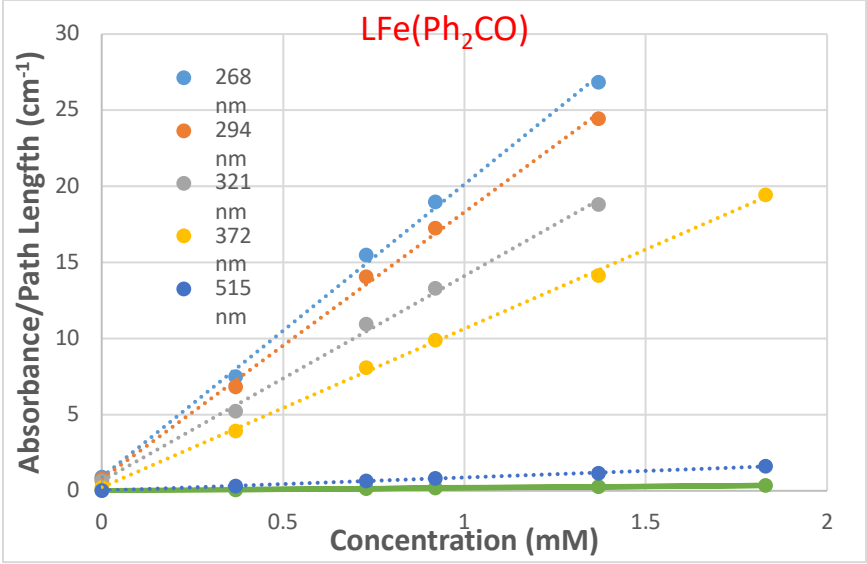


Figure S-8: ^{1}H NMR spectrum of $L^{Me}Fe(OCPh_2CHCPh)$ **(6)** in C_6D_6. ^{1}H NMR (C_6D_6, 400 MHz) 37, 35, 34, 24, 17, 8, 5, 4, 2, -40 ppm. There are at least three missing or overlapping signals, which is unsurprising given the broadness of the peaks as is typical for the iron(III) oxidation state.



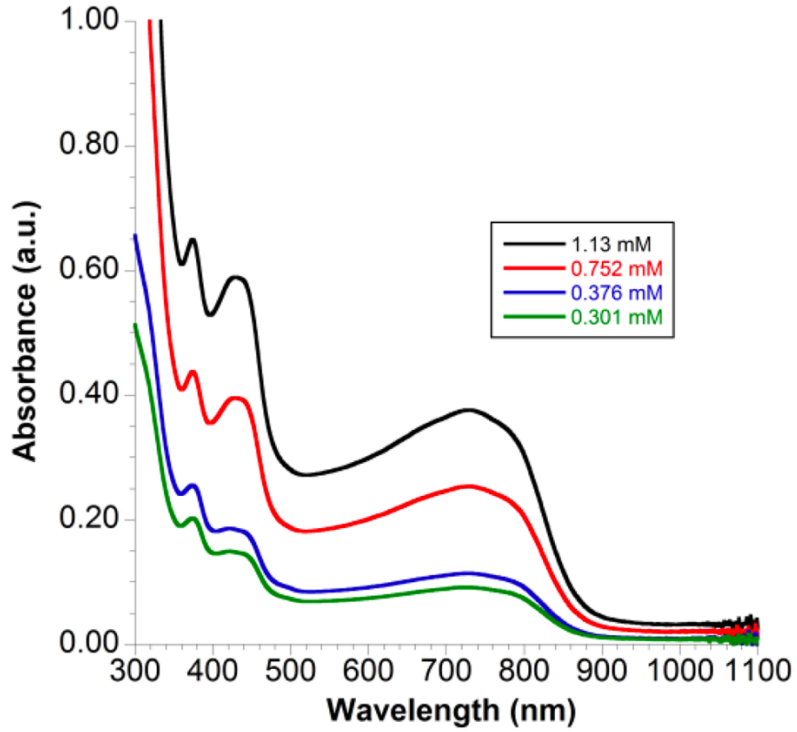
		Value	Error
Peak at 486 nm	y-int	-0.4080	0.1487
	slope	2460.1805	140.2989
	R^2	0.9903	
Peak at 372 nm	y-int	-1.1953	0.3945
	slope	7826.3101	372.2403
	R^2	0.9933	
Peak at 325 nm	y-int	-2.3682	0.8057
	slope	15870.1106	760.3451
	R^2	0.9932	
Peak at 236 nm	y-int	-4.89	2.07
	slope	26669.54	2460.74
	R^2	0.9833	

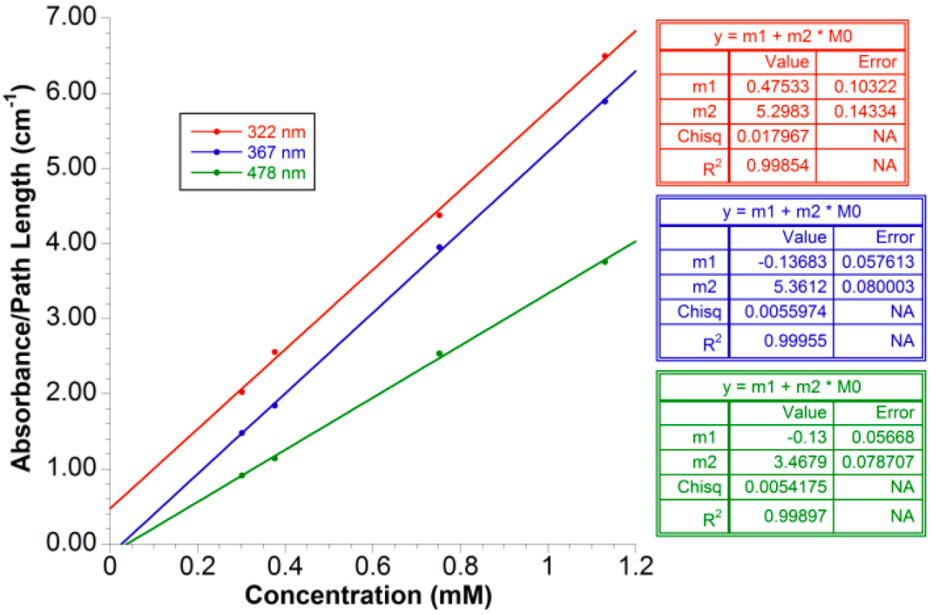
Figure S-9: Beer-Lambert Law plot of selected UV-vis spectral features for $L^{Me}Fe(CPh_3)$ **(1)** in hexanes.



		Value	Error
Peak at 817 nm	y-int	0.004948	0.009304
	slope	188.4428	8.012423
	R^2	0.9946	
Peak at 515 nm	y-int	0.009976	0.031076
	slope	866.3141	26.76175
	R^2	0.9971	
Peak at 372 nm	y-int	0.227078	0.296108
	slope	10416.74	255.0006
	R^2	0.9982	
Peak at 321 nm	y-int	0.640788	0.653175
	slope	13473.72	709.1879
	R^2	0.9945	
Peak at 294 nm	y-int	0.773263	0.729542
	slope	17529.95	792.1041
	R^2	0.9959	
Peak at 268 nm	y-int	0.888233	0.85134
	slope	19248.08	924.3458
	R^2	0.9954	

Figure S-10: Beer-Lambert Law plot of selected UV-vis spectral features for $L^{Me}Fe(Ph_2CO)$ (**2**) in hexanes solutions.



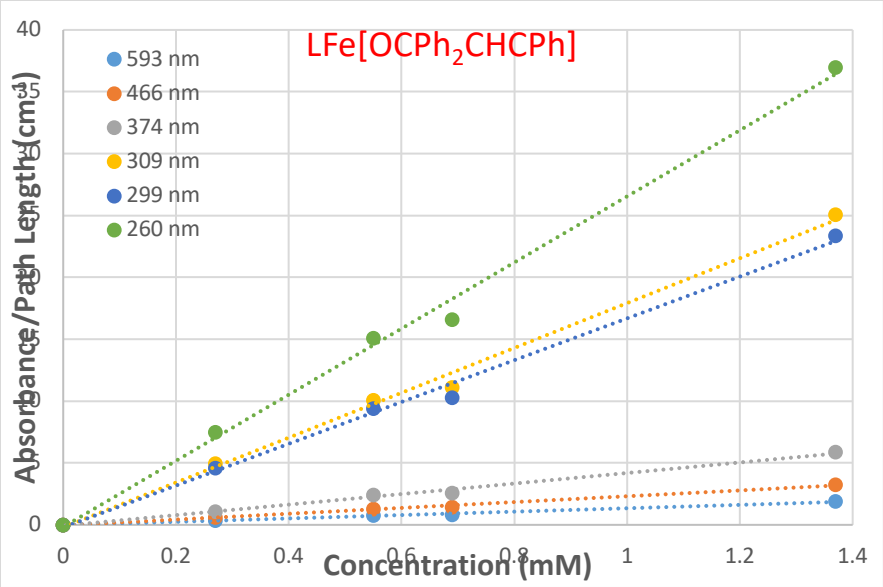


y = m1 + m2 * M0		
	Value	Error
m1	0.47533	0.10322
m2	5.2983	0.14334
Chisq	0.017967	NA
R^2	0.99854	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.13683	0.057613
m2	5.3612	0.080003
Chisq	0.0055974	NA
R^2	0.99955	NA

y = m1 + m2 * M0		
	Value	Error
m1	-0.13	0.05668
m2	3.4679	0.078707
Chisq	0.0054175	NA
R^2	0.99897	NA

Figure S-11: UV-vis spectra and Beer-Lambert Law plot of [K(18-crown-6)][$L^{Me}FeCH_3$] **(3)**.



		Value	Error
Peak at 593 nm	y-int	-0.0310	0.04551
	slope	1.3712	0.06161
	R^2	0.9940	
Peak at 466 nm	y-int	-0.0435	0.07676
	slope	2.3544	0.10392
	R^2	0.9942	
Peak at 374 nm	y-int	-0.0668	0.14701
	slope	4.25707	0.19901
	R^2	0.9935	
Peak at 309 nm	y-int	-0.2043	0.56737
	slope	18.1270	0.76806
	R^2	0.9946	
Peak at 299 nm	y-int	-0.2057	0.53804
	slope	16.8942	0.72836
	R^2	0.9945	
Peak at 260 nm	y-int	-0.1679	0.7940
	slope	26.7166	1.0748
	R^2	0.9952	

Figure S-12: Beer-Lambert Law plot of selected UV-vis spectral features for $L^{Me}Fe(OCPh_2CHCPh)$ (**6**) in hexanes.

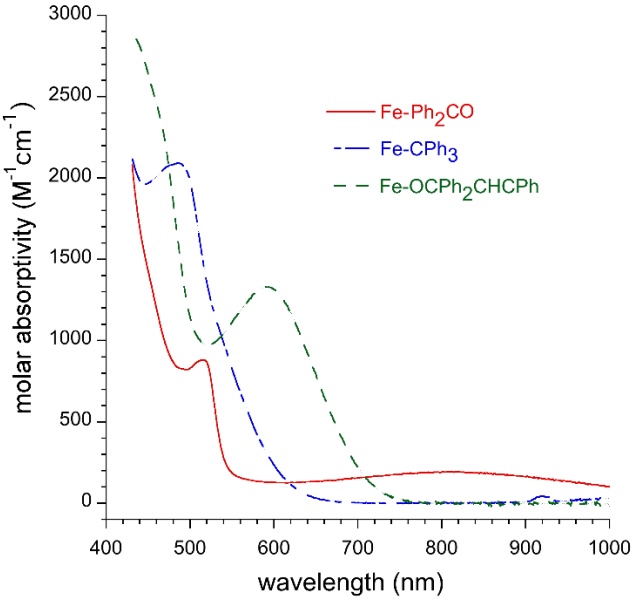


Figure S-13. Overlaid UV-vis spectra of **1** (blue), **2** (red), and **6** (green).

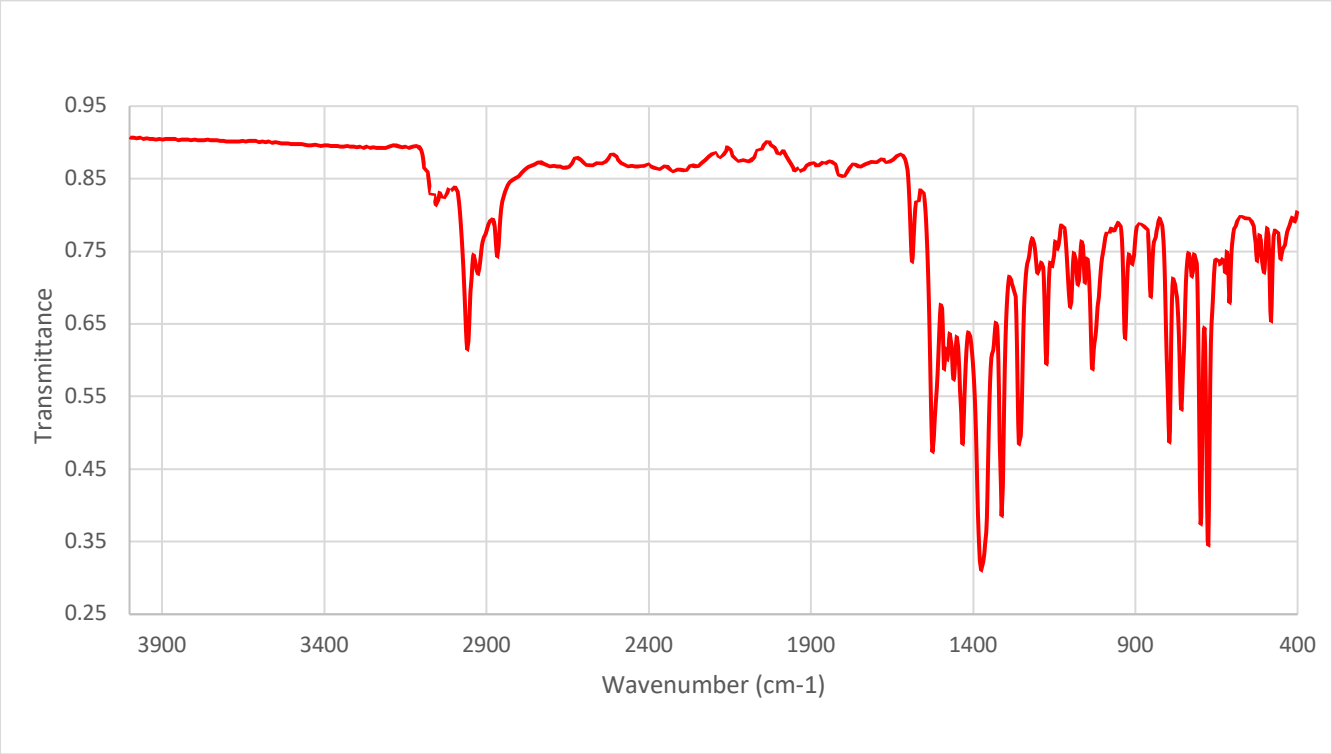


Figure S-14: FTIR spectrum of solid $L^{Me}Fe(CPh_3)$ **(1)**.

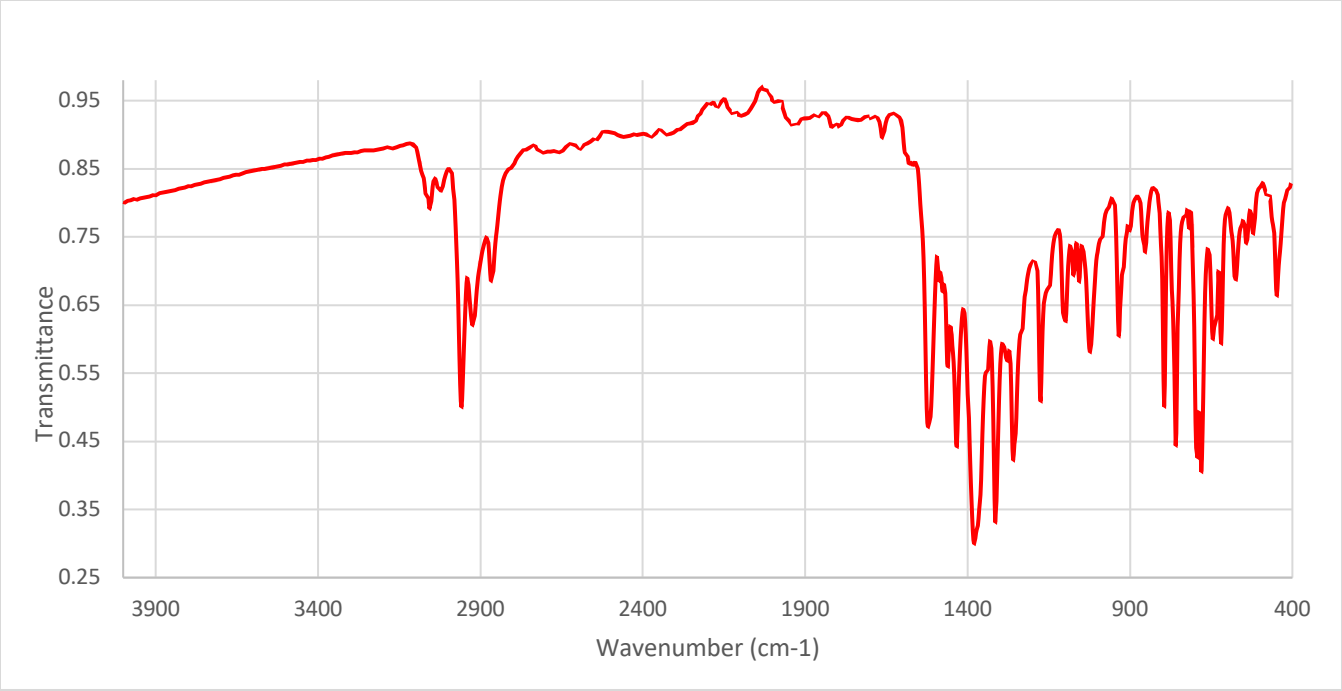


Figure S-15: FTIR spectrum of solid $L^{Me}Fe(Ph_2CO)$ **(2)**.

Figure S-16: FTIR spectrum of [K(18-crown-6)][$L^{Me}FeCH_3$] **(3)**.

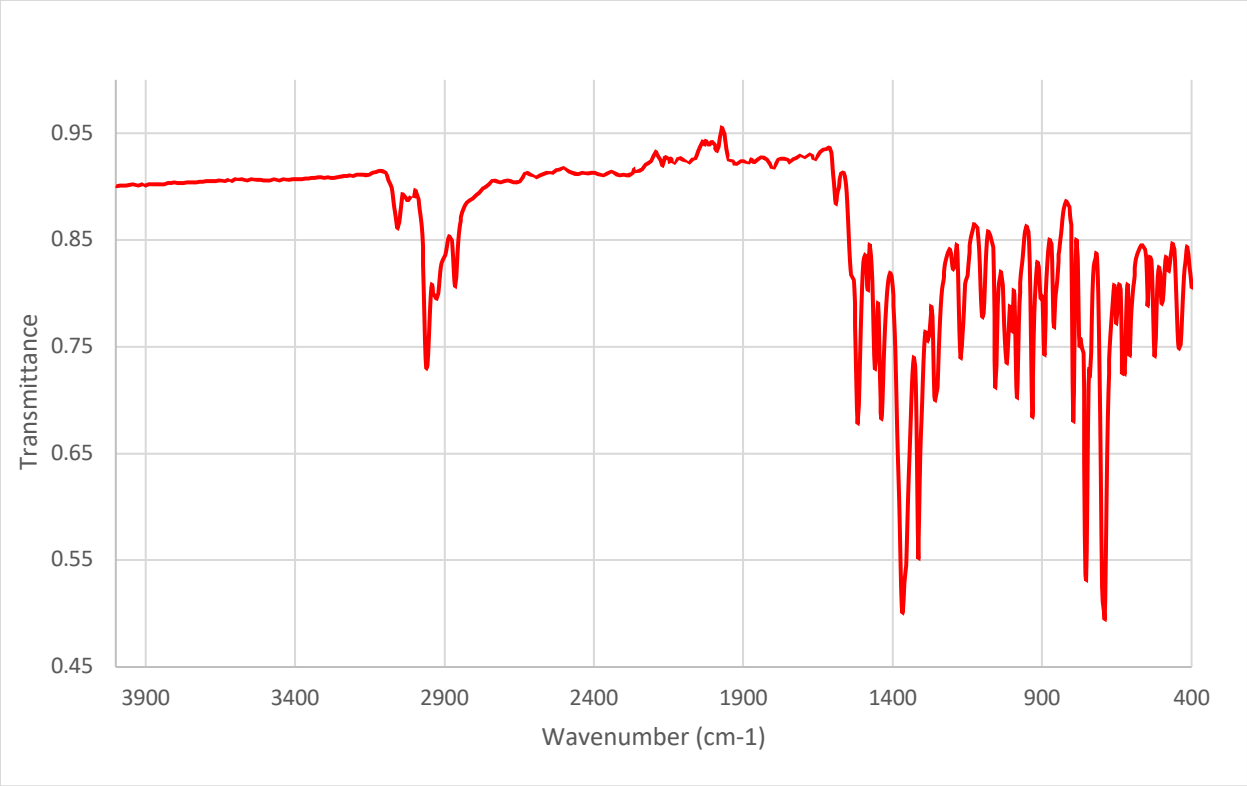


Figure S-17: FTIR spectrum of $L^{Me}Fe(OCPh_2CHCPh)$ **(6)**.

X-Ray Absorption Data Collection. Fe K-edge XAS spectra were collected on the 16 pole, 2 T wiggler beamline 9-3 at the Stanford Synchrotron Radiation Lightsource (SSRL) under ring conditions of 3 GeV and 500 mA. Samples were diluted in BN, pressed into 1 mm aluminum spacers and sealed with 37 μm Kapton tape. Samples were maintained at 10 K in a liquid He cryostat during data collection. A Si(220) double-crystal monochromator was used for energy selection and a Rh-coated mirror (set to an energy cutoff of 13 keV) was used for harmonic rejection. Internal energy calibration was performed by assigning the first inflection point of an Fe foil spectrum to 7112.6 eV.[1]Spectra were collected in fluorescence mode with a Lytle detector, attenuating elastic scatter into the detector using a Soller slit with an upstream Mn filter. The raw data were averaged and energy shifted using EXAFSPAK.[1] Data were calibrated using an internal Fe foil standard. Spectra were shifted such that the Fe foil rising edge inflection point matched the value of 7112.6 eV. The averaged data file was then normalized in Igor by applying a linear normalization to the pre-edge and a quad normalization to the post-edge to produce the final spectra.

Computational Details. All electronic structure and spectroscopic calculations were performed using the ORCA 4.04 computational chemistry package.[2] Geometry optimizations were performed using the BP86 functional,[3] the zeroth-order regular approximation for relativistic effects (ZORA)[4] as implemented by van Wüllen,[5] and the CP(PPP) basis set.[6] Optimized crystal structure coordinates were used for TDDFT calculations[7] of Fe K-edge XAS utilizing the B3LYP[9] functional. Calculated excitation energies were plotted against experimental energies for the B3LYP functional.[8] This correlation (Figure S-18) was used to shift the calculated energy of the spectra and produce calculated spectra that correlate well to experimental spectra.

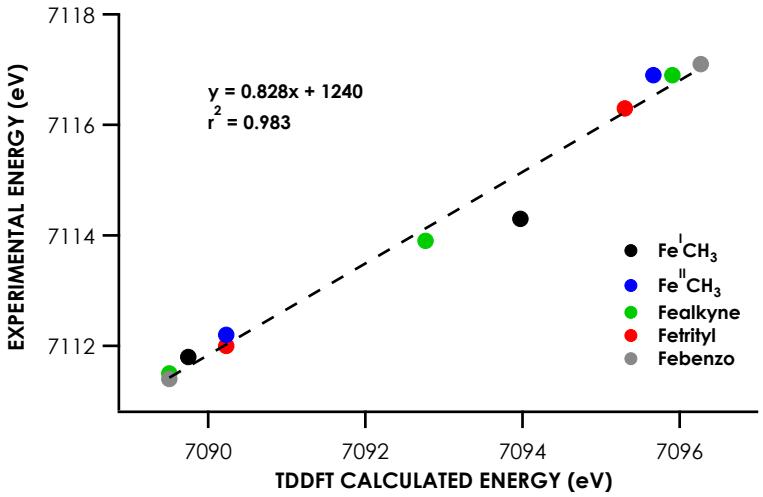


Figure S-18: Correlation curve of experimentally collected pre-edge energy to B3LYP calculated energy for compounds **1-5** used to shift calculated spectra.

Multireference character in the ground states of **2** and **5** was evaluated using SORCI calculations. SORCI was performed on a complete active space (CAS) for models of **2** and **5** comprising 15 electrons and 11 orbitals [CAS(15,11)]. Sufficiency of the active space was evaluated by ensuring that it captured ca. 90% of chosen state references without requiring holes or particles outside the active orbitals. The ZORA-def2-TZVPP(-f) basis set[9] was used on Fe, and ZORA-def2-SVP was used on all other atoms. The ZORA relativistic correction[10] was used in all SORCI calculations. As described elsewhere,[11] individual selection was used to ease the computational burden. The size of the first-order interacting space was reduced with a threshold: $T_{sel} = 10^{-6}$ E_h. A further approximation involved reducing the reference space through another selection: all initial references that contributed less than a second threshold ($T_{pre} = 10^{-5}$) to the zeroth-order states were rejected from the reference space. Starting orbitals were taken from unrestricted Kohn–Sham orbitals generated via B3LYP calculations using the aforementioned basis sets that were subsequently transformed to quasi-restricted orbitals (QROs).[12] These orbitals were then used in a CASSCF calculation, whereupon the resulting orbitals were used in the SORCI procedure.

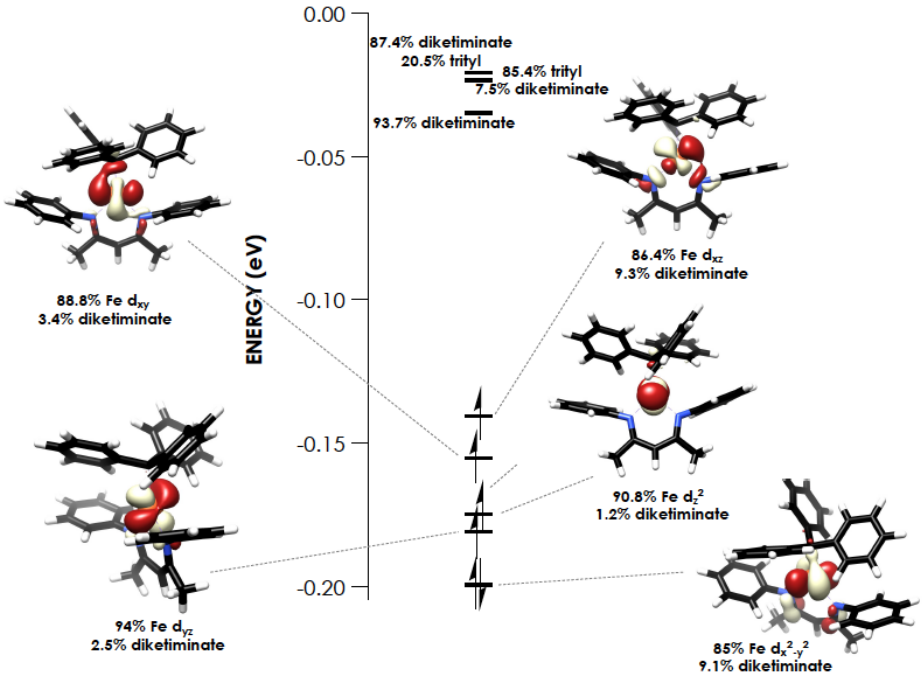


Figure S-19. (left) Overlay of experimental and TDDFT calculated spectra of **1** showing acceptor molecular orbitals for pre-edge transitions. (right) Molecular orbital diagram for **1** generated with QROs calculated with the B3LYP functional. Orbitals are plotted at an isovalue of 0.03 au.

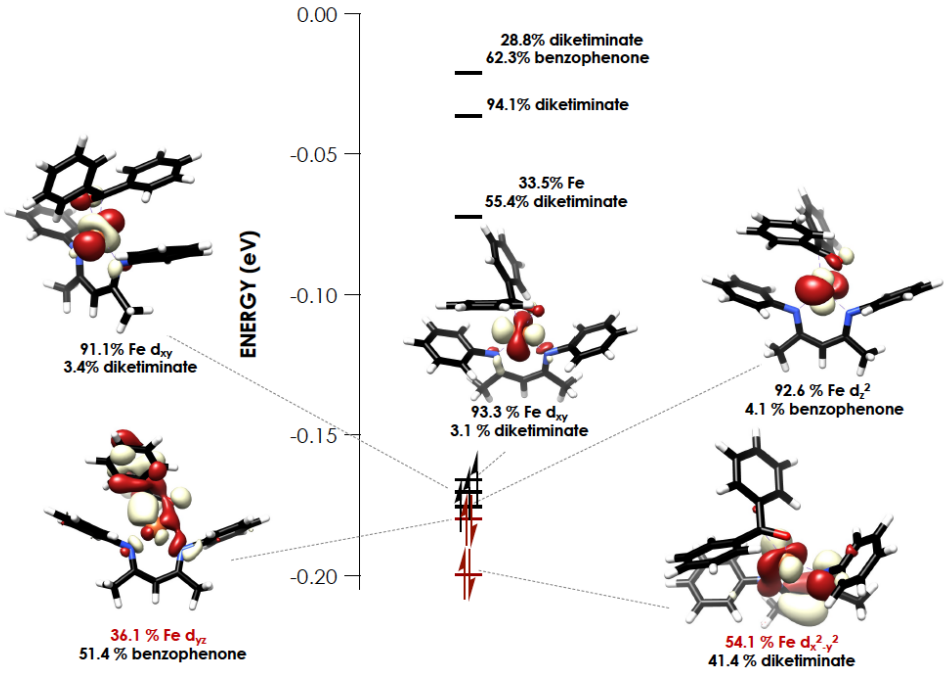


Figure S-20. Molecular orbital diagram for **2** generated with QROs calculated with the B3LYP functional. Orbitals with low Fe percentage are shown in red. Orbitals are plotted at an isovalue of 0.03 au.

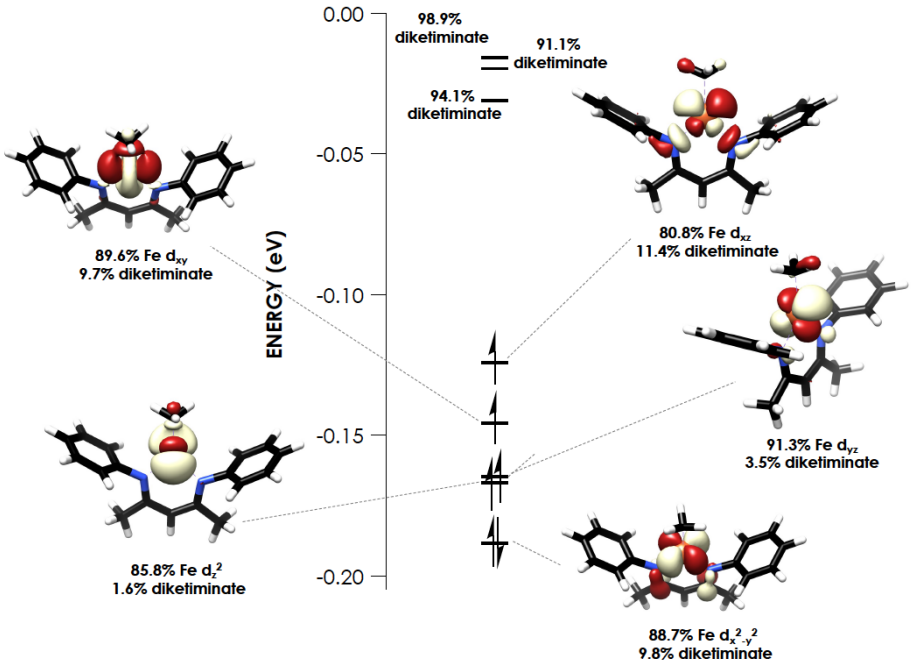


Figure S-21. Molecular orbital diagram for **3** generated with QROs calculated with the B3LYP functional. Orbitals are plotted at an isovalue of 0.03 au.

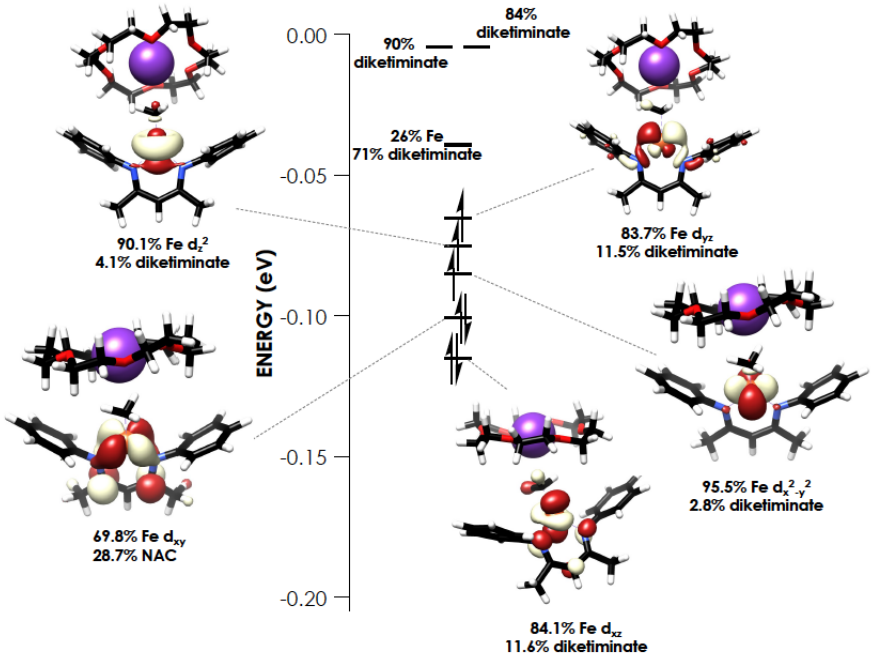


Figure S-22. Molecular orbital diagram for **4** generated with QROs calculated with the B3LYP functional. Orbitals are plotted at an isovalue of 0.03 au.

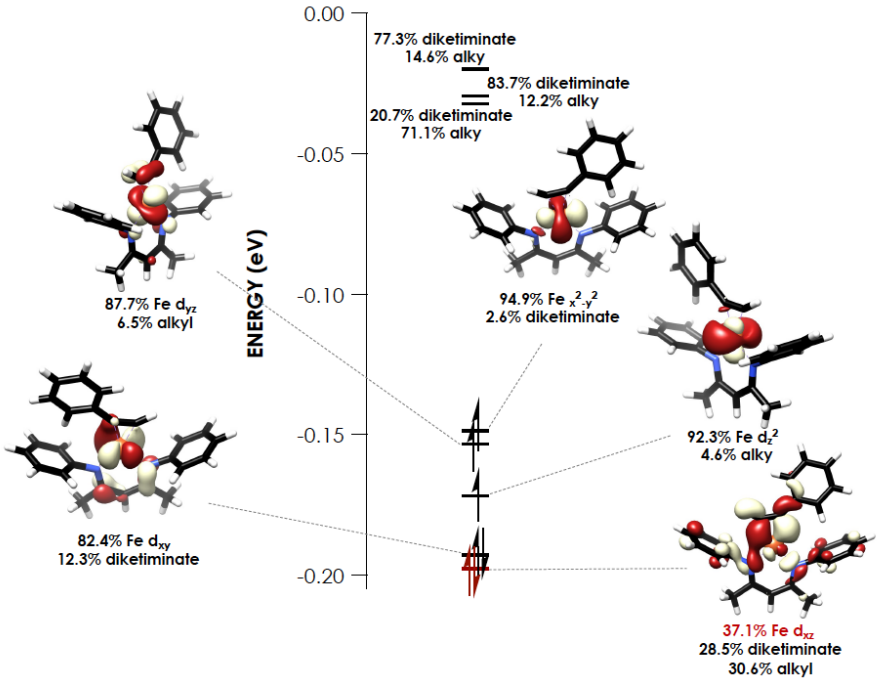


Figure S-23. Molecular orbital diagram for **5** generated with QROs calculated with the B3LYP functional. Orbitals are plotted at an isovalue of 0.03 au.

Example input file: geometry optimizations

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!NormalPrint TightSCF SlowConv Grid4 NoFinalGrid
!PrintBasis
%geom
     optimizehydrogens true
      end
%MaxCore 4000
%SCF
      MaxIter 500
      end

* xyz CHARGE MULTIPLICITY
COORDINATES
*
```

Example input file: TD-DFT for K-edge spectra

```
!B3LYP KDIIS RIJCOSX ZORA-def2-TZVP(-f) def2/J ZORA CPCM UKS
PAL6
!NormalPrint VeryTightSCF SlowConv Grid4 NoFinalGrid UNO UCO
!PrintBasis
%output print[p_mos] 1 end
%basis newgto Fe "CP(PPP)" end  end
%method SpecialGridAtoms 26
        SpecialGridIntAcc 7
        end
%tddft   NRoots 150
         MaxDim 500
         OrbWin[0] = 0, 0, -1, -1
         OrbWin[1] = 0, 0, -1, -1
         DoQuad true
         end
%MaxCore 4000
%SCF
      MaxIter 500
      end

* xyz CHARGE MULTIPLICITY
COORDINATES
*
```

Example input file: SORCI

```
!ROHF ZORA-def2-SVP def2-SVP/C ZORA
!NormalPrint Grid4
!MOREAD NOITER
!PrintBasis
%pal nprocs 3 end
%maxcore 30000
%moinp "FILENAME.gbw"
%basis NewGTO Fe "ZORA-def2-TZVPP" end
                      NewAuxGTO Fe "def2-TZVPP/C" end end
%mrci CIType         sorci
      UseIVOs         false
      IntMode      RITrafo
      Maxdim          100
      TSel            1e-6
      TPre            1e-5
      TNat            1e-5
      ETol            1e-6
        RTol            1e-6
        MaxDIIS           35
        MaxIter           400
        allsingles false
        soc
        printlevel 5
     GTensor True
     NDoubGTensor 1
        end
        NewBlock 4 *
         NRoots    5
        excitations cisd
        Refs CAS(15,11)
           end end
        NewBlock 6 *
         NRoots    5
        excitations cisd
        Refs CAS(15,11)
           end end end
%method SpecialGridAtoms 26
        SpecialGridIntAcc 7
        end

* xyz CHARGE MULTIPLICITY
COORDINATES
*
```

Example input file: CASSCF

```
!RI-JK ZORA-def2-SVP AutoAux ZORA
!TightSCF SlowConv NormalPrint CPCM(THF) Grid4
!PrintBasis
!Conv MOREAD
%casscf nel 15
     norb 11
     mult 4, 6
     MaxIter 250
     nroots 5, 5
     orbstep SuperCI
     cistep CSFCI
     switchstep DIIS
     etol 1e-7
     end
%scf
    Rotate
       { ORBITAL #1, ORBITAL #2, 90 }
          end
        end
%moinp "FILENAME.qro"
%basis NewGTO Fe "ZORA-def2-TZVPP" end end
%pal nprocs 12 end
%method SpecialGridAtoms 26
        SpecialGridIntAcc 7
        end
%MaxCore 4000


* xyz CHARGE MULTIPLICITY
COORDINATES
*
```

Optimized, Truncated Structure for 1

Fe	0.000000	0.000000	0.000000
N	-1.212610	-0.734180	-1.428340
N	1.307280	0.790110	-1.303680
C	0.402220	-0.386710	-3.200820
H	0.576390	-0.586360	-4.256580
C	3.496010	-2.104410	3.579800
H	4.341510	-2.671230	3.974690
C	0.961720	2.343010	2.275240
H	1.882490	1.952840	1.841150
C	-1.261270	2.040580	3.078810
H	-2.121360	1.410740	3.303630
C	2.015820	-0.213300	3.699240
H	1.703480	0.694770	4.216750
C	1.559540	3.193750	-0.983620
C	-1.168720	-0.843930	2.596430
C	2.117610	1.906690	-0.878260
C	3.402180	1.711760	-0.347800
C	-2.576740	-1.114220	-1.146850
C	-3.546860	-0.094450	-1.029310
C	-2.914790	-2.459720	-0.985630
C	1.741620	-1.820950	1.963780
H	1.197160	-2.208190	1.094860
C	-0.114400	1.471440	2.501660
C	-0.825060	-0.844440	-2.708400
C	1.335040	0.461560	-2.595150
C	0.000000	-0.000000	2.123500
C	3.564160	4.090790	0.026430
H	4.129670	4.949880	0.390820
C	-1.047600	-1.863550	3.535300
H	-0.078290	-2.065410	3.992060

C	-3.380930	-2.426350	3.357630
H	-4.233300	-3.043940	3.646010
C	0.893290	3.687610	2.590580
H	1.756830	4.324950	2.395450
C	1.303510	-0.647100	2.579630
C	2.303920	4.271650	-0.524230
H	1.882230	5.277540	-0.586870
C	-0.257020	4.226980	3.147830
H	-0.311060	5.289100	3.394120
C	3.100460	-0.928000	4.182890
H	3.626410	-0.565270	5.069290
C	2.823050	-2.544260	2.458440
H	3.128720	-3.465130	1.957250
C	-5.213590	-1.782880	-0.632920
H	-6.252890	-2.051310	-0.433620
C	-3.528250	-1.391900	2.442690
H	-4.505080	-1.191320	2.001270
C	-1.761350	-1.444430	-3.726860
H	-2.012750	-2.487900	-3.489920
H	-1.310730	-1.414120	-4.725140
H	-2.712050	-0.891620	-3.757730
C	2.370440	1.050420	-3.509730
H	2.182900	2.122990	-3.675170
H	2.354470	0.549790	-4.484050
H	3.381760	0.971470	-3.085960
C	-4.257760	-2.773810	-0.730900
H	-4.543600	-3.820270	-0.603730
C	-2.452980	-0.632760	2.067840
H	-2.600140	0.168400	1.343120
C	-1.328230	3.389290	3.392750
H	-2.241160	3.784830	3.844660

C	-2.127180	-2.641300	3.911130
H	-1.983720	-3.434730	4.648650
C	-4.861500	-0.469570	-0.778380
H	-5.624860	0.308160	-0.693570
C	4.104210	2.825530	0.095390
H	5.102540	2.687880	0.518060
H	0.561680	3.321170	-1.403180
H	3.819840	0.707140	-0.281310
H	-3.257970	0.948940	-1.157380
H	-2.151060	-3.233880	-1.056940

Optimized, Truncated Structure for 2

Fe	-0.000000	0.000000	0.000000
O	0.870430	0.799950	1.404460
N	0.794430	1.053570	-1.504760
N	-1.076220	-1.214980	-1.070730
C	1.082640	1.613680	-3.864170
H	1.093430	2.693520	-3.657930
H	0.584650	1.441860	-4.825130
H	2.134540	1.305010	-3.964960
C	0.414960	0.851270	-2.768570
C	-0.554450	-0.086880	-3.140510
H	-0.783350	-0.101760	-4.204920
C	-1.206650	-1.060120	-2.392830
C	-2.061140	-2.031350	-3.167930
H	-3.041690	-2.174520	-2.691990
H	-1.584550	-3.021960	-3.213460
H	-2.212880	-1.678380	-4.193690
C	1.862400	1.980620	-1.221490
C	3.187410	1.508490	-1.236280
C	4.193040	2.424180	-0.912020

H	5.231500	2.082030	-0.917370
C	3.915920	3.722390	-0.614730
H	4.727710	4.412200	-0.375040
C	2.609420	4.165960	-0.579480
H	2.388580	5.203940	-0.321850
C	1.561680	3.297800	-0.881900
C	-1.624570	-2.392420	-0.450750
C	-2.849870	-2.310160	0.249060
C	-3.336220	-3.467470	0.843200
H	-4.287480	-3.427340	1.379590
C	-2.638220	-4.661620	0.782050
H	-3.034610	-5.553300	1.269760
C	-1.434430	-4.711560	0.110290
H	-0.878750	-5.651490	0.068760
C	-0.915050	-3.595580	-0.526760
C	-0.000000	-0.000000	2.072940
C	-1.110500	0.701250	2.763590
C	-1.792930	1.757000	2.165070
H	-1.547420	2.031420	1.134810
C	-2.780470	2.449740	2.834850
H	-3.311460	3.261650	2.334580
C	-3.086030	2.114940	4.146810
H	-3.863260	2.662900	4.683360
C	-2.408430	1.091220	4.764660
H	-2.638290	0.835690	5.801730
C	-1.432990	0.387290	4.096050
H	-0.899610	-0.415550	4.605120
C	0.519380	-1.266140	2.619330
C	-0.308570	-2.353910	2.870700
H	-1.372200	-2.283610	2.637430
C	0.197860	-3.516170	3.396770

H	-0.470050	-4.360260	3.580310
C	1.543230	-3.625390	3.697690
H	1.938310	-4.549660	4.123680
C	2.379630	-2.565240	3.442020
H	3.444810	-2.647210	3.673390
C	1.896880	-1.391830	2.901310
H	2.561550	-0.552200	2.697030
H	3.405070	0.469530	-1.480680
H	0.523340	3.629580	-0.862090
H	-3.387970	-1.363840	0.299950
H	0.035990	-3.632840	-1.058480

Full Structure of 2 for SORCI and CASSCF

Fe	0.000000	0.000000	0.000000
O	-0.820530	0.526180	-1.555620
N	-1.334090	0.705430	1.314540
N	1.201140	-0.845390	1.274160
C	-2.188660	1.076960	3.571810
H	-2.461160	1.983130	3.321510
H	-1.831210	1.084380	4.484300
H	-2.963670	0.478420	3.528420
C	-1.135500	0.595880	2.630100
C	-0.000000	0.000000	3.190260
H	0.068310	0.087190	4.134040
C	1.044760	-0.696180	2.594090
C	2.013510	-1.371420	3.532060
H	2.931380	-1.180080	3.249010
H	1.862880	-2.339260	3.516410
H	1.874940	-1.035330	4.442580
C	-2.573450	1.257160	0.824830
C	-3.663760	0.391810	0.621970

C	-4.834260	0.953580	0.103060
H	-5.583920	0.390970	-0.057230
C	-4.932900	2.281170	-0.176790
H	-5.753440	2.636090	-0.498740
C	-3.847320	3.114200	0.003500
H	-3.917900	4.033840	-0.216980
C	-2.648700	2.611410	0.506930
C	-3.600070	-1.092490	0.893370
H	-2.749080	-1.273980	1.386870
C	-3.545260	-1.870880	-0.422250
H	-2.761580	-1.586740	-0.937020
H	-4.358210	-1.693450	-0.939980
H	-3.480410	-2.830530	-0.231460
C	-4.749820	-1.583250	1.762610
H	-4.724180	-1.123910	2.627550
H	-4.664280	-2.550090	1.903200
H	-5.601100	-1.391770	1.315720
C	-1.460920	3.552900	0.652030
H	-0.651900	2.998120	0.849910
C	-1.187710	4.338740	-0.619700
H	-1.097260	3.720980	-1.374130
H	-0.357450	4.848790	-0.515190
H	-1.931380	4.952540	-0.789580
C	-1.662710	4.523450	1.824660
H	-1.689400	4.019300	2.664130
H	-2.507590	5.007870	1.705420
H	-0.920750	5.161660	1.851000
C	2.191130	-1.771720	0.791210
C	3.430000	-1.287550	0.313020
C	4.351320	-2.215050	-0.155810
H	5.197180	-1.913850	-0.466250

C	4.065410	-3.569450	-0.184400
H	4.707490	-4.187800	-0.514500
C	2.841310	-4.015360	0.269030
H	2.644070	-4.945790	0.235520
C	1.894740	-3.138720	0.775490
C	3.782060	0.176990	0.305000
H	2.936570	0.702440	0.400530
C	4.458410	0.588970	-1.007430
H	3.960210	0.213310	-1.764320
H	5.377330	0.249900	-1.022060
H	4.468810	1.567260	-1.077150
C	4.696550	0.526380	1.473710
H	4.219050	0.378200	2.317050
H	4.961660	1.466830	1.409790
H	5.494960	-0.041630	1.445100
C	0.542320	-3.665320	1.245140
H	0.145190	-2.986420	1.863070
C	-0.392560	-3.821960	0.061330
H	-0.529900	-2.950800	-0.364620
H	-1.254140	-4.173130	0.368410
H	0.000890	-4.441590	-0.587030
C	0.660430	-4.984120	2.005130
H	1.312690	-4.884760	2.729120
H	0.957320	-5.689990	1.391500
H	-0.211560	-5.222010	2.381230
C	0.359560	0.060770	-2.040610
C	1.294790	1.095800	-2.546590
C	1.495330	2.294650	-1.867550
H	1.059380	2.436280	-1.035220
C	2.314880	3.282300	-2.374120
H	2.454180	4.083860	-1.884640

C	2.933000	3.099290	-3.603400
H	3.494170	3.776490	-3.960260
C	2.730240	1.932920	-4.301500
H	3.150580	1.812740	-5.144790
C	1.925710	0.938490	-3.793680
H	1.795530	0.140070	-4.290310
C	0.368380	-1.287900	-2.634270
C	1.527110	-2.051970	-2.708200
H	2.339510	-1.705550	-2.356370
C	1.511780	-3.298600	-3.282430
H	2.311510	-3.812010	-3.316360
C	0.342950	-3.816800	-3.809500
H	0.340700	-4.672940	-4.220740
C	-0.815720	-3.081720	-3.732050
H	-1.620450	-3.438930	-4.086740
C	-0.828530	-1.832390	-3.147830
H	-1.639390	-1.340320	-3.091340

Optimized, Truncated Structure of 3 for TD-DFT

Fe	0.000000	0.000000	0.000000
C	-1.775740	-1.559020	-3.631860
H	-1.714570	-2.639840	-3.432470
H	-1.482930	-1.381930	-4.673040
H	-2.832940	-1.276470	-3.517260
C	-2.142680	-1.732070	-0.852790
C	2.121900	1.814540	-0.701130
C	0.000000	-0.000000	2.002830
H	-0.810570	0.648510	2.379680
H	0.954570	0.380120	2.403520

H	-0.168010	-1.012380	2.408560
C	-0.894170	-0.784300	-2.688970
C	-3.425320	-1.182370	-0.701080
C	1.763680	3.142850	-0.418570
C	0.085730	0.036390	-3.258110
H	0.117850	0.039600	-4.346860
C	-4.396290	-1.940350	-0.051760
H	-5.393930	-1.516730	0.086920
C	2.682280	3.930480	0.286680
H	2.418080	4.962800	0.528750
C	1.034960	0.850510	-2.627370
C	-4.115770	-3.198480	0.428680
H	-4.888150	-3.769360	0.947530
C	3.905260	3.429780	0.670250
H	4.604800	4.065420	1.216690
C	1.959700	1.659110	-3.505380
H	1.823960	2.737410	-3.333920
H	1.772150	1.451850	-4.565180
H	3.013830	1.434310	-3.284470
C	-2.868310	-3.741570	0.244710
H	-2.653200	-4.746750	0.615760
C	4.245460	2.133390	0.375340
H	5.216370	1.741910	0.689220
C	-1.852100	-3.028980	-0.398530
C	3.362840	1.288360	-0.302020
N	-1.077970	-0.913970	-1.375800
N	1.146830	0.939320	-1.301850
H	-3.631980	-0.173840	-1.059480
H	0.788870	3.525970	-0.717140
H	-0.852260	-3.443760	-0.526310
H	3.613830	0.250410	-0.520280

Optimized, Truncated Structure of 4 for TD-DFT

Fe	0.000000	0.000000	0.000000
C	-0.000000	-0.000000	2.036910
H	0.287140	-0.986350	2.440760
H	0.647690	0.777350	2.479060
H	-1.042290	0.218870	2.331620
N	0.513630	-1.400500	-1.227490
N	-0.366230	1.393280	-1.267970
C	1.099150	-2.308400	-3.490750
H	1.937160	-2.874100	-3.055180
H	1.420000	-1.894210	-4.454700
H	0.295010	-3.036230	-3.687500
C	0.644050	-1.179080	-2.564380
C	0.437500	0.079760	-3.156350
H	0.651450	0.127220	-4.224840
C	-0.033900	1.258030	-2.593590
C	-0.155160	2.483760	-3.487750
H	-1.198010	2.823830	-3.585610
H	0.223750	2.258550	-4.492590
H	0.415860	3.336220	-3.087020
C	0.639770	-2.606600	-0.675150
C	-0.346540	-3.590860	-0.922360
C	-0.259610	-4.831290	-0.300940
H	-1.024220	-5.589670	-0.486900
C	0.782050	-5.089780	0.592490
H	0.837140	-6.048990	1.110320
C	1.741650	-4.121930	0.816820
H	2.560330	-4.340500	1.508920
C	1.722450	-2.896460	0.170080
C	-0.779340	2.545750	-0.804130

C	-2.103880	2.913120	-0.982700
C	-2.754650	3.973510	-0.359200
H	-3.828690	4.120470	-0.478840
C	-1.944640	4.907000	0.281760
H	-2.374290	5.801680	0.738800
C	-0.595920	4.642070	0.422550
H	0.039070	5.354630	0.955260
C	-0.015190	3.487340	-0.090190
K	-0.997450	-0.501750	4.951920
O	-3.186540	-1.354000	3.331290
O	-0.925020	-3.291940	4.230950
O	0.924840	-2.374010	6.236900
O	1.077490	0.426060	6.445270
O	-0.997730	2.102850	6.087340
O	-2.960080	1.093630	4.261440
C	-2.805660	-2.670480	2.792390
H	-3.709210	-3.200410	2.442510
H	-2.205930	-2.436230	1.892260
C	-2.090180	-3.654570	3.605850
H	-2.788060	-4.070730	4.368860
H	-1.913060	-4.486470	2.888900
C	-0.230300	-3.876470	5.212950
H	-0.237850	-4.983840	5.025940
H	-0.794280	-3.802080	6.173510
C	1.122340	-3.549490	5.539150
H	1.559250	-4.342560	6.173490
H	1.783250	-3.393340	4.663660
C	2.092790	-1.731580	6.457470
H	2.637980	-1.587560	5.496370
H	2.777760	-2.330610	7.097810
C	1.924780	-0.409390	7.124780

H	1.539050	-0.597660	8.147040
H	2.933370	0.037260	7.243970
C	1.023200	1.513680	7.321930
H	1.900470	2.159120	7.112170
H	1.116230	1.197000	8.371640
C	-0.230840	2.266510	7.226810
H	-0.871080	1.976680	8.086060
H	-0.001900	3.338580	7.402030
C	-1.816840	2.844640	5.209330
H	-1.255620	2.924470	4.258650
H	-1.903260	3.888050	5.581750
C	-3.158370	2.387490	4.855800
H	-3.875530	2.305370	5.690660
H	-3.543060	3.104750	4.111060
C	-4.037730	0.939380	3.466900
H	-3.900530	1.547170	2.541810
H	-4.972680	1.305910	3.932490
C	-4.223380	-0.447230	3.177380
H	-5.051910	-0.815840	3.825750
H	-4.654520	-0.527470	2.154820
H	-1.177290	-3.348670	-1.586890
H	2.483890	-2.136590	0.347730
H	-2.725330	2.201490	-1.539490
H	1.046820	3.289820	0.080590

Optimized Truncated Structure of 5 for TD-DFT

Fe	0.000000	0.000000	0.000000
N	-1.435360	0.017150	1.353610
N	1.455130	-0.003590	1.357390
C	3.510860	-1.100380	0.594130
C	-1.256920	0.017020	2.676350

C	2.804780	0.075410	0.852660
C	3.345100	1.338040	0.563250
C	1.265300	0.019190	2.679050
C	-0.000000	0.000000	3.277830
H	-0.001020	0.001580	4.366640
C	-2.766250	0.103780	0.824430
C	-1.248730	0.280690	-3.020670
C	-2.455360	0.021950	3.596070
H	-3.098440	0.894500	3.407450
H	-2.137980	0.043310	4.644420
H	-3.079150	-0.870410	3.438530
C	2.460780	0.074380	3.604520
H	3.125840	-0.787360	3.446800
H	2.137790	0.078830	4.651720
H	3.062160	0.976690	3.420710
C	-3.500430	-1.075810	0.603580
C	-3.268150	1.359200	0.457870
C	4.774620	-0.995860	0.012270
H	5.340140	-1.904500	-0.206500
C	4.608160	1.381840	-0.019910
H	5.041760	2.355200	-0.264440
C	-4.543680	1.412760	-0.119310
H	-4.954470	2.383130	-0.406960
C	-0.285760	0.120350	-1.932810
C	0.949380	0.020230	-1.665860
C	-2.600660	0.117650	-2.829870
H	-2.975610	-0.155090	-1.845060
C	-4.754910	-0.957660	0.005290
H	-5.335970	-1.863070	-0.186010
C	-0.817460	0.609110	-4.281480
H	0.252380	0.740110	-4.462420

C	-5.269490	0.266450	-0.346600
H	-6.254080	0.328990	-0.813340
C	5.313860	0.241560	-0.291290
H	6.300700	0.304910	-0.753530
C	-3.489620	0.290850	-3.878730
H	-4.557940	0.156840	-3.695470
C	-3.043160	0.631820	-5.112670
H	-3.751670	0.775330	-5.932250
C	-1.705810	0.783330	-5.332210
H	-1.325480	1.048530	-6.320480
H	1.957530	-0.027510	-2.072640
H	3.064870	-2.068410	0.823760
H	2.772460	2.242000	0.769600
H	-3.080560	-2.043360	0.877710
H	-2.674470	2.257840	0.624160

Full Structure of 5 for SORCI and CASSCF

Fe	0.000000	0.000000	0.000000
N	-1.435350	0.017630	1.353610
N	1.455130	-0.004080	1.357390
C	3.510500	-1.101550	0.594130
C	-1.256910	0.017440	2.676350
C	2.804810	0.074470	0.852660
C	3.345550	1.336930	0.563250
C	1.265310	0.018760	2.679050
C	0.000000	-0.000000	3.277830
H	-0.001260	-0.029130	4.207520
C	-2.766210	0.104700	0.824430
C	-1.248630	0.281110	-3.020670
C	-2.455350	0.022760	3.596070
H	-3.059050	0.717460	3.330240

H	-2.165110	0.176830	4.498410
H	-2.900860	-0.826770	3.544670
C	2.460810	0.073560	3.604520
H	3.039260	-0.672530	3.424730
H	2.162200	0.034780	4.516780
H	2.940490	0.892300	3.459700
C	-3.500780	-1.074640	0.603580
C	-3.267700	1.360290	0.457870
C	2.921970	-2.472050	0.877630
H	2.124110	-2.340930	1.431670
C	4.774290	-0.997460	0.012270
H	5.259270	-1.768590	-0.173730
C	4.608620	1.380300	-0.019910
H	4.981380	2.207020	-0.230490
C	-4.543210	1.414270	-0.119300
H	-4.905160	2.239220	-0.353790
C	-0.285720	0.120450	-1.932810
C	0.949390	0.019920	-1.665860
C	2.593410	2.615750	0.885670
H	1.850480	2.384090	1.482080
C	-2.600620	0.118520	-2.829870
H	-2.921150	-0.110890	-1.987890
C	3.870080	-3.396790	1.647030
H	4.660800	-3.550640	1.124980
H	3.430510	-4.233330	1.817610
H	4.112260	-2.987930	2.480550
C	-2.929910	-2.439220	0.937150
H	-2.214780	-2.304000	1.594630
C	-2.445360	2.628180	0.655600
H	-1.549350	2.355530	0.945150
C	2.476530	-3.133660	-0.411980

H	1.864570	-2.553160	-0.873870
H	2.039680	-3.963770	-0.209890
H	3.240940	-3.299820	-0.966840
C	-4.755230	-0.956080	0.005290
H	-5.254770	-1.721830	-0.159220
C	-0.817250	0.609380	-4.281480
H	0.093640	0.717120	-4.435570
C	3.474260	3.625550	1.612210
H	3.851370	3.216840	2.394270
H	2.946120	4.383850	1.870170
H	4.180530	3.911810	1.027930
C	-5.269400	0.268210	-0.346600
H	-6.111500	0.323730	-0.739110
C	5.313940	0.239780	-0.291290
H	6.156570	0.295110	-0.680010
C	-3.014300	3.524120	1.726640
H	-2.460100	4.301770	1.821890
H	-3.042620	3.048340	2.560050
H	-3.902810	3.793230	1.480570
C	-3.489520	0.292010	-3.878720
H	-4.401080	0.173050	-3.734870
C	2.001030	3.260930	-0.372700
H	2.712720	3.522870	-0.962500
H	1.489070	4.031940	-0.125280
H	1.432750	2.629920	-0.819560
C	-3.042940	0.632840	-5.112670
H	-3.646210	0.763680	-5.807950
C	-1.705540	0.783900	-5.332200
H	-1.391580	1.002240	-6.180690
C	-3.943570	-3.383210	1.561750
H	-4.327740	-2.969640	2.338980

H	-3.507420	-4.199020	1.814070
H	-4.637280	-3.572950	0.925800
C	-2.302280	-3.076530	-0.288310
H	-2.979680	-3.233460	-0.950160
H	-1.895700	-3.912020	-0.042800
H	-1.634140	-2.487790	-0.647430
C	-2.289830	3.411950	-0.625590
H	-3.148420	3.724840	-0.913790
H	-1.911820	2.845930	-1.302390
H	-1.708330	4.160030	-0.472560
H	1.861770	-0.054790	-2.025300

X-ray crystallography:

[L^{Me}Fe(CPh_3] (1)

A crystal (0.48 x 0.14 x 0.06 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(5) K.[13] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 90 seconds and a detector distance of 3.99 cm. A randomly oriented region of reciprocal space was surveyed: six major sections of frames were collected with 0.50º steps in ω at six different ϕ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.[14] Final cell constants were calculated from the xyz centroids of 4024 strong reflections from the actual data collection after integration.[15] See Table S-1 for additional crystal and refinement information.

The structure was solved using SIR97[16] and refined using SHELXL-97.[17] The space group $P2_1/n$ was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0502$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1307$ (F^2, all data).

The structure is the one suggested. The asymmetric unit contains one iron molecule and one-half molecule of cocrystallized diethyl ether solvent. The diethyl ether molecule is modeled as disordered over a special position. Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

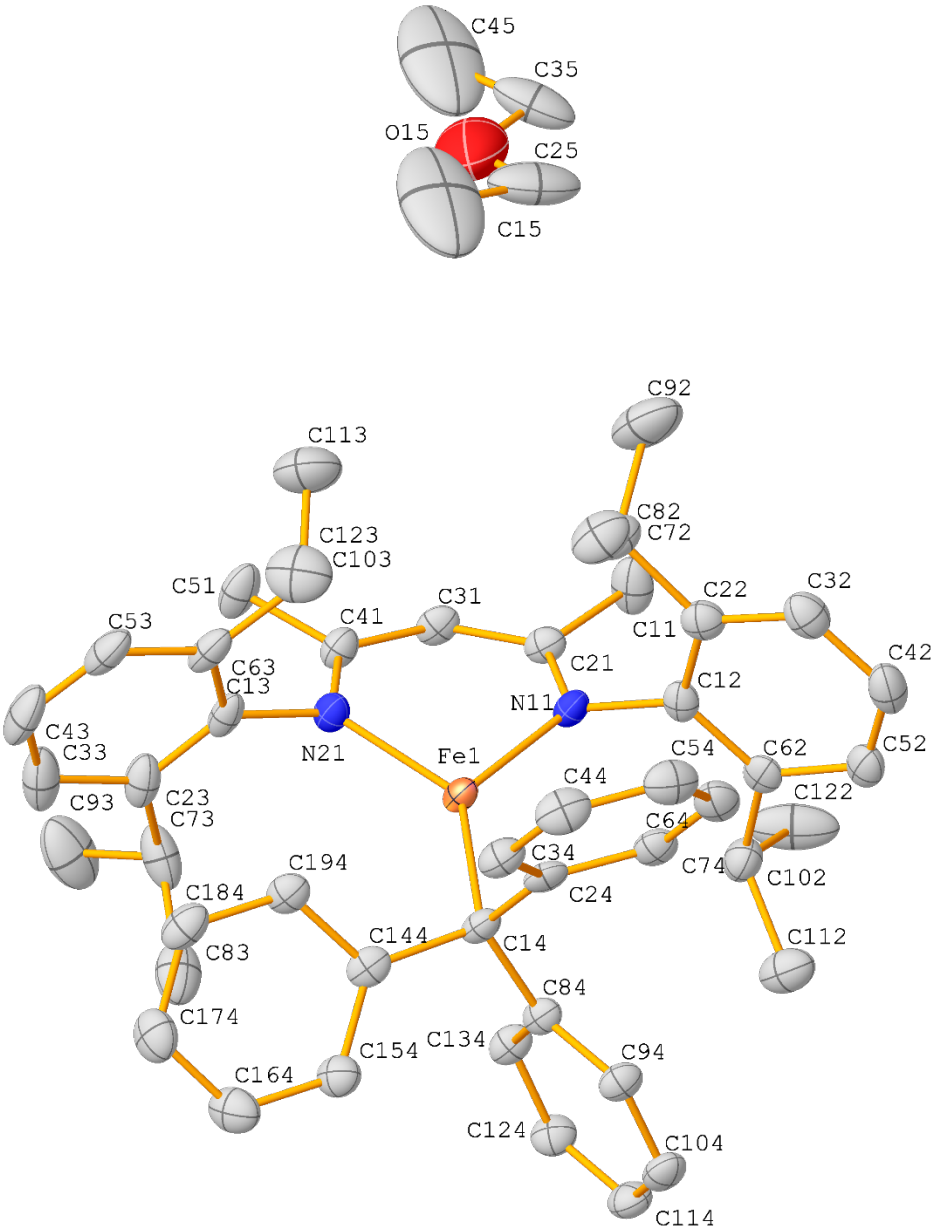

Figure S-24: The complete numbering scheme of $L^{Me}Fe(CPh_3)$ (**1**) with 50% thermal ellipsoid probability levels. The hydrogen atoms are omitted for clarity.

Table S-1. Crystal data and structure refinement for $L^{Me}Fe(CPh_3]$ (**1**).

Identification code	holkcm06	
CSD Deposition Number	1944808	
Empirical formula	$C_{50}\ H_{61}\ Fe\ N_2\ O_{0.5}$	
Formula weight	753.86	
Temperature	100.0(5) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 19.946(4) Å	α = 90°
	b = 10.0572(18) Å	β = 108.414(4)°
	c = 22.639(4) Å	γ = 90°
Volume	4308.9(13) Å^3	
Z	4	
Density (calculated)	1.162 g/cm^3	
Absorption coefficient	0.386 mm^{-1}	
F(000)	1620	
Crystal color, morphology	orange, needle	
Crystal size	0.48 x 0.14 x 0.06 mm^3	
Theta range for data collection	1.90 to 24.99°	
Index ranges	$-23 \le h \le 23$, $-11 \le k \le 11$, $-26 \le l \le 26$	
Reflections collected	57089	
Independent reflections	7554 [R(int) = 0.1431]	
Observed reflections	5083	
Completeness to theta = 24.99°	99.7%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9772 and 0.8364	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7554 / 5 / 509	
Goodness-of-fit on F^2	1.008	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1124	
R indices (all data)	R1 = 0.0891, wR2 = 0.1307	
Largest diff. peak and hole	0.522 and -0.321 e.Å^{-3}	

Table S-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $L^{Me}Fe(CPh_3]$ (**1**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	7166(1)	2398(1)	4172(1)	19(1)
N21	6398(1)	3723(2)	4137(1)	23(1)
N11	7948(1)	3743(2)	4440(1)	22(1)
C31	7163(2)	5628(3)	4207(1)	25(1)
C114	8035(2)	-318(3)	2473(2)	30(1)
C74	8350(2)	-7(3)	4875(1)	26(1)
C34	7327(2)	-1058(3)	4989(1)	30(1)
C94	8009(2)	-899(3)	3496(1)	25(1)
C22	8821(2)	3137(3)	5428(1)	28(1)
C144	6446(2)	-180(3)	3756(1)	24(1)
C12	8651(2)	3288(3)	4779(1)	23(1)
C62	9141(2)	2976(3)	4471(1)	24(1)
C13	5706(2)	3311(3)	4140(2)	26(1)
C63	5620(2)	2922(3)	4711(2)	30(1)
C23	5139(2)	3291(3)	3586(2)	33(1)
C134	7357(2)	975(3)	2974(1)	26(1)
C24	7623(2)	-258(3)	4627(1)	23(1)
C41	6507(2)	5040(3)	4139(1)	25(1)
C21	7836(2)	5051(3)	4397(1)	23(1)
C14	7200(2)	328(3)	4000(1)	23(1)
C42	9968(2)	2308(3)	5457(2)	35(1)
C154	6189(2)	-939(3)	3218(1)	30(1)
C174	5022(2)	-1013(4)	3313(2)	37(1)
C64	8752(2)	-508(3)	5446(2)	32(1)
C84	7553(2)	153(3)	3498(1)	22(1)
C32	9484(2)	2645(3)	5757(2)	33(1)
C112	9196(2)	1992(3)	3461(2)	40(1)
C103	6242(2)	2905(3)	5308(2)	34(1)
C54	8445(2)	-1285(3)	5797(2)	37(1)
C104	8249(2)	-1122(3)	2993(2)	29(1)
C102	8984(2)	3180(3)	3774(2)	31(1)
C124	7593(2)	742(3)	2466(1)	28(1)

C43	4387(2)	2535(4)	4175(2)	46(1)
C184	5272(2)	-283(3)	3860(2)	33(1)
C51	5905(2)	5985(3)	4091(2)	36(1)
C11	8445(2)	6006(3)	4584(2)	39(1)
C82	8176(2)	2379(4)	6158(2)	44(1)
C72	8308(2)	3522(3)	5775(2)	34(1)
C33	4476(2)	2899(3)	3617(2)	44(1)
C194	5961(2)	128(3)	4071(2)	27(1)
C44	7731(2)	-1558(3)	5562(2)	36(1)
C164	5492(2)	-1349(4)	2999(2)	37(1)
C83	5270(2)	2317(4)	2613(2)	46(1)
C122	9352(3)	4411(4)	3635(2)	65(1)
C73	5236(2)	3604(4)	2961(2)	42(1)
C53	4950(2)	2546(3)	4711(2)	38(1)
C52	9797(2)	2489(3)	4823(2)	30(1)
C93	4668(2)	4543(4)	2556(2)	63(1)
C123	6199(2)	1792(4)	5749(2)	54(1)
C113	6353(2)	4242(4)	5631(2)	59(1)
C92	8577(2)	4740(4)	6186(2)	65(1)
C15	7319(8)	4170(20)	7697(7)	168(8)
C25	7948(6)	4984(10)	7654(4)	76(3)
O15	7587(4)	6180(9)	7405(4)	118(3)
C35	8036(5)	7321(9)	7402(4)	63(3)
C45	7478(8)	8393(16)	7215(7)	168(8)

Table S-3. Bond lengths [Å] and angles [°] for $L^{Me}Fe(CPh_3]$ (**1**).

Fe(1)-N(11)	2.008(2)	C(23)-C(33)	1.403(5)
Fe(1)-N(21)	2.013(2)	C(23)-C(73)	1.520(5)
Fe(1)-C(14)	2.123(3)	C(134)-C(124)	1.392(4)
N(21)-C(41)	1.342(4)	C(134)-C(84)	1.396(4)
N(21)-C(13)	1.444(4)	C(134)-H(134)	0.9500
N(11)-C(21)	1.333(4)	C(24)-C(14)	1.524(4)
N(11)-C(12)	1.444(4)	C(41)-C(51)	1.508(4)
C(31)-C(21)	1.399(4)	C(21)-C(11)	1.501(4)
C(31)-C(41)	1.400(4)	C(14)-C(84)	1.525(4)
C(31)-H(31)	0.9500	C(42)-C(52)	1.378(5)
C(114)-C(124)	1.380(5)	C(42)-C(32)	1.387(5)
C(114)-C(104)	1.380(4)	C(42)-H(42)	0.9500
C(114)-H(114)	0.9500	C(154)-C(164)	1.383(4)
C(74)-C(64)	1.383(4)	C(154)-H(154)	0.9500
C(74)-C(24)	1.403(4)	C(174)-C(164)	1.387(5)
C(74)-H(74)	0.9500	C(174)-C(184)	1.389(5)
C(34)-C(44)	1.386(4)	C(174)-H(174)	0.9500
C(34)-C(24)	1.405(4)	C(64)-C(54)	1.387(5)
C(34)-H(34)	0.9500	C(64)-H(64)	0.9500
C(94)-C(104)	1.386(4)	C(32)-H(32)	0.9500
C(94)-C(84)	1.396(4)	C(112)-C(102)	1.517(5)
C(94)-H(94)	0.9500	C(112)-H(11A)	0.9800
C(22)-C(32)	1.388(4)	C(112)-H(11B)	0.9800
C(22)-C(12)	1.407(4)	C(112)-H(11C)	0.9800
C(22)-C(72)	1.525(4)	C(103)-C(113)	1.513(5)
C(144)-C(154)	1.391(4)	C(103)-C(123)	1.519(5)
C(144)-C(194)	1.405(4)	C(103)-H(103)	1.0000
C(144)-C(14)	1.517(4)	C(54)-C(44)	1.382(5)
C(12)-C(62)	1.403(4)	C(54)-H(54)	0.9500
C(62)-C(52)	1.389(4)	C(104)-H(104)	0.9500
C(62)-C(102)	1.522(4)	C(102)-C(122)	1.521(5)
C(13)-C(23)	1.397(4)	C(102)-H(102)	1.0000
C(13)-C(63)	1.412(4)	C(124)-H(124)	0.9500
C(63)-C(53)	1.390(4)	C(43)-C(53)	1.368(5)
C(63)-C(103)	1.519(5)	C(43)-C(33)	1.380(5)

C(43)-H(43)	0.9500	C(113)-H(11H)	0.9800
C(184)-C(194)	1.368(4)	C(113)-H(11I)	0.9800
C(184)-H(184)	0.9500	C(92)-H(92A)	0.9800
C(51)-H(51A)	0.9800	C(92)-H(92B)	0.9800
C(51)-H(51B)	0.9800	C(92)-H(92C)	0.9800
C(51)-H(51C)	0.9800	C(15)-C(25)	1.524(9)
C(11)-H(11D)	0.9800	C(15)-H(15A)	0.9800
C(11)-H(11E)	0.9800	C(15)-H(15B)	0.9800
C(11)-H(11F)	0.9800	C(15)-H(15C)	0.9800
C(82)-C(72)	1.511(5)	C(25)-O(15)	1.423(10)
C(82)-H(82A)	0.9800	C(25)-H(25A)	0.9900
C(82)-H(82B)	0.9800	C(25)-H(25B)	0.9900
C(82)-H(82C)	0.9800	O(15)-C(35)	1.457(10)
C(72)-C(92)	1.530(5)	C(35)-C(45)	1.512(9)
C(72)-H(72)	1.0000	C(35)-H(35A)	0.9900
C(33)-H(33)	0.9500	C(35)-H(35B)	0.9900
C(194)-H(194)	0.9500	C(45)-H(45A)	0.9800
C(44)-H(44)	0.9500	C(45)-H(45B)	0.9800
C(164)-H(164)	0.9500	C(45)-H(45C)	0.9800
C(83)-C(73)	1.528(5)	N(11)-Fe(1)-N(21)	94.29(10)
C(83)-H(83A)	0.9800	N(11)-Fe(1)-C(14)	130.49(11)
C(83)-H(83B)	0.9800	N(21)-Fe(1)-C(14)	135.23(11)
C(83)-H(83C)	0.9800	C(41)-N(21)-C(13)	116.0(2)
C(122)-H(12A)	0.9800	C(41)-N(21)-Fe(1)	122.2(2)
C(122)-H(12B)	0.9800	C(13)-N(21)-Fe(1)	121.77(19)
C(122)-H(12C)	0.9800	C(21)-N(11)-C(12)	117.7(2)
C(73)-C(93)	1.537(5)	C(21)-N(11)-Fe(1)	123.1(2)
C(73)-H(73)	1.0000	C(12)-N(11)-Fe(1)	118.58(18)
C(53)-H(53)	0.9500	C(21)-C(31)-C(41)	129.1(3)
C(52)-H(52)	0.9500	C(21)-C(31)-H(31)	115.4
C(93)-H(93A)	0.9800	C(41)-C(31)-H(31)	115.4
C(93)-H(93B)	0.9800	C(124)-C(114)-C(104)	119.2(3)
C(93)-H(93C)	0.9800	C(124)-C(114)-H(114)	120.4
C(123)-H(12D)	0.9800	C(104)-C(114)-H(114)	120.4
C(123)-H(12E)	0.9800	C(64)-C(74)-C(24)	122.0(3)
C(123)-H(12F)	0.9800	C(64)-C(74)-H(74)	119.0
C(113)-H(11G)	0.9800	C(24)-C(74)-H(74)	119.0

C(44)-C(34)-C(24)	121.8(3)	N(11)-C(21)-C(11)	120.5(3)
C(44)-C(34)-H(34)	119.1	C(31)-C(21)-C(11)	115.7(3)
C(24)-C(34)-H(34)	119.1	C(144)-C(14)-C(24)	113.7(2)
C(104)-C(94)-C(84)	121.3(3)	C(144)-C(14)-C(84)	109.2(2)
C(104)-C(94)-H(94)	119.4	C(24)-C(14)-C(84)	113.6(2)
C(84)-C(94)-H(94)	119.4	C(144)-C(14)-Fe(1)	108.19(19)
C(32)-C(22)-C(12)	118.2(3)	C(24)-C(14)-Fe(1)	104.37(19)
C(32)-C(22)-C(72)	119.6(3)	C(84)-C(14)-Fe(1)	107.41(19)
C(12)-C(22)-C(72)	122.1(3)	C(52)-C(42)-C(32)	119.7(3)
C(154)-C(144)-C(194)	116.3(3)	C(52)-C(42)-H(42)	120.1
C(154)-C(144)-C(14)	123.5(3)	C(32)-C(42)-H(42)	120.1
C(194)-C(144)-C(14)	120.2(3)	C(164)-C(154)-C(144)	121.9(3)
C(62)-C(12)-C(22)	121.2(3)	C(164)-C(154)-H(154)	119.1
C(62)-C(12)-N(11)	121.2(3)	C(144)-C(154)-H(154)	119.1
C(22)-C(12)-N(11)	117.6(3)	C(164)-C(174)-C(184)	118.3(3)
C(52)-C(62)-C(12)	118.2(3)	C(164)-C(174)-H(174)	120.8
C(52)-C(62)-C(102)	119.3(3)	C(184)-C(174)-H(174)	120.8
C(12)-C(62)-C(102)	122.5(3)	C(74)-C(64)-C(54)	120.7(3)
C(23)-C(13)-C(63)	121.3(3)	C(74)-C(64)-H(64)	119.6
C(23)-C(13)-N(21)	120.3(3)	C(54)-C(64)-H(64)	119.6
C(63)-C(13)-N(21)	118.4(3)	C(134)-C(84)-C(94)	117.0(3)
C(53)-C(63)-C(13)	118.0(3)	C(134)-C(84)-C(14)	119.6(3)
C(53)-C(63)-C(103)	120.8(3)	C(94)-C(84)-C(14)	123.0(3)
C(13)-C(63)-C(103)	121.2(3)	C(42)-C(32)-C(22)	121.2(3)
C(13)-C(23)-C(33)	117.9(3)	C(42)-C(32)-H(32)	119.4
C(13)-C(23)-C(73)	121.8(3)	C(22)-C(32)-H(32)	119.4
C(33)-C(23)-C(73)	120.1(3)	C(102)-C(112)-H(11A)	109.5
C(124)-C(134)-C(84)	121.6(3)	C(102)-C(112)-H(11B)	109.5
C(124)-C(134)-H(134)	119.2	H(11A)-C(112)-H(11B)	109.5
C(84)-C(134)-H(134)	119.2	C(102)-C(112)-H(11C)	109.5
C(74)-C(24)-C(34)	116.1(3)	H(11A)-C(112)-H(11C)	109.5
C(74)-C(24)-C(14)	120.2(3)	H(11B)-C(112)-H(11C)	109.5
C(34)-C(24)-C(14)	123.7(3)	C(113)-C(103)-C(123)	111.6(3)
N(21)-C(41)-C(31)	124.2(3)	C(113)-C(103)-C(63)	111.9(3)
N(21)-C(41)-C(51)	119.8(3)	C(123)-C(103)-C(63)	113.2(3)
C(31)-C(41)-C(51)	115.9(3)	C(113)-C(103)-H(103)	106.5
N(11)-C(21)-C(31)	123.7(3)	C(123)-C(103)-H(103)	106.5

C(63)-C(103)-H(103)	106.5	C(72)-C(82)-H(82C)	109.5
C(44)-C(54)-C(64)	118.6(3)	H(82A)-C(82)-H(82C)	109.5
C(44)-C(54)-H(54)	120.7	H(82B)-C(82)-H(82C)	109.5
C(64)-C(54)-H(54)	120.7	C(82)-C(72)-C(22)	111.7(3)
C(114)-C(104)-C(94)	120.8(3)	C(82)-C(72)-C(92)	110.6(3)
C(114)-C(104)-H(104)	119.6	C(22)-C(72)-C(92)	110.6(3)
C(94)-C(104)-H(104)	119.6	C(82)-C(72)-H(72)	107.9
C(112)-C(102)-C(122)	108.7(3)	C(22)-C(72)-H(72)	107.9
C(112)-C(102)-C(62)	112.4(3)	C(92)-C(72)-H(72)	107.9
C(122)-C(102)-C(62)	111.7(3)	C(43)-C(33)-C(23)	121.0(3)
C(112)-C(102)-H(102)	107.9	C(43)-C(33)-H(33)	119.5
C(122)-C(102)-H(102)	107.9	C(23)-C(33)-H(33)	119.5
C(62)-C(102)-H(102)	107.9	C(184)-C(194)-C(144)	122.1(3)
C(114)-C(124)-C(134)	120.1(3)	C(184)-C(194)-H(194)	118.9
C(114)-C(124)-H(124)	119.9	C(144)-C(194)-H(194)	118.9
C(134)-C(124)-H(124)	119.9	C(54)-C(44)-C(34)	120.8(3)
C(53)-C(43)-C(33)	120.3(3)	C(54)-C(44)-H(44)	119.6
C(53)-C(43)-H(43)	119.9	C(34)-C(44)-H(44)	119.6
C(33)-C(43)-H(43)	119.9	C(154)-C(164)-C(174)	120.7(3)
C(194)-C(184)-C(174)	120.7(3)	C(154)-C(164)-H(164)	119.7
C(194)-C(184)-H(184)	119.7	C(174)-C(164)-H(164)	119.7
C(174)-C(184)-H(184)	119.7	C(73)-C(83)-H(83A)	109.5
C(41)-C(51)-H(51A)	109.5	C(73)-C(83)-H(83B)	109.5
C(41)-C(51)-H(51B)	109.5	H(83A)-C(83)-H(83B)	109.5
H(51A)-C(51)-H(51B)	109.5	C(73)-C(83)-H(83C)	109.5
C(41)-C(51)-H(51C)	109.5	H(83A)-C(83)-H(83C)	109.5
H(51A)-C(51)-H(51C)	109.5	H(83B)-C(83)-H(83C)	109.5
H(51B)-C(51)-H(51C)	109.5	C(102)-C(122)-H(12A)	109.5
C(21)-C(11)-H(11D)	109.5	C(102)-C(122)-H(12B)	109.5
C(21)-C(11)-H(11E)	109.5	H(12A)-C(122)-H(12B)	109.5
H(11D)-C(11)-H(11E)	109.5	C(102)-C(122)-H(12C)	109.5
C(21)-C(11)-H(11F)	109.5	H(12A)-C(122)-H(12C)	109.5
H(11D)-C(11)-H(11F)	109.5	H(12B)-C(122)-H(12C)	109.5
H(11E)-C(11)-H(11F)	109.5	C(23)-C(73)-C(83)	110.1(3)
C(72)-C(82)-H(82A)	109.5	C(23)-C(73)-C(93)	113.4(3)
C(72)-C(82)-H(82B)	109.5	C(83)-C(73)-C(93)	110.9(3)
H(82A)-C(82)-H(82B)	109.5	C(23)-C(73)-H(73)	107.4

C(83)-C(73)-H(73)	107.4	C(72)-C(92)-H(92C)	109.5
C(93)-C(73)-H(73)	107.4	H(92A)-C(92)-H(92C)	109.5
C(43)-C(53)-C(63)	121.4(3)	H(92B)-C(92)-H(92C)	109.5
C(43)-C(53)-H(53)	119.3	C(25)-C(15)-H(15A)	109.5
C(63)-C(53)-H(53)	119.3	C(25)-C(15)-H(15B)	109.5
C(42)-C(52)-C(62)	121.5(3)	H(15A)-C(15)-H(15B)	109.5
C(42)-C(52)-H(52)	119.3	C(25)-C(15)-H(15C)	109.5
C(62)-C(52)-H(52)	119.3	H(15A)-C(15)-H(15C)	109.5
C(73)-C(93)-H(93A)	109.5	H(15B)-C(15)-H(15C)	109.5
C(73)-C(93)-H(93B)	109.5	O(15)-C(25)-C(15)	98.9(11)
H(93A)-C(93)-H(93B)	109.5	O(15)-C(25)-H(25A)	112.0
C(73)-C(93)-H(93C)	109.5	C(15)-C(25)-H(25A)	112.0
H(93A)-C(93)-H(93C)	109.5	O(15)-C(25)-H(25B)	112.0
H(93B)-C(93)-H(93C)	109.5	C(15)-C(25)-H(25B)	112.0
C(103)-C(123)-H(12D)	109.5	H(25A)-C(25)-H(25B)	109.7
C(103)-C(123)-H(12E)	109.5	C(25)-O(15)-C(35)	115.7(8)
H(12D)-C(123)-H(12E)	109.5	O(15)-C(35)-C(45)	99.4(10)
C(103)-C(123)-H(12F)	109.5	O(15)-C(35)-H(35A)	111.9
H(12D)-C(123)-H(12F)	109.5	C(45)-C(35)-H(35A)	111.9
H(12E)-C(123)-H(12F)	109.5	O(15)-C(35)-H(35B)	111.9
C(103)-C(113)-H(11G)	109.5	C(45)-C(35)-H(35B)	111.9
C(103)-C(113)-H(11H)	109.5	H(35A)-C(35)-H(35B)	109.6
H(11G)-C(113)-H(11H)	109.5	C(35)-C(45)-H(45A)	109.5
C(103)-C(113)-H(11I)	109.5	C(35)-C(45)-H(45B)	109.5
H(11G)-C(113)-H(11I)	109.5	H(45A)-C(45)-H(45B)	109.5
H(11H)-C(113)-H(11I)	109.5	C(35)-C(45)-H(45C)	109.5
C(72)-C(92)-H(92A)	109.5	H(45A)-C(45)-H(45C)	109.5
C(72)-C(92)-H(92B)	109.5	H(45B)-C(45)-H(45C)	109.5
H(92A)-C(92)-H(92B)	109.5		

Table S-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $L^{Me}Fe(CPh_3]$ (**1**). 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	20(1)	16(1)	26(1)	-1(1)	12(1)	0(1)
N21	21(1)	19(1)	31(1)	-1(1)	11(1)	-3(1)
N11	22(1)	19(1)	28(1)	-1(1)	13(1)	2(1)
C31	32(2)	13(2)	33(2)	2(1)	16(1)	0(1)
C114	32(2)	33(2)	30(2)	-7(2)	17(2)	-3(2)
C74	32(2)	16(2)	32(2)	-3(1)	14(2)	0(1)
C34	36(2)	26(2)	32(2)	0(2)	19(2)	1(2)
C94	31(2)	19(2)	29(2)	1(1)	14(1)	2(1)
C22	31(2)	22(2)	30(2)	-2(1)	10(1)	-3(2)
C144	32(2)	17(2)	30(2)	5(1)	16(2)	0(1)
C12	20(2)	15(2)	33(2)	0(1)	7(1)	-3(1)
C62	23(2)	15(2)	34(2)	-5(1)	10(1)	-8(1)
C13	22(2)	14(2)	49(2)	-2(1)	20(2)	0(1)
C63	33(2)	18(2)	51(2)	-3(2)	29(2)	0(1)
C23	22(2)	24(2)	54(2)	5(2)	15(2)	1(2)
C134	30(2)	19(2)	32(2)	2(1)	17(1)	1(1)
C24	33(2)	15(2)	26(2)	-3(1)	15(1)	3(1)
C41	25(2)	22(2)	32(2)	2(1)	13(1)	4(1)
C21	28(2)	18(2)	28(2)	-2(1)	14(1)	-4(1)
C14	26(2)	18(2)	29(2)	-3(1)	16(1)	0(1)
C42	24(2)	26(2)	48(2)	-1(2)	3(2)	0(2)
C154	31(2)	30(2)	32(2)	-2(2)	16(2)	-5(2)
C174	30(2)	43(2)	42(2)	4(2)	15(2)	-10(2)
C64	34(2)	22(2)	38(2)	-5(2)	8(2)	1(2)
C84	24(2)	17(2)	29(2)	-2(1)	14(1)	-4(1)
C32	33(2)	27(2)	35(2)	1(2)	5(2)	-4(2)
C112	50(2)	32(2)	48(2)	-7(2)	29(2)	-8(2)
C103	45(2)	28(2)	39(2)	-2(2)	28(2)	-5(2)
C54	50(2)	29(2)	31(2)	4(2)	12(2)	8(2)
C104	31(2)	20(2)	41(2)	-7(2)	17(2)	1(2)
C102	25(2)	33(2)	37(2)	-3(2)	14(2)	0(2)
C124	34(2)	28(2)	27(2)	2(1)	14(1)	-2(2)

C43	31(2)	35(2)	84(3)	-1(2)	37(2)	0(2)
C184	38(2)	27(2)	42(2)	3(2)	25(2)	2(2)
C51	30(2)	19(2)	66(2)	4(2)	25(2)	5(2)
C11	29(2)	21(2)	65(2)	3(2)	12(2)	-4(2)
C82	57(2)	38(2)	50(2)	6(2)	33(2)	1(2)
C72	39(2)	37(2)	30(2)	4(2)	17(2)	8(2)
C33	23(2)	30(2)	75(3)	7(2)	10(2)	3(2)
C194	31(2)	18(2)	35(2)	-1(1)	16(2)	-3(1)
C44	52(2)	30(2)	33(2)	7(2)	22(2)	3(2)
C164	41(2)	39(2)	36(2)	-4(2)	18(2)	-14(2)
C83	34(2)	68(3)	36(2)	17(2)	10(2)	5(2)
C122	131(4)	29(2)	45(2)	-3(2)	41(3)	-17(3)
C73	24(2)	43(2)	51(2)	16(2)	0(2)	-8(2)
C53	38(2)	27(2)	61(2)	-8(2)	36(2)	-2(2)
C52	23(2)	25(2)	44(2)	-7(2)	11(1)	-7(2)
C93	52(3)	47(3)	70(3)	17(2)	-9(2)	1(2)
C123	70(3)	51(3)	49(2)	5(2)	29(2)	-12(2)
C113	76(3)	46(3)	58(3)	-17(2)	27(2)	-3(2)
C92	83(3)	42(3)	89(3)	-20(2)	53(3)	-4(2)
C15	114(9)	340(20)	43(5)	30(9)	14(5)	-29(11)
C25	138(10)	51(6)	34(5)	-9(4)	21(5)	5(6)
O15	90(6)	185(11)	81(5)	-50(6)	29(5)	14(7)
C35	99(8)	53(6)	29(4)	-4(4)	6(4)	-31(6)
C45	114(9)	340(20)	43(5)	30(9)	14(5)	-29(11)

Table S-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $L^{Me}Fe(CPh_3]$ (**1**).

	x	y	z	U(eq)
H31	7150	6549	4110	30
H114	8189	-492	2124	36
H74	8573	522	4644	31
H34	6838	-1262	4838	35
H94	8158	-1473	3847	30
H134	7055	1711	2963	31
H42	10416	1953	5687	42
H154	6501	-1182	2995	36
H174	4540	-1275	3159	45
H64	9243	-319	5599	38
H32	9608	2537	6195	40
H11A	9712	1905	3605	60
H11B	9029	2118	3009	60
H11C	8985	1184	3568	60
H103	6673	2728	5185	41
H54	8720	-1622	6191	44
H104	8565	-1836	3006	35
H102	8463	3310	3585	37
H124	7450	1314	2115	34
H43	3934	2276	4187	55
H184	4962	-66	4089	39
H51A	5542	5876	3685	54
H51B	6081	6901	4134	54
H51C	5701	5791	4422	54
H11D	8862	5556	4861	58
H11E	8324	6766	4801	58
H11F	8548	6317	4211	58
H82A	7951	1646	5881	67
H82B	7864	2675	6391	67
H82C	8626	2077	6449	67
H72	7847	3763	5459	41

H33	4082	2884	3247	53
H194	6117	637	4443	32
H44	7514	-2095	5795	44
H164	5335	-1866	2630	45
H83A	5649	1752	2873	69
H83B	5364	2527	2224	69
H83C	4817	1848	2519	69
H12A	9176	5201	3792	98
H12B	9254	4492	3184	98
H12C	9862	4331	3839	98
H73	5702	4061	3047	51
H53	4880	2292	5091	45
H52	10136	2276	4622	36
H93A	4207	4100	2439	95
H93B	4784	4777	2180	95
H93C	4650	5353	2792	95
H12D	5816	1978	5922	82
H12E	6648	1733	6089	82
H12F	6107	948	5522	82
H11G	6406	4928	5341	88
H11H	6781	4213	5994	88
H11I	5945	4452	5767	88
H92A	9028	4526	6502	98
H92B	8231	4996	6391	98
H92C	8645	5478	5929	98
H15A	7482	3296	7873	252
H15B	6977	4067	7281	252
H15C	7094	4635	7966	252
H25A	8303	5125	8068	91
H25B	8176	4572	7369	91
H35A	8290	7218	7093	76
H35B	8381	7490	7818	76
H45A	7702	9250	7191	252
H45B	7229	8447	7525	252
H45C	7140	8178	6807	252

Table S-6. Torsion angles [°] for $L^{Me}Fe(CPh_3]$ (**1**).

N11-Fe1-N21-C41	15.0(2)	C44-C34-C24-C14	-179.2(3)
C14-Fe1-N21-C41	-164.9(2)	C13-N21-C41-C31	172.6(3)
N11-Fe1-N21-C13	-161.9(2)	Fe1-N21-C41-C31	-4.6(4)
C14-Fe1-N21-C13	18.1(3)	C13-N21-C41-C51	-4.9(4)
N21-Fe1-N11-C21	-15.3(2)	Fe1-N21-C41-C51	178.0(2)
C14-Fe1-N11-C21	164.6(2)	C21-C31-C41-N21	-13.2(5)
N21-Fe1-N11-C12	155.0(2)	C21-C31-C41-C51	164.4(3)
C14-Fe1-N11-C12	-25.0(3)	C12-N11-C21-C31	-165.5(3)
C32-C22-C12-C62	-1.2(4)	Fe1-N11-C21-C31	4.9(4)
C72-C22-C12-C62	177.6(3)	C12-N11-C21-C11	11.8(4)
C32-C22-C12-N11	177.2(3)	Fe1-N11-C21-C11	-177.8(2)
C72-C22-C12-N11	-4.1(4)	C41-C31-C21-N11	13.0(5)
C21-N11-C12-C62	-95.5(3)	C41-C31-C21-C11	-164.5(3)
Fe1-N11-C12-C62	93.6(3)	C154-C144-C14-C24	-115.2(3)
C21-N11-C12-C22	86.1(3)	C194-C144-C14-C24	65.9(4)
Fe1-N11-C12-C22	-84.7(3)	C154-C144-C14-C84	12.7(4)
C22-C12-C62-C52	1.1(4)	C194-C144-C14-C84	-166.1(3)
N11-C12-C62-C52	-177.2(3)	C154-C144-C14-Fe1	129.4(3)
C22-C12-C62-C102	-177.5(3)	C194-C144-C14-Fe1	-49.5(3)
N11-C12-C62-C102	4.1(4)	C74-C24-C14-C144	172.3(3)
C41-N21-C13-C23	81.1(4)	C34-C24-C14-C144	-7.8(4)
Fe1-N21-C13-C23	-101.8(3)	C74-C24-C14-C84	46.6(4)
C41-N21-C13-C63	-99.4(3)	C34-C24-C14-C84	-133.5(3)
Fe1-N21-C13-C63	77.8(3)	C74-C24-C14-Fe1	-70.1(3)
C23-C13-C63-C53	-1.4(5)	C34-C24-C14-Fe1	109.8(3)
N21-C13-C63-C53	179.0(3)	N11-Fe1-C14-C144	-175.31(16)
C23-C13-C63-C103	178.1(3)	N21-Fe1-C14-C144	4.6(3)
N21-C13-C63-C103	-1.4(4)	N11-Fe1-C14-C24	63.3(2)
C63-C13-C23-C33	1.3(5)	N21-Fe1-C14-C24	-116.8(2)
N21-C13-C23-C33	-179.2(3)	N11-Fe1-C14-C84	-57.5(2)
C63-C13-C23-C73	-175.2(3)	N21-Fe1-C14-C84	122.4(2)
N21-C13-C23-C73	4.3(5)	C194-C144-C154-C164	1.1(5)
C64-C74-C24-C34	-0.6(4)	C14-C144-C154-C164	-177.8(3)
C64-C74-C24-C14	179.3(3)	C24-C74-C64-C54	0.0(5)
C44-C34-C24-C74	0.7(4)	C124-C134-C84-C94	1.3(4)

C124-C134-C84-C14	-171.3(3)	C24-C34-C44-C54	-0.1(5)
C104-C94-C84-C134	-0.7(4)	C144-C154-C164-C174	0.0(5)
C104-C94-C84-C14	171.7(3)	C184-C174-C164-C154	-1.5(5)
C144-C14-C84-C134	72.2(3)	C13-C23-C73-C83	100.0(4)
C24-C14-C84-C134	-159.7(3)	C33-C23-C73-C83	-76.5(4)
Fe1-C14-C84-C134	-44.9(3)	C13-C23-C73-C93	-135.1(3)
C144-C14-C84-C94	-99.9(3)	C33-C23-C73-C93	48.5(5)
C24-C14-C84-C94	28.1(4)	C33-C43-C53-C63	0.1(6)
Fe1-C14-C84-C94	143.0(3)	C13-C63-C53-C43	0.7(5)
C52-C42-C32-C22	1.4(5)	C103-C63-C53-C43	-178.9(3)
C12-C22-C32-C42	-0.1(5)	C32-C42-C52-C62	-1.5(5)
C72-C22-C32-C42	-178.9(3)	C12-C62-C52-C42	0.3(5)
C53-C63-C103-C113	-93.3(4)	C102-C62-C52-C42	178.9(3)
C13-C63-C103-C113	87.2(4)	C15-C25-O15-C35	168.9(9)
C53-C63-C103-C123	33.9(4)	C25-O15-C35-C45	-171.1(9)
C13-C63-C103-C123	-145.7(3)		
C74-C64-C54-C44	0.6(5)		
C124-C114-C104-C94	2.0(5)		
C84-C94-C104-C114	-1.0(5)		
C52-C62-C102-C112	47.1(4)		
C12-C62-C102-C112	-134.3(3)		
C52-C62-C102-C122	-75.4(4)		
C12-C62-C102-C122	103.2(4)		
C104-C114-C124-C134	-1.4(5)		
C84-C134-C124-C114	-0.3(5)		
C164-C174-C184-C194	2.0(5)		
C32-C22-C72-C82	-55.9(4)		
C12-C22-C72-C82	125.4(3)		
C32-C22-C72-C92	67.8(4)		
C12-C22-C72-C92	-110.9(4)		
C53-C43-C33-C23	-0.2(6)		
C13-C23-C33-C43	-0.5(5)		
C73-C23-C33-C43	176.1(3)		
C174-C184-C194-C144	-1.0(5)		
C154-C144-C194-C184	-0.6(5)		
C14-C144-C194-C184	178.4(3)		
C64-C54-C44-C34	-0.5(5)		

[L^{Me}Fe(Ph_2CO] (2)

A crystal (0.28 x 0.12 x 0.05 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD platform diffractometer for a data collection at 100.0(5) K.[13] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 90 seconds and a detector distance of 4.00 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with 0.50º steps in ω at three different ϕ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.[14] Final cell constants were calculated from the xyz centroids of 2904 strong reflections from the actual data collection after integration.[15] See Table S-7 for additional crystal and refinement information.

The structure was solved using SIR2011[16] and refined using SHELXL-2013.[17] The space group *C*2/*c* was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0655$ (F^2, $I > 2\sigma(I)$) and $wR^2 = 0.1579$ (F^2, all data).

The asymmetric unit contains one iron molecule in a general position and one cocrystallized *n*-hexane solvent molecule in a crystallographic inversion center. The unique portion of the latter is modeled as disordered over two general positions (71:29).

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

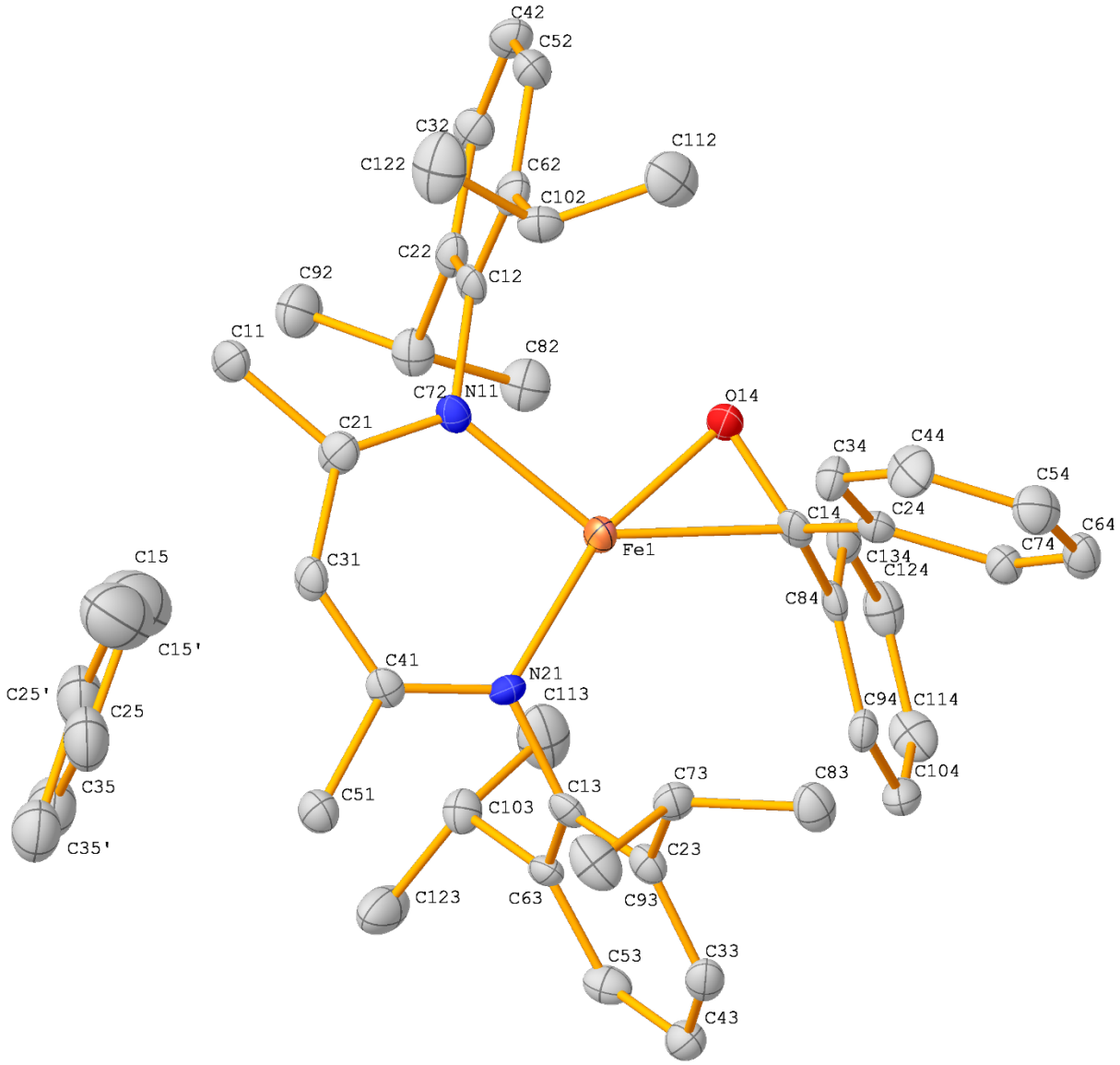

Figure S-25: The complete numbering scheme of $L^{Me}Fe(Ph_2CO)$ (**2**) with 50% thermal ellipsoid probability levels. The hydrogen atoms are omitted for clarity.

Table S-7. Crystal data and structure refinement for $L^{Me}Fe(Ph_2CO)$ (**2**).

Identification code	holkcm09	
CSD Deposition Number	1944809	
Empirical formula	C45 H58 Fe N2 O	
Formula weight	698.78	
Temperature	100.0(5) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 39.564(5) Å	α = 90°
	b = 11.3678(13) Å	β = 107.263(2)°
	c = 17.931(2) Å	γ = 90°
Volume	7701.2(16) Å^3	
Z	8	
Density (calculated)	1.205 g/cm^3	
Absorption coefficient	0.428 mm^{-1}	
F(000)	3008	
Crystal color, morphology	orange, plate	
Crystal size	0.28 x 0.12 x 0.05 mm^3	
Theta range for data collection	1.078 to 25.086°	
Index ranges	$-46 \le h \le 46$, $-13 \le k \le 12$, $-21 \le l \le 21$	
Reflections collected	29328	
Independent reflections	6852 [*R*(int) = 0.1658]	
Observed reflections	3906	
Completeness to theta = 25.030°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7452 and 0.5466	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6852 / 4 / 464	
Goodness-of-fit on F^2	1.026	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0655, *wR*2 = 0.1235	
R indices (all data)	*R*1 = 0.1381, *wR*2 = 0.1579	
Largest diff. peak and hole	0.426 and -0.450 e.Å^{-3}	

Table S-8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	3564(1)	1298(1)	1246(1)	17(1)
O14	3490(1)	888(3)	2175(2)	21(1)
N11	3400(1)	2971(3)	1181(2)	16(1)
N21	3714(1)	1284(3)	307(2)	16(1)
C11	3286(1)	4903(4)	562(3)	25(1)
C21	3393(1)	3644(4)	567(2)	22(1)
C31	3496(1)	3245(4)	-72(2)	20(1)
C41	3652(1)	2194(4)	-188(2)	17(1)
C51	3773(1)	2128(4)	-909(3)	25(1)
C12	3311(1)	3477(4)	1837(2)	18(1)
C22	3581(1)	4010(4)	2435(3)	21(1)
C32	3488(1)	4455(4)	3074(2)	22(1)
C42	3151(1)	4397(4)	3116(3)	25(1)
C52	2890(1)	3852(4)	2532(3)	25(1)
C62	2967(1)	3382(4)	1883(3)	22(1)
C72	3961(1)	4079(4)	2424(3)	23(1)
C82	4191(1)	3212(4)	3012(3)	30(1)
C92	4112(1)	5318(4)	2571(3)	33(1)
C102	2675(1)	2755(4)	1263(3)	22(1)
C112	2487(1)	1836(4)	1611(3)	33(1)
C122	2403(2)	3635(5)	777(3)	42(2)
C13	3930(1)	328(4)	186(2)	18(1)
C23	3769(1)	-729(4)	-158(3)	20(1)
C33	3988(1)	-1633(4)	-257(2)	22(1)
C43	4353(1)	-1521(4)	-14(3)	23(1)
C53	4504(1)	-487(4)	331(3)	22(1)
C63	4298(1)	454(4)	429(2)	18(1)
C73	3374(1)	-901(4)	-422(3)	20(1)
C83	3270(1)	-2114(4)	-188(3)	26(1)
C93	3224(1)	-753(5)	-1304(3)	33(1)
C103	4475(1)	1576(4)	826(3)	22(1)
C113	4576(2)	1439(5)	1706(3)	39(2)

C123	4799(1)	1915(4)	577(3)	36(1)
C14	3579(1)	-172(4)	1939(2)	19(1)
C24	3285(1)	-1033(4)	1682(2)	18(1)
C34	2950(1)	-700(4)	1218(3)	23(1)
C44	2673(1)	-1490(4)	1012(3)	30(1)
C54	2725(1)	-2638(4)	1286(3)	28(1)
C64	3052(1)	-2980(4)	1756(3)	24(1)
C74	3330(1)	-2199(4)	1956(3)	21(1)
C84	3944(1)	-591(4)	2296(2)	18(1)
C94	4103(1)	-1398(4)	1924(2)	19(1)
C104	4441(1)	-1786(4)	2274(3)	25(1)
C114	4630(1)	-1388(5)	3008(3)	28(1)
C124	4479(1)	-580(4)	3381(3)	26(1)
C134	4140(1)	-168(4)	3038(3)	22(1)
C15	4385(3)	5200(20)	816(9)	65(5)
C25	4527(2)	4944(7)	123(5)	44(2)
C35	4925(2)	5157(8)	328(4)	41(2)
C15'	4310(8)	5210(70)	550(30)	65(5)
C25'	4711(6)	5369(17)	676(11)	44(2)
C35'	4803(2)	5050(20)	-78(11)	41(2)

Table S-9. Bond lengths [Å] and angles [°] for **2**.

Fe(1)-O(14)	1.836(3)	C(82)-H(82B)	0.9800
Fe(1)-N(21)	1.945(4)	C(82)-H(82C)	0.9800
Fe(1)-N(11)	2.001(4)	C(92)-H(92A)	0.9800
Fe(1)-C(14)	2.073(4)	C(92)-H(92B)	0.9800
O(14)-C(14)	1.358(5)	C(92)-H(92C)	0.9800
N(11)-C(21)	1.335(5)	C(102)-C(112)	1.520(7)
N(11)-C(12)	1.443(5)	C(102)-C(122)	1.535(7)
N(21)-C(41)	1.337(5)	C(102)-H(10A)	1.0000
N(21)-C(13)	1.440(5)	C(112)-H(11D)	0.9800
C(11)-C(21)	1.492(6)	C(112)-H(11E)	0.9800
C(11)-H(11A)	0.9800	C(112)-H(11F)	0.9800
C(11)-H(11B)	0.9800	C(122)-H(12A)	0.9800
C(11)-H(11C)	0.9800	C(122)-H(12B)	0.9800
C(21)-C(31)	1.400(6)	C(122)-H(12C)	0.9800
C(31)-C(41)	1.390(6)	C(13)-C(63)	1.399(7)
C(31)-H(31A)	0.9500	C(13)-C(23)	1.413(6)
C(41)-C(51)	1.507(6)	C(23)-C(33)	1.389(6)
C(51)-H(51A)	0.9800	C(23)-C(73)	1.506(6)
C(51)-H(51B)	0.9800	C(33)-C(43)	1.385(7)
C(51)-H(51C)	0.9800	C(33)-H(33A)	0.9500
C(12)-C(62)	1.393(7)	C(43)-C(53)	1.380(6)
C(12)-C(22)	1.407(6)	C(43)-H(43A)	0.9500
C(22)-C(32)	1.398(6)	C(53)-C(63)	1.386(6)
C(22)-C(72)	1.511(7)	C(53)-H(53A)	0.9500
C(32)-C(42)	1.361(7)	C(63)-C(103)	1.525(6)
C(32)-H(32A)	0.9500	C(73)-C(93)	1.524(6)
C(42)-C(52)	1.380(6)	C(73)-C(83)	1.533(6)
C(42)-H(42A)	0.9500	C(73)-H(73A)	1.0000
C(52)-C(62)	1.395(6)	C(83)-H(83A)	0.9800
C(52)-H(52A)	0.9500	C(83)-H(83B)	0.9800
C(62)-C(102)	1.523(6)	C(83)-H(83C)	0.9800
C(72)-C(92)	1.523(6)	C(93)-H(93A)	0.9800
C(72)-C(82)	1.530(6)	C(93)-H(93B)	0.9800
C(72)-H(72A)	1.0000	C(93)-H(93C)	0.9800
C(82)-H(82A)	0.9800	C(103)-C(113)	1.517(6)

C(103)-C(123)	1.527(7)	C(25)-H(25A)	0.9900
C(103)-H(10B)	1.0000	C(25)-H(25B)	0.9900
C(113)-H(11G)	0.9800	C(35)-C(35)#1	1.507(13)
C(113)-H(11H)	0.9800	C(35)-H(35A)	0.9900
C(113)-H(11I)	0.9800	C(35)-H(35B)	0.9900
C(123)-H(12D)	0.9800	C(15')-C(25')	1.55(2)
C(123)-H(12E)	0.9800	C(15')-H(15D)	0.9800
C(123)-H(12F)	0.9800	C(15')-H(15E)	0.9800
C(14)-C(84)	1.474(7)	C(15')-H(15F)	0.9800
C(14)-C(24)	1.483(6)	C(25')-C(35')	1.542(17)
C(24)-C(34)	1.392(6)	C(25')-H(25C)	0.9900
C(24)-C(74)	1.407(6)	C(25')-H(25D)	0.9900
C(34)-C(44)	1.379(7)	C(35')-C(35')#1	1.504(15)
C(34)-H(34A)	0.9500	C(35')-H(35C)	0.9900
C(44)-C(54)	1.388(7)	C(35')-H(35D)	0.9900
C(44)-H(44A)	0.9500	O(14)-Fe(1)-N(21)	162.96(15)
C(54)-C(64)	1.375(7)	O(14)-Fe(1)-N(11)	99.05(14)
C(54)-H(54A)	0.9500	N(21)-Fe(1)-N(11)	97.73(15)
C(64)-C(74)	1.376(6)	O(14)-Fe(1)-C(14)	40.10(15)
C(64)-H(64A)	0.9500	N(21)-Fe(1)-C(14)	123.42(17)
C(74)-H(74A)	0.9500	N(11)-Fe(1)-C(14)	138.75(16)
C(84)-C(94)	1.389(6)	C(14)-O(14)-Fe(1)	79.4(2)
C(84)-C(134)	1.412(6)	C(21)-N(11)-C(12)	119.5(4)
C(94)-C(104)	1.373(6)	C(21)-N(11)-Fe(1)	121.3(3)
C(94)-H(94A)	0.9500	C(12)-N(11)-Fe(1)	119.0(3)
C(104)-C(114)	1.383(6)	C(41)-N(21)-C(13)	118.9(4)
C(104)-H(10C)	0.9500	C(41)-N(21)-Fe(1)	121.8(3)
C(114)-C(124)	1.374(7)	C(13)-N(21)-Fe(1)	119.0(3)
C(114)-H(11J)	0.9500	C(21)-C(11)-H(11A)	109.5
C(124)-C(134)	1.379(7)	C(21)-C(11)-H(11B)	109.5
C(124)-H(12G)	0.9500	H(11A)-C(11)-H(11B)	109.5
C(134)-H(13A)	0.9500	C(21)-C(11)-H(11C)	109.5
C(15)-C(25)	1.536(13)	H(11A)-C(11)-H(11C)	109.5
C(15)-H(15A)	0.9800	H(11B)-C(11)-H(11C)	109.5
C(15)-H(15B)	0.9800	N(11)-C(21)-C(31)	123.3(4)
C(15)-H(15C)	0.9800	N(11)-C(21)-C(11)	119.4(4)
C(25)-C(35)	1.527(10)	C(31)-C(21)-C(11)	117.2(4)

C(41)-C(31)-C(21)	130.7(4)	C(72)-C(82)-H(82B)	109.5
C(41)-C(31)-H(31A)	114.7	H(82A)-C(82)-H(82B)	109.5
C(21)-C(31)-H(31A)	114.7	C(72)-C(82)-H(82C)	109.5
N(21)-C(41)-C(31)	124.5(4)	H(82A)-C(82)-H(82C)	109.5
N(21)-C(41)-C(51)	119.3(4)	H(82B)-C(82)-H(82C)	109.5
C(31)-C(41)-C(51)	116.1(4)	C(72)-C(92)-H(92A)	109.5
C(41)-C(51)-H(51A)	109.5	C(72)-C(92)-H(92B)	109.5
C(41)-C(51)-H(51B)	109.5	H(92A)-C(92)-H(92B)	109.5
H(51A)-C(51)-H(51B)	109.5	C(72)-C(92)-H(92C)	109.5
C(41)-C(51)-H(51C)	109.5	H(92A)-C(92)-H(92C)	109.5
H(51A)-C(51)-H(51C)	109.5	H(92B)-C(92)-H(92C)	109.5
H(51B)-C(51)-H(51C)	109.5	C(112)-C(102)-C(62)	112.4(4)
C(62)-C(12)-C(22)	121.6(4)	C(112)-C(102)-C(122)	109.6(4)
C(62)-C(12)-N(11)	119.7(4)	C(62)-C(102)-C(122)	111.2(4)
C(22)-C(12)-N(11)	118.7(4)	C(112)-C(102)-H(10A)	107.9
C(32)-C(22)-C(12)	117.1(5)	C(62)-C(102)-H(10A)	107.9
C(32)-C(22)-C(72)	119.8(4)	C(122)-C(102)-H(10A)	107.9
C(12)-C(22)-C(72)	123.0(4)	C(102)-C(112)-H(11D)	109.5
C(42)-C(32)-C(22)	122.0(4)	C(102)-C(112)-H(11E)	109.5
C(42)-C(32)-H(32A)	119.0	H(11D)-C(112)-H(11E)	109.5
C(22)-C(32)-H(32A)	119.0	C(102)-C(112)-H(11F)	109.5
C(32)-C(42)-C(52)	120.3(4)	H(11D)-C(112)-H(11F)	109.5
C(32)-C(42)-H(42A)	119.8	H(11E)-C(112)-H(11F)	109.5
C(52)-C(42)-H(42A)	119.8	C(102)-C(122)-H(12A)	109.5
C(42)-C(52)-C(62)	120.4(5)	C(102)-C(122)-H(12B)	109.5
C(42)-C(52)-H(52A)	119.8	H(12A)-C(122)-H(12B)	109.5
C(62)-C(52)-H(52A)	119.8	C(102)-C(122)-H(12C)	109.5
C(12)-C(62)-C(52)	118.6(4)	H(12A)-C(122)-H(12C)	109.5
C(12)-C(62)-C(102)	122.5(4)	H(12B)-C(122)-H(12C)	109.5
C(52)-C(62)-C(102)	118.8(4)	C(63)-C(13)-C(23)	121.1(4)
C(22)-C(72)-C(92)	112.8(4)	C(63)-C(13)-N(21)	119.1(4)
C(22)-C(72)-C(82)	110.3(4)	C(23)-C(13)-N(21)	119.7(4)
C(92)-C(72)-C(82)	110.7(4)	C(33)-C(23)-C(13)	117.8(4)
C(22)-C(72)-H(72A)	107.6	C(33)-C(23)-C(73)	119.5(4)
C(92)-C(72)-H(72A)	107.6	C(13)-C(23)-C(73)	122.7(4)
C(82)-C(72)-H(72A)	107.6	C(43)-C(33)-C(23)	121.6(4)
C(72)-C(82)-H(82A)	109.5	C(43)-C(33)-H(33A)	119.2

C(23)-C(33)-H(33A)	119.2	C(103)-C(113)-H(11I)	109.5
C(53)-C(43)-C(33)	119.5(4)	H(11G)-C(113)-H(11I)	109.5
C(53)-C(43)-H(43A)	120.3	H(11H)-C(113)-H(11I)	109.5
C(33)-C(43)-H(43A)	120.3	C(103)-C(123)-H(12D)	109.5
C(43)-C(53)-C(63)	121.5(5)	C(103)-C(123)-H(12E)	109.5
C(43)-C(53)-H(53A)	119.3	H(12D)-C(123)-H(12E)	109.5
C(63)-C(53)-H(53A)	119.3	C(103)-C(123)-H(12F)	109.5
C(53)-C(63)-C(13)	118.5(4)	H(12D)-C(123)-H(12F)	109.5
C(53)-C(63)-C(103)	120.0(4)	H(12E)-C(123)-H(12F)	109.5
C(13)-C(63)-C(103)	121.5(4)	O(14)-C(14)-C(84)	117.6(4)
C(23)-C(73)-C(93)	111.0(4)	O(14)-C(14)-C(24)	115.5(4)
C(23)-C(73)-C(83)	111.7(4)	C(84)-C(14)-C(24)	119.8(4)
C(93)-C(73)-C(83)	109.3(4)	O(14)-C(14)-Fe(1)	60.5(2)
C(23)-C(73)-H(73A)	108.2	C(84)-C(14)-Fe(1)	111.8(3)
C(93)-C(73)-H(73A)	108.2	C(24)-C(14)-Fe(1)	117.8(3)
C(83)-C(73)-H(73A)	108.2	C(34)-C(24)-C(74)	117.6(4)
C(73)-C(83)-H(83A)	109.5	C(34)-C(24)-C(14)	121.7(4)
C(73)-C(83)-H(83B)	109.5	C(74)-C(24)-C(14)	120.5(4)
H(83A)-C(83)-H(83B)	109.5	C(44)-C(34)-C(24)	121.6(4)
C(73)-C(83)-H(83C)	109.5	C(44)-C(34)-H(34A)	119.2
H(83A)-C(83)-H(83C)	109.5	C(24)-C(34)-H(34A)	119.2
H(83B)-C(83)-H(83C)	109.5	C(34)-C(44)-C(54)	119.7(5)
C(73)-C(93)-H(93A)	109.5	C(34)-C(44)-H(44A)	120.2
C(73)-C(93)-H(93B)	109.5	C(54)-C(44)-H(44A)	120.2
H(93A)-C(93)-H(93B)	109.5	C(64)-C(54)-C(44)	119.7(5)
C(73)-C(93)-H(93C)	109.5	C(64)-C(54)-H(54A)	120.1
H(93A)-C(93)-H(93C)	109.5	C(44)-C(54)-H(54A)	120.1
H(93B)-C(93)-H(93C)	109.5	C(54)-C(64)-C(74)	120.8(4)
C(113)-C(103)-C(63)	110.0(4)	C(54)-C(64)-H(64A)	119.6
C(113)-C(103)-C(123)	110.3(4)	C(74)-C(64)-H(64A)	119.6
C(63)-C(103)-C(123)	112.5(4)	C(64)-C(74)-C(24)	120.6(5)
C(113)-C(103)-H(10B)	108.0	C(64)-C(74)-H(74A)	119.7
C(63)-C(103)-H(10B)	108.0	C(24)-C(74)-H(74A)	119.7
C(123)-C(103)-H(10B)	108.0	C(94)-C(84)-C(134)	118.4(4)
C(103)-C(113)-H(11G)	109.5	C(94)-C(84)-C(14)	122.0(4)
C(103)-C(113)-H(11H)	109.5	C(134)-C(84)-C(14)	119.6(4)
H(11G)-C(113)-H(11H)	109.5	C(104)-C(94)-C(84)	120.8(4)

C(104)-C(94)-H(94A)	119.6
C(84)-C(94)-H(94A)	119.6
C(94)-C(104)-C(114)	120.6(5)
C(94)-C(104)-H(10C)	119.7
C(114)-C(104)-H(10C)	119.7
C(124)-C(114)-C(104)	119.4(5)
C(124)-C(114)-H(11J)	120.3
C(104)-C(114)-H(11J)	120.3
C(114)-C(124)-C(134)	121.1(5)
C(114)-C(124)-H(12G)	119.5
C(134)-C(124)-H(12G)	119.5
C(124)-C(134)-C(84)	119.7(5)
C(124)-C(134)-H(13A)	120.2
C(84)-C(134)-H(13A)	120.2
C(25)-C(15)-H(15A)	109.5
C(25)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(25)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(35)-C(25)-C(15)	112.1(8)
C(35)-C(25)-H(25A)	109.2
C(15)-C(25)-H(25A)	109.2
C(35)-C(25)-H(25B)	109.2
C(15)-C(25)-H(25B)	109.2
H(25A)-C(25)-H(25B)	107.9
C(35)#1-C(35)-C(25)	113.0(9)
C(35)#1-C(35)-H(35A)	109.0
C(25)-C(35)-H(35A)	109.0
C(35)#1-C(35)-H(35B)	109.0
C(25)-C(35)-H(35B)	109.0
H(35A)-C(35)-H(35B)	107.8
C(25')-C(15')-H(15D)	109.5
C(25')-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(25')-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5
H(15E)-C(15')-H(15F)	109.5
C(35')-C(25')-C(15')	109.9(19)
C(35')-C(25')-H(25C)	109.7
C(15')-C(25')-H(25C)	109.7
C(35')-C(25')-H(25D)	109.7
C(15')-C(25')-H(25D)	109.7
H(25C)-C(25')-H(25D)	108.2
C(35')#1-C(35')-C(25')	110.9(19)
C(35')#1-C(35')-H(35C)	109.5
C(25')-C(35')-H(35C)	109.5
C(35')#1-C(35')-H(35D)	109.5
C(25')-C(35')-H(35D)	109.5
H(35C)-C(35')-H(35D)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table S-10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **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	25(1)	15(1)	13(1)	1(1)	7(1)	1(1)
O14	33(2)	17(2)	15(2)	0(1)	11(2)	2(1)
N11	19(2)	17(2)	11(2)	0(2)	4(2)	-2(2)
N21	20(2)	14(2)	18(2)	-1(2)	8(2)	4(2)
C11	40(3)	22(3)	16(2)	5(2)	12(2)	7(2)
C21	30(3)	21(3)	14(2)	1(2)	4(2)	4(2)
C31	30(3)	17(3)	12(2)	3(2)	5(2)	0(2)
C41	20(3)	18(3)	11(2)	-3(2)	3(2)	-5(2)
C51	32(3)	22(3)	21(3)	2(2)	11(2)	1(2)
C12	30(3)	16(3)	10(2)	3(2)	8(2)	0(2)
C22	33(3)	14(3)	15(2)	2(2)	6(2)	0(2)
C32	30(3)	21(3)	13(2)	0(2)	5(2)	2(2)
C42	41(3)	20(3)	15(2)	-3(2)	10(2)	4(2)
C52	36(3)	20(3)	24(3)	2(2)	17(2)	1(2)
C62	30(3)	16(3)	19(2)	5(2)	6(2)	5(2)
C72	27(3)	23(3)	17(2)	-1(2)	3(2)	-3(2)
C82	29(3)	30(3)	28(3)	0(2)	5(3)	-1(2)
C92	39(3)	23(3)	39(3)	-2(2)	15(3)	-6(2)
C102	27(3)	23(3)	20(3)	-4(2)	10(2)	1(2)
C112	35(3)	31(3)	34(3)	-8(2)	10(3)	-12(3)
C122	47(4)	39(3)	31(3)	4(3)	-4(3)	-4(3)
C13	26(3)	22(3)	11(2)	3(2)	10(2)	2(2)
C23	24(3)	21(3)	15(2)	3(2)	8(2)	0(2)
C33	35(3)	17(3)	16(2)	-2(2)	9(2)	-1(2)
C43	28(3)	21(3)	21(2)	2(2)	10(2)	4(2)
C53	18(3)	30(3)	19(3)	-1(2)	6(2)	2(2)
C63	24(3)	18(3)	14(2)	3(2)	11(2)	5(2)
C73	26(3)	17(3)	19(2)	-4(2)	8(2)	-1(2)
C83	34(3)	23(3)	22(3)	-2(2)	9(2)	-7(2)
C93	29(3)	42(3)	27(3)	3(2)	8(3)	-6(3)
C103	23(3)	19(3)	24(3)	1(2)	7(2)	-2(2)
C113	51(4)	33(3)	29(3)	-6(2)	6(3)	-15(3)

C123	35(3)	23(3)	57(4)	-6(3)	23(3)	-3(3)
C14	34(3)	18(3)	9(2)	0(2)	10(2)	-2(2)
C24	24(3)	17(3)	15(2)	-1(2)	10(2)	1(2)
C34	29(3)	15(3)	24(3)	4(2)	9(2)	2(2)
C44	24(3)	32(3)	30(3)	11(2)	4(2)	11(2)
C54	27(3)	27(3)	31(3)	-2(2)	10(3)	-5(2)
C64	39(3)	19(3)	17(2)	1(2)	10(2)	-1(2)
C74	28(3)	18(3)	18(2)	1(2)	10(2)	1(2)
C84	27(3)	15(2)	12(2)	5(2)	7(2)	-3(2)
C94	27(3)	12(2)	19(2)	3(2)	8(2)	-1(2)
C104	27(3)	19(3)	33(3)	5(2)	18(3)	5(2)
C114	20(3)	36(3)	25(3)	6(2)	4(2)	1(2)
C124	29(3)	27(3)	20(3)	4(2)	3(2)	-7(2)
C134	28(3)	16(3)	22(3)	1(2)	10(2)	-4(2)
C15	78(9)	61(6)	69(13)	-12(11)	39(9)	-15(7)
C25	62(6)	31(5)	43(5)	9(3)	20(5)	-2(4)
C35	55(6)	31(4)	38(6)	5(5)	14(5)	0(4)
C15'	78(9)	61(6)	69(13)	-12(11)	39(9)	-15(7)
C25'	62(6)	31(5)	43(5)	9(3)	20(5)	-2(4)
C35'	55(6)	31(4)	38(6)	5(5)	14(5)	0(4)

Table S-11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [$L^{Me}Fe(Ph_2CO]$ (**2**).

	x	y	z	U(eq)
H11A	3064	4957	698	38
H11B	3251	5234	40	38
H11C	3471	5344	944	38
H31A	3450	3781	-497	24
H51A	3696	1382	-1179	37
H51B	4032	2177	-759	37
H51C	3671	2784	-1258	37
H32A	3666	4810	3491	26
H42A	3095	4733	3550	30
H52A	2657	3797	2573	30
H72A	3967	3835	1892	28
H82A	4099	2413	2884	45
H82B	4185	3417	3539	45
H82C	4435	3251	2989	45
H92A	3973	5847	2164	50
H92B	4359	5313	2561	50
H92C	4103	5591	3083	50
H10A	2786	2343	902	27
H11D	2661	1295	1939	50
H11E	2321	1394	1189	50
H11F	2357	2226	1929	50
H12A	2518	4145	484	64
H12B	2310	4115	1126	64
H12C	2209	3206	412	64
H33A	3885	-2346	-496	27
H43A	4498	-2152	-84	27
H53A	4755	-418	504	27
H73A	3265	-288	-165	25
H83A	3402	-2275	358	39
H83B	3325	-2717	-524	39
H83C	3015	-2126	-247	39

H93A	3262	58	-1447	49
H93B	2970	-924	-1465	49
H93C	3344	-1297	-1566	49
H10B	4299	2230	673	26
H11G	4362	1299	1863	59
H11H	4692	2158	1957	59
H11I	4737	771	1868	59
H12D	4734	1948	6	54
H12E	4986	1326	771	54
H12F	4885	2687	794	54
H34A	2911	89	1038	27
H44A	2448	-1249	685	36
H54A	2535	-3185	1149	34
H64A	3086	-3765	1945	29
H74A	3554	-2450	2282	25
H94A	3975	-1684	1421	23
H10C	4547	-2332	2009	29
H11J	4863	-1670	3252	33
H12G	4609	-301	3883	32
H13A	4040	398	3300	26
H15A	4513	4717	1264	98
H15B	4132	5009	670	98
H15C	4419	6033	955	98
H25A	4476	4115	-42	53
H25B	4404	5454	-322	53
H35A	4974	5998	462	49
H35B	5047	4686	794	49
H15D	4178	5541	42	98
H15E	4242	5609	965	98
H15F	4256	4366	556	98
H25C	4779	6195	821	53
H25D	4846	4856	1108	53
H35C	4689	4298	-286	49
H35D	4710	5668	-476	49

Table S-12. Torsion angles [°] for **2**.

N21-Fe1-O14-C14	-16.9(6)
N11-Fe1-O14-C14	173.1(3)
C12-N11-C21-C31	176.0(4)
Fe1-N11-C21-C31	0.5(6)
C12-N11-C21-C11	-1.5(6)
Fe1-N11-C21-C11	-177.0(3)
N11-C21-C31-C41	-7.4(8)
C11-C21-C31-C41	170.1(5)
C13-N21-C41-C31	-169.6(4)
Fe1-N21-C41-C31	3.4(6)
C13-N21-C41-C51	7.2(6)
Fe1-N21-C41-C51	-179.7(3)
C21-C31-C41-N21	5.3(8)
C21-C31-C41-C51	-171.7(5)
C21-N11-C12-C62	95.2(5)
Fe1-N11-C12-C62	-89.1(4)
C21-N11-C12-C22	-87.8(5)
Fe1-N11-C12-C22	87.9(4)
C62-C12-C22-C32	-0.9(6)
N11-C12-C22-C32	-177.9(4)
C62-C12-C22-C72	177.1(4)
N11-C12-C22-C72	0.1(6)
C12-C22-C32-C42	-0.9(7)
C72-C22-C32-C42	-179.0(4)
C22-C32-C42-C52	2.2(7)
C32-C42-C52-C62	-1.7(7)
C22-C12-C62-C52	1.4(7)
N11-C12-C62-C52	178.3(4)
C22-C12-C62-C102	-176.8(4)
N11-C12-C62-C102	0.1(6)
C42-C52-C62-C12	-0.1(7)
C42-C52-C62-C102	178.2(4)
C32-C22-C72-C92	-52.7(6)
C12-C22-C72-C92	129.3(5)
C32-C22-C72-C82	71.6(5)
C12-C22-C72-C82	-106.3(5)

C12-C62-C102-C112	127.9(5)
C52-C62-C102-C112	-50.3(6)
C12-C62-C102-C122	-108.8(5)
C52-C62-C102-C122	73.0(5)
C41-N21-C13-C63	79.4(5)
Fe1-N21-C13-C63	-93.8(4)
C41-N21-C13-C23	-102.0(5)
Fe1-N21-C13-C23	84.8(4)
C63-C13-C23-C33	-0.8(6)
N21-C13-C23-C33	-179.3(4)
C63-C13-C23-C73	179.6(4)
N21-C13-C23-C73	1.0(6)
C13-C23-C33-C43	1.2(7)
C73-C23-C33-C43	-179.2(4)
C23-C33-C43-C53	-0.3(7)
C33-C43-C53-C63	-1.1(7)
C43-C53-C63-C13	1.5(7)
C43-C53-C63-C103	178.9(4)
C23-C13-C63-C53	-0.5(6)
N21-C13-C63-C53	178.0(4)
C23-C13-C63-C103	-177.9(4)
N21-C13-C63-C103	0.7(6)
C33-C23-C73-C93	-78.5(5)
C13-C23-C73-C93	101.1(5)
C33-C23-C73-C83	43.7(6)
C13-C23-C73-C83	-136.6(4)
C53-C63-C103-C113	-82.9(6)
C13-C63-C103-C113	94.4(5)
C53-C63-C103-C123	40.5(6)
C13-C63-C103-C123	-142.2(4)
Fe1-O14-C14-C84	100.7(4)
Fe1-O14-C14-C24	-108.9(3)
O14-C14-C24-C34	42.2(6)
C84-C14-C24-C34	-168.1(4)
Fe1-C14-C24-C34	-26.4(6)
O14-C14-C24-C74	-132.6(4)
C84-C14-C24-C74	17.1(6)

Fe1-C14-C24-C74	158.8(3)
C74-C24-C34-C44	-1.8(7)
C14-C24-C34-C44	-176.8(4)
C24-C34-C44-C54	1.5(7)
C34-C44-C54-C64	-0.3(8)
C44-C54-C64-C74	-0.4(7)
C54-C64-C74-C24	0.0(7)
C34-C24-C74-C64	1.1(7)
C14-C24-C74-C64	176.1(4)
O14-C14-C84-C94	-155.9(4)
C24-C14-C84-C94	54.9(6)
Fe1-C14-C84-C94	-88.8(4)
O14-C14-C84-C134	24.1(6)
C24-C14-C84-C134	-125.0(4)
Fe1-C14-C84-C134	91.2(4)
C134-C84-C94-C104	0.9(7)
C14-C84-C94-C104	-179.1(4)
C84-C94-C104-C114	0.5(7)
C94-C104-C114-C124	-1.2(7)
C104-C114-C124-C134	0.5(7)
C114-C124-C134-C84	0.8(7)
C94-C84-C134-C124	-1.5(6)
C14-C84-C134-C124	178.5(4)
C15-C25-C35-C35#1	176.5(13)
C15'-C25'-C35'-C35'#1	-168(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

[$L^{Me}FeCH_3$][K(18-crown-6)] (4). Low-temperature diffraction data (ω-scans) were collected on a Rigaku R-AXIS RAPID diffractometer coupled to an R-AXIS RAPID imaging plate detector with Mo Kα radiation (λ = 0.71073 Å) for the structure of **4**. The diffraction images were processed and scaled using the Rigaku CrystalClear software (CrystalClear and CrystalStructure; Rigaku/MSC: The Woodlands, TX, 2005). The structure was solved with SHELXT and was refined against F2 on all data by full-matrix least squares with SHELXL (Sheldrick, G. M. Acta Cryst. 2008, A64, 112–122). All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups). The N-aryl groups of the diketiminate supporting ligand are disordered. The site occupancies of the disordered groups were freely refined and converged to benearly equal occupiancies. Chemically identical 1,2 C-C distances were restrained to be similar. An attempt was made to model the 18-crown-6 as disordered, but a stable model was not obtained. Some 1,3 C-C distances of the crown ether converged at chemically unreasonable distances, and were subsequently restrained to 2.4(2)Å. Many of the geometrically generated solvent atoms caused close contact with those generated by symmetry. The program SQUEEZE was used to compensate for the contribution of disordered solvents contained in voids within the crystal lattice from the diffraction intensities. This procedure was applied to the data file and the submitted model is based on the solvent-removed data. Based on the total electron density found in the voids (198 e/$Å^3$), it is likely that ~4 toluene molecules are present in the unit cell. See "_platon_squeeze_details" in this .cif for more information. The full numbering scheme of compound **4** can be found in the full details of the X-ray structure determination (CIF), which is included as Supporting Information.

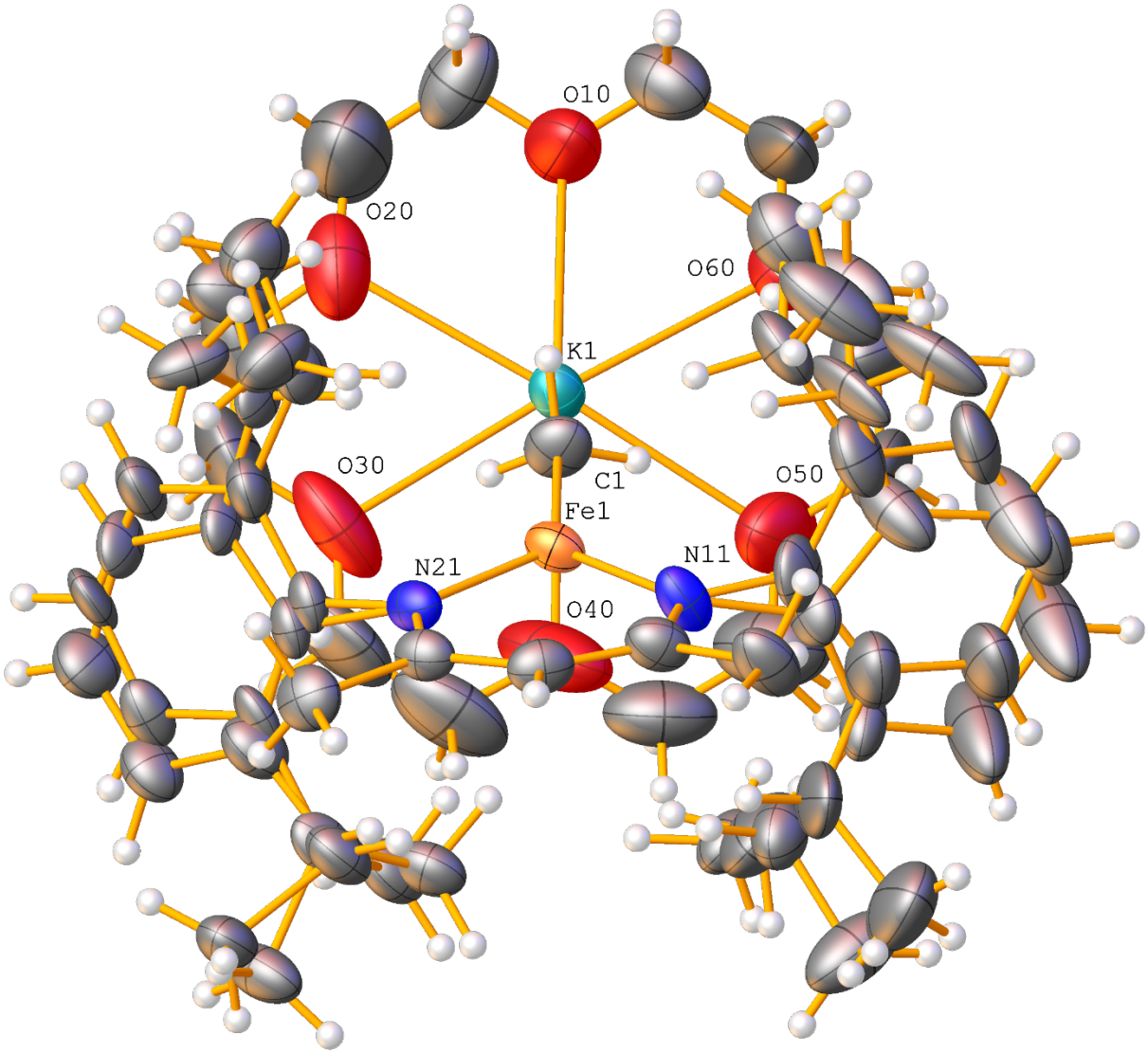

Figure S-26: A partial numbering scheme of **4** with 50% thermal ellipsoid probability levels. The hydrogen atoms are shown as circles for clarity.

Table S-13. Crystal data and structure refinement for **4**.

Identification code	spider-16053	
CSD Deposition Number	1944810	
Empirical formula	$C_{42}H_{68}FeKN_2O_6$	
Formula weight	791.93	
Temperature	93(2) K	
Wavelength	0.71075 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 16.6896(5) Å	α= 90°.
	b = 24.5737(17) Å	β= 90°.
	c = 12.2392(4) Å	γ = 90°.
Volume	5019.6(4) Å^3	
Z	4	
Density (calculated)	1.048 g/cm^3	
Absorption coefficient	0.422 mm^{-1}	
F(000)	1708	
Crystal size	0.250 x 0.150 x 0.100 mm^3	
Crystal color and habit	Red block	
Diffractometer	Rigaku R-AXIS RAPID imaging plate	
Theta range for data collection	2.992 to 25.028°.	
Index ranges	-19<=h<=19, -29<=k<=29, -14<=l<=14	
Reflections collected	77966	
Independent reflections	8866 [R(int) = 0.1154]	
Observed reflections (I > 2sigma(I))	7995	
Completeness to theta = 25.028°	99.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.663	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	8866 / 950 / 700	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0868, wR2 = 0.2196	
R indices (all data)	R1 = 0.0933, wR2 = 0.2252	
Absolute structure parameter	0.08(5)	
Largest diff. peak and hole	0.858 and -0.371 e Å^{-3}	

Table S-14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4819(1)	6406(1)	3342(1)	37(1)
C(1)	5543(5)	7051(3)	3062(8)	50(2)
N(11)	4863(4)	5832(3)	4395(5)	43(2)
N(21)	3803(4)	6229(3)	2673(6)	38(2)
C(11)	4251(6)	5116(4)	5577(8)	59(3)
C(21)	4212(5)	5497(3)	4590(7)	44(2)
C(31)	3515(5)	5510(3)	3993(7)	42(2)
C(41)	3318(4)	5832(3)	3059(7)	38(2)
C(51)	2508(5)	5718(4)	2505(8)	49(2)
C(1A)	5669(13)	5663(11)	4880(20)	43(6)
C(2A)	6185(13)	5268(12)	4432(18)	54(5)
C(3A)	6964(15)	5170(19)	4790(20)	115(13)
C(4A)	7224(18)	5461(19)	5720(20)	120(12)
C(5A)	6734(14)	5840(20)	6240(30)	95(12)
C(6A)	5977(13)	5933(13)	5808(19)	69(6)
C(7A)	5970(15)	5002(8)	3359(19)	57(5)
C(8A)	6399(16)	5284(11)	2391(19)	56(6)
C(9A)	6210(20)	4404(10)	3410(30)	93(9)
C(10A)	5452(14)	6365(10)	6331(17)	69(6)
C(11A)	5852(15)	6929(12)	6320(20)	80(7)
C(12A)	5249(19)	6173(13)	7503(17)	88(8)
C(1B)	5482(15)	5811(9)	5052(17)	56(5)
C(2B)	6052(14)	5407(10)	4870(20)	73(6)
C(3B)	6810(14)	5358(9)	5340(20)	81(7)
C(4B)	6959(16)	5716(9)	6200(20)	75(7)
C(5B)	6411(11)	6130(8)	6463(15)	65(5)
C(6B)	5680(12)	6167(9)	5923(15)	59(5)
C(7B)	5913(16)	5003(9)	3950(20)	97(8)
C(8B)	6290(30)	5174(14)	2850(30)	132(13)
C(9B)	6110(20)	4402(10)	4180(30)	128(11)
C(10B)	5062(12)	6603(8)	6194(13)	60(4)

C(11B)	5446(15)	7183(9)	6280(20)	73(6)
C(12B)	4631(18)	6482(12)	7278(15)	95(8)
C(1C)	3660(20)	6510(8)	1759(16)	34(3)
C(2C)	3463(14)	7066(7)	1789(16)	47(4)
C(3C)	3350(13)	7351(8)	815(16)	53(5)
C(4C)	3444(13)	7091(7)	-204(17)	51(5)
C(5C)	3576(13)	6522(8)	-223(15)	44(4)
C(6C)	3700(16)	6226(7)	751(15)	36(4)
C(7C)	3336(10)	7367(7)	2376(17)	41(4)
C(8C)	3626(19)	7968(8)	2240(20)	72(8)
C(9C)	2438(11)	7385(8)	2670(20)	56(6)
C(10C)	4001(12)	5637(8)	612(19)	40(5)
C(11C)	4927(12)	5541(14)	700(20)	51(6)
C(12C)	3702(15)	5187(12)	-200(30)	60(8)
C(1D)	3650(20)	6458(10)	1490(20)	34(3)
C(2D)	3459(15)	7011(9)	1376(15)	36(5)
C(3D)	3426(14)	7219(10)	311(18)	45(6)
C(4D)	3531(17)	6885(10)	-600(20)	62(6)
C(5D)	3672(18)	6319(10)	-500(19)	51(6)
C(6D)	3740(30)	6124(12)	560(20)	54(7)
C(7D)	3337(11)	7334(6)	2896(16)	55(4)
C(8D)	3393(16)	7962(7)	2840(20)	69(6)
C(9D)	2536(11)	7185(8)	3451(19)	67(5)
C(10D)	4003(18)	5541(11)	730(30)	54(7)
C(11D)	4879(19)	5630(20)	360(30)	59(8)
C(12D)	3450(20)	5328(12)	-200(30)	54(8)
K(1)	6893(1)	7755(1)	1957(1)	42(1)
O(10)	7033(7)	8761(4)	2847(10)	135(5)
O(20)	6032(6)	8600(5)	1058(8)	106(3)
O(30)	6041(7)	7580(5)	38(8)	119(3)
O(40)	6940(7)	6726(5)	851(10)	130(4)
O(50)	7989(8)	6930(4)	2549(8)	120(4)
O(60)	7950(5)	7928(3)	3667(6)	79(2)
C(10)	6527(7)	9150(5)	2540(12)	88(3)
C(20)	6147(16)	9069(7)	1503(18)	167(9)
C(30)	5720(11)	8516(8)	85(12)	131(6)

C(40)	5603(17)	7978(8)	-340(20)	195(12)
C(50)	5903(13)	7066(7)	-251(17)	155(8)
C(60)	6464(11)	6652(7)	23(14)	126(5)
C(70)	7542(10)	6399(6)	1100(12)	108(4)
C(80)	7896(12)	6451(7)	2144(15)	134(6)
C(90)	8335(12)	6989(6)	3531(13)	136(7)
C(100)	8375(14)	7507(6)	3906(14)	144(7)
C(110)	7963(17)	8423(7)	4140(20)	235(17)
C(120)	7420(7)	8840(5)	3783(10)	84(3)

Table S-15. Bond lengths [Å] and angles [°] for **4**.

Fe(1)-N(11)	1.912(6)
Fe(1)-N(21)	1.932(6)
Fe(1)-C(1)	2.024(8)
C(1)-K(1)	3.146(8)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
N(11)-C(1B)	1.31(2)
N(11)-C(21)	1.385(11)
N(11)-C(1A)	1.53(2)
N(21)-C(1C)	1.34(2)
N(21)-C(41)	1.352(10)
N(21)-C(1D)	1.58(3)
C(11)-C(21)	1.529(12)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(21)-C(31)	1.374(12)
C(31)-C(41)	1.429(12)
C(31)-H(31)	0.9500
C(41)-C(51)	1.539(11)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(1A)-C(2A)	1.409(18)
C(1A)-C(6A)	1.414(17)
C(2A)-C(3A)	1.393(18)
C(2A)-C(7A)	1.51(2)
C(3A)-C(4A)	1.407(19)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.394(19)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.391(19)
C(5A)-H(5A)	0.9500

C(6A)-C(10A)	1.52(2)
C(7A)-C(9A)	1.522(18)
C(7A)-C(8A)	1.548(19)
C(7A)-H(7A)	1.0000
C(8A)-H(8AA)	0.9800
C(8A)-H(8AB)	0.9800
C(8A)-H(8AC)	0.9800
C(9A)-H(9AA)	0.9800
C(9A)-H(9AB)	0.9800
C(9A)-H(9AC)	0.9800
C(10A)-C(11A)	1.537(19)
C(10A)-C(12A)	1.548(19)
C(10A)-H(10A)	1.0000
C(11A)-H(11D)	0.9800
C(11A)-H(11E)	0.9800
C(11A)-H(11F)	0.9800
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(1B)-C(2B)	1.392(18)
C(1B)-C(6B)	1.419(18)
C(2B)-C(3B)	1.396(17)
C(2B)-C(7B)	1.52(2)
C(3B)-C(4B)	1.393(18)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.404(18)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.390(17)
C(5B)-H(5B)	0.9500
C(6B)-C(10B)	1.52(2)
C(7B)-C(9B)	1.538(18)
C(7B)-C(8B)	1.55(2)
C(7B)-H(7B)	1.0000
C(8B)-H(8BA)	0.9800
C(8B)-H(8BB)	0.9800
C(8B)-H(8BC)	0.9800

C(9B)-H(9BA)	0.9800
C(9B)-H(9BB)	0.9800
C(9B)-H(9BC)	0.9800
C(10B)-C(12B)	1.538(17)
C(10B)-C(11B)	1.568(17)
C(10B)-H(10B)	1.0000
C(11B)-H(11G)	0.9800
C(11B)-H(11H)	0.9800
C(11B)-H(11I)	0.9800
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(1C)-C(2C)	1.405(16)
C(1C)-C(6C)	1.419(16)
C(2C)-C(3C)	1.395(16)
C(2C)-C(7D)	1.520(18)
C(3C)-C(4C)	1.410(17)
C(3C)-H(3C)	0.9500
C(4C)-C(5C)	1.416(17)
C(4C)-K(1)#1	3.383(17)
C(4C)-H(4C)	0.9500
C(5C)-C(6C)	1.412(15)
C(5C)-H(5C)	0.9500
C(6C)-C(10C)	1.541(17)
C(7C)-C(2D)	1.518(19)
C(7C)-C(9C)	1.542(18)
C(7C)-C(8C)	1.563(18)
C(7C)-H(7C)	1.0000
C(8C)-H(8CA)	0.9800
C(8C)-H(8CB)	0.9800
C(8C)-H(8CC)	0.9800
C(9C)-H(9CA)	0.9800
C(9C)-H(9CB)	0.9800
C(9C)-H(9CC)	0.9800
C(10C)-C(12C)	1.567(17)
C(10C)-C(11C)	1.568(17)

C(10C)-H(10C)	1.0000
C(11C)-H(11J)	0.9800
C(11C)-H(11K)	0.9800
C(11C)-H(11L)	0.9800
C(12C)-H(12G)	0.9800
C(12C)-H(12H)	0.9800
C(12C)-H(12I)	0.9800
C(1D)-C(2D)	1.400(17)
C(1D)-C(6D)	1.404(17)
C(2D)-C(3D)	1.401(17)
C(3D)-C(4D)	1.396(18)
C(3D)-H(3D)	0.9500
C(4D)-C(5D)	1.416(19)
C(4D)-K(1)#1	3.32(3)
C(4D)-H(4D)	0.9500
C(5D)-C(6D)	1.393(18)
C(5D)-H(5D)	0.9500
C(6D)-C(10D)	1.51(2)
C(7D)-C(9D)	1.542(18)
C(7D)-C(8D)	1.548(17)
C(7D)-H(7D)	1.0000
C(8D)-H(8DA)	0.9800
C(8D)-H(8DB)	0.9800
C(8D)-H(8DC)	0.9800
C(9D)-H(9DA)	0.9800
C(9D)-H(9DB)	0.9800
C(9D)-H(9DC)	0.9800
C(10D)-C(11D)	1.55(2)
C(10D)-C(12D)	1.557(19)
C(10D)-H(10D)	1.0000
C(11D)-H(11M)	0.9800
C(11D)-H(11N)	0.9800
C(11D)-H(11O)	0.9800
C(12D)-H(12J)	0.9800
C(12D)-H(12K)	0.9800
C(12D)-H(12L)	0.9800

K(1)-O(10)	2.712(9)
K(1)-O(20)	2.756(10)
K(1)-O(60)	2.770(7)
K(1)-O(30)	2.779(9)
K(1)-O(50)	2.824(10)
K(1)-O(40)	2.870(10)
O(10)-C(120)	1.330(13)
O(10)-C(10)	1.330(12)
O(20)-C(20)	1.287(15)
O(20)-C(30)	1.316(13)
O(30)-C(40)	1.306(16)
O(30)-C(50)	1.333(15)
O(40)-C(60)	1.300(14)
O(40)-C(70)	1.322(14)
O(50)-C(80)	1.287(14)
O(50)-C(90)	1.341(14)
O(60)-C(100)	1.287(13)
O(60)-C(110)	1.347(13)
C(10)-C(20)	1.432(17)
C(10)-H(10E)	0.9900
C(10)-H(10F)	0.9900
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(30)-C(40)	1.436(18)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(50)-C(60)	1.424(18)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(70)-C(80)	1.415(17)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900

C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(90)-C(100)	1.355(16)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(100)-H(10G)	0.9900
C(100)-H(10H)	0.9900
C(110)-C(120)	1.437(16)
C(110)-H(11P)	0.9900
C(110)-H(11Q)	0.9900
C(120)-H(12M)	0.9900
C(120)-H(12N)	0.9900

N(11)-Fe(1)-N(21)	98.9(3)
N(11)-Fe(1)-C(1)	132.0(3)
N(21)-Fe(1)-C(1)	128.9(3)
Fe(1)-C(1)-K(1)	158.7(4)
Fe(1)-C(1)-H(1A)	109.5
K(1)-C(1)-H(1A)	58.0
Fe(1)-C(1)-H(1B)	109.5
K(1)-C(1)-H(1B)	64.6
H(1A)-C(1)-H(1B)	109.5
Fe(1)-C(1)-H(1C)	109.5
K(1)-C(1)-H(1C)	91.6
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(1B)-N(11)-C(21)	119.3(12)
C(21)-N(11)-C(1A)	117.5(13)
C(1B)-N(11)-Fe(1)	118.3(11)
C(21)-N(11)-Fe(1)	121.6(6)
C(1A)-N(11)-Fe(1)	119.8(12)
C(1C)-N(21)-C(41)	123.7(15)
C(41)-N(21)-C(1D)	118.6(15)
C(1C)-N(21)-Fe(1)	113.6(14)
C(41)-N(21)-Fe(1)	122.6(5)
C(1D)-N(21)-Fe(1)	117.1(15)

C(21)-C(11)-H(11A)	109.5
C(21)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(21)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(31)-C(21)-N(11)	124.0(8)
C(31)-C(21)-C(11)	118.1(8)
N(11)-C(21)-C(11)	117.8(8)
C(21)-C(31)-C(41)	129.3(7)
C(21)-C(31)-H(31)	115.4
C(41)-C(31)-H(31)	115.4
N(21)-C(41)-C(31)	122.8(7)
N(21)-C(41)-C(51)	120.2(7)
C(31)-C(41)-C(51)	117.0(7)
C(41)-C(51)-H(51A)	109.5
C(41)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(41)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(2A)-C(1A)-C(6A)	114(2)
C(2A)-C(1A)-N(11)	125.1(15)
C(6A)-C(1A)-N(11)	120.3(17)
C(3A)-C(2A)-C(1A)	124(2)
C(3A)-C(2A)-C(7A)	115(2)
C(1A)-C(2A)-C(7A)	119.4(16)
C(2A)-C(3A)-C(4A)	117(3)
C(2A)-C(3A)-H(3A)	121.5
C(4A)-C(3A)-H(3A)	121.5
C(5A)-C(4A)-C(3A)	122(3)
C(5A)-C(4A)-H(4A)	119.0
C(3A)-C(4A)-H(4A)	119.0
C(6A)-C(5A)-C(4A)	118(3)
C(6A)-C(5A)-H(5A)	121.1
C(4A)-C(5A)-H(5A)	121.1

C(5A)-C(6A)-C(1A)	124(2)
C(5A)-C(6A)-C(10A)	119(2)
C(1A)-C(6A)-C(10A)	117.3(18)
C(2A)-C(7A)-C(9A)	109(2)
C(2A)-C(7A)-C(8A)	111.3(18)
C(9A)-C(7A)-C(8A)	110(2)
C(2A)-C(7A)-H(7A)	108.9
C(9A)-C(7A)-H(7A)	108.9
C(8A)-C(7A)-H(7A)	108.9
C(7A)-C(8A)-H(8AA)	109.5
C(7A)-C(8A)-H(8AB)	109.5
H(8AA)-C(8A)-H(8AB)	109.5
C(7A)-C(8A)-H(8AC)	109.5
H(8AA)-C(8A)-H(8AC)	109.5
H(8AB)-C(8A)-H(8AC)	109.5
C(7A)-C(9A)-H(9AA)	109.5
C(7A)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(7A)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
C(6A)-C(10A)-C(11A)	112(2)
C(6A)-C(10A)-C(12A)	108(2)
C(11A)-C(10A)-C(12A)	112.2(18)
C(6A)-C(10A)-H(10A)	108.2
C(11A)-C(10A)-H(10A)	108.2
C(12A)-C(10A)-H(10A)	108.2
C(10A)-C(11A)-H(11D)	109.5
C(10A)-C(11A)-H(11E)	109.5
H(11D)-C(11A)-H(11E)	109.5
C(10A)-C(11A)-H(11F)	109.5
H(11D)-C(11A)-H(11F)	109.5
H(11E)-C(11A)-H(11F)	109.5
C(10A)-C(12A)-H(12A)	109.5
C(10A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5

C(10A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
N(11)-C(1B)-C(2B)	117.9(16)
N(11)-C(1B)-C(6B)	128.4(18)
C(2B)-C(1B)-C(6B)	113.6(19)
C(1B)-C(2B)-C(3B)	128(2)
C(1B)-C(2B)-C(7B)	118.7(16)
C(3B)-C(2B)-C(7B)	112.8(19)
C(4B)-C(3B)-C(2B)	115(2)
C(4B)-C(3B)-H(3B)	122.6
C(2B)-C(3B)-H(3B)	122.6
C(3B)-C(4B)-C(5B)	121(2)
C(3B)-C(4B)-H(4B)	119.6
C(5B)-C(4B)-H(4B)	119.6
C(6B)-C(5B)-C(4B)	120.7(19)
C(6B)-C(5B)-H(5B)	119.7
C(4B)-C(5B)-H(5B)	119.7
C(5B)-C(6B)-C(1B)	121.4(19)
C(5B)-C(6B)-C(10B)	122.5(17)
C(1B)-C(6B)-C(10B)	116.1(15)
C(2B)-C(7B)-C(9B)	117(2)
C(2B)-C(7B)-C(8B)	114(2)
C(9B)-C(7B)-C(8B)	109.3(18)
C(2B)-C(7B)-H(7B)	105.0
C(9B)-C(7B)-H(7B)	105.0
C(8B)-C(7B)-H(7B)	105.0
C(7B)-C(8B)-H(8BA)	109.5
C(7B)-C(8B)-H(8BB)	109.5
H(8BA)-C(8B)-H(8BB)	109.5
C(7B)-C(8B)-H(8BC)	109.5
H(8BA)-C(8B)-H(8BC)	109.5
H(8BB)-C(8B)-H(8BC)	109.5
C(7B)-C(9B)-H(9BA)	109.5
C(7B)-C(9B)-H(9BB)	109.5
H(9BA)-C(9B)-H(9BB)	109.5

C(7B)-C(9B)-H(9BC)	109.5
H(9BA)-C(9B)-H(9BC)	109.5
H(9BB)-C(9B)-H(9BC)	109.5
C(6B)-C(10B)-C(12B)	111.7(19)
C(6B)-C(10B)-C(11B)	112.1(16)
C(12B)-C(10B)-C(11B)	107.8(16)
C(6B)-C(10B)-H(10B)	108.3
C(12B)-C(10B)-H(10B)	108.3
C(11B)-C(10B)-H(10B)	108.3
C(10B)-C(11B)-H(11G)	109.5
C(10B)-C(11B)-H(11H)	109.5
H(11G)-C(11B)-H(11H)	109.5
C(10B)-C(11B)-H(11I)	109.5
H(11G)-C(11B)-H(11I)	109.5
H(11H)-C(11B)-H(11I)	109.5
C(10B)-C(12B)-H(12D)	109.5
C(10B)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(10B)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
N(21)-C(1C)-C(2C)	121.5(14)
N(21)-C(1C)-C(6C)	117.6(14)
C(2C)-C(1C)-C(6C)	120.9(16)
C(3C)-C(2C)-C(1C)	119.7(16)
C(3C)-C(2C)-C(7D)	121.8(15)
C(1C)-C(2C)-C(7D)	118.4(14)
C(2C)-C(3C)-C(4C)	120.9(16)
C(2C)-C(3C)-H(3C)	119.5
C(4C)-C(3C)-H(3C)	119.5
C(3C)-C(4C)-C(5C)	118.6(16)
C(3C)-C(4C)-K(1)#1	115.1(13)
C(5C)-C(4C)-K(1)#1	102.7(11)
C(3C)-C(4C)-H(4C)	120.7
C(5C)-C(4C)-H(4C)	120.7
K(1)#1-C(4C)-H(4C)	50.9

C(6C)-C(5C)-C(4C)	121.1(16)
C(6C)-C(5C)-H(5C)	119.4
C(4C)-C(5C)-H(5C)	119.4
C(5C)-C(6C)-C(1C)	118.3(15)
C(5C)-C(6C)-C(10C)	115.9(16)
C(1C)-C(6C)-C(10C)	125.1(16)
C(2D)-C(7C)-C(9C)	109.9(17)
C(2D)-C(7C)-C(8C)	114.4(17)
C(9C)-C(7C)-C(8C)	107.4(17)
C(2D)-C(7C)-H(7C)	108.3
C(9C)-C(7C)-H(7C)	108.3
C(8C)-C(7C)-H(7C)	108.3
C(7C)-C(8C)-H(8CA)	109.5
C(7C)-C(8C)-H(8CB)	109.5
H(8CA)-C(8C)-H(8CB)	109.5
C(7C)-C(8C)-H(8CC)	109.5
H(8CA)-C(8C)-H(8CC)	109.5
H(8CB)-C(8C)-H(8CC)	109.5
C(7C)-C(9C)-H(9CA)	109.5
C(7C)-C(9C)-H(9CB)	109.5
H(9CA)-C(9C)-H(9CB)	109.5
C(7C)-C(9C)-H(9CC)	109.5
H(9CA)-C(9C)-H(9CC)	109.5
H(9CB)-C(9C)-H(9CC)	109.5
C(6C)-C(10C)-C(12C)	129(2)
C(6C)-C(10C)-C(11C)	117(2)
C(12C)-C(10C)-C(11C)	105(2)
C(6C)-C(10C)-H(10C)	100.1
C(12C)-C(10C)-H(10C)	100.1
C(11C)-C(10C)-H(10C)	100.1
C(10C)-C(11C)-H(11J)	109.5
C(10C)-C(11C)-H(11K)	109.5
H(11J)-C(11C)-H(11K)	109.5
C(10C)-C(11C)-H(11L)	109.5
H(11J)-C(11C)-H(11L)	109.5
H(11K)-C(11C)-H(11L)	109.5

C(10C)-C(12C)-H(12G)	109.5
C(10C)-C(12C)-H(12H)	109.5
H(12G)-C(12C)-H(12H)	109.5
C(10C)-C(12C)-H(12I)	109.5
H(12G)-C(12C)-H(12I)	109.5
H(12H)-C(12C)-H(12I)	109.5
C(2D)-C(1D)-C(6D)	121(2)
C(2D)-C(1D)-N(21)	118.1(16)
C(6D)-C(1D)-N(21)	120.7(17)
C(1D)-C(2D)-C(3D)	116.9(19)
C(1D)-C(2D)-C(7C)	120.7(16)
C(3D)-C(2D)-C(7C)	122.4(18)
C(4D)-C(3D)-C(2D)	122(2)
C(4D)-C(3D)-H(3D)	119.2
C(2D)-C(3D)-H(3D)	119.2
C(3D)-C(4D)-C(5D)	122(2)
C(3D)-C(4D)-K(1)#1	98.0(15)
C(5D)-C(4D)-K(1)#1	116.3(17)
C(3D)-C(4D)-H(4D)	119.0
C(5D)-C(4D)-H(4D)	119.0
K(1)#1-C(4D)-H(4D)	53.1
C(6D)-C(5D)-C(4D)	116(2)
C(6D)-C(5D)-H(5D)	122.2
C(4D)-C(5D)-H(5D)	122.2
C(5D)-C(6D)-C(1D)	123(2)
C(5D)-C(6D)-C(10D)	118(2)
C(1D)-C(6D)-C(10D)	119(2)
C(2C)-C(7D)-C(9D)	114.2(16)
C(2C)-C(7D)-C(8D)	112.6(15)
C(9D)-C(7D)-C(8D)	107.9(16)
C(2C)-C(7D)-H(7D)	107.3
C(9D)-C(7D)-H(7D)	107.3
C(8D)-C(7D)-H(7D)	107.3
C(7D)-C(8D)-H(8DA)	109.5
C(7D)-C(8D)-H(8DB)	109.5
H(8DA)-C(8D)-H(8DB)	109.5

C(7D)-C(8D)-H(8DC)	109.5
H(8DA)-C(8D)-H(8DC)	109.5
H(8DB)-C(8D)-H(8DC)	109.5
C(7D)-C(9D)-H(9DA)	109.5
C(7D)-C(9D)-H(9DB)	109.5
H(9DA)-C(9D)-H(9DB)	109.5
C(7D)-C(9D)-H(9DC)	109.5
H(9DA)-C(9D)-H(9DC)	109.5
H(9DB)-C(9D)-H(9DC)	109.5
C(6D)-C(10D)-C(11D)	96(3)
C(6D)-C(10D)-C(12D)	93(2)
C(11D)-C(10D)-C(12D)	113(3)
C(6D)-C(10D)-H(10D)	116.9
C(11D)-C(10D)-H(10D)	116.9
C(12D)-C(10D)-H(10D)	116.9
C(10D)-C(11D)-H(11M)	109.5
C(10D)-C(11D)-H(11N)	109.5
H(11M)-C(11D)-H(11N)	109.5
C(10D)-C(11D)-H(11O)	109.5
H(11M)-C(11D)-H(11O)	109.5
H(11N)-C(11D)-H(11O)	109.5
C(10D)-C(12D)-H(12J)	109.5
C(10D)-C(12D)-H(12K)	109.5
H(12J)-C(12D)-H(12K)	109.5
C(10D)-C(12D)-H(12L)	109.5
H(12J)-C(12D)-H(12L)	109.5
H(12K)-C(12D)-H(12L)	109.5
O(10)-K(1)-O(20)	61.2(3)
O(10)-K(1)-O(60)	60.1(2)
O(20)-K(1)-O(60)	121.2(3)
O(10)-K(1)-O(30)	121.6(3)
O(20)-K(1)-O(30)	60.8(4)
O(60)-K(1)-O(30)	171.2(3)
O(10)-K(1)-O(50)	119.7(3)
O(20)-K(1)-O(50)	168.9(4)
O(60)-K(1)-O(50)	60.3(3)

O(30)-K(1)-O(50)	116.0(3)
O(10)-K(1)-O(40)	172.2(4)
O(20)-K(1)-O(40)	119.4(4)
O(60)-K(1)-O(40)	118.3(3)
O(30)-K(1)-O(40)	58.6(4)
O(50)-K(1)-O(40)	58.1(3)
C(120)-O(10)-C(10)	116.6(11)
C(120)-O(10)-K(1)	121.4(8)
C(10)-O(10)-K(1)	119.1(8)
C(20)-O(20)-C(30)	125.6(15)
C(20)-O(20)-K(1)	115.3(10)
C(30)-O(20)-K(1)	116.7(11)
C(40)-O(30)-C(50)	121.2(14)
C(40)-O(30)-K(1)	118.2(10)
C(50)-O(30)-K(1)	117.3(10)
C(60)-O(40)-C(70)	123.9(14)
C(60)-O(40)-K(1)	118.3(11)
C(70)-O(40)-K(1)	116.6(8)
C(80)-O(50)-C(90)	119.7(13)
C(80)-O(50)-K(1)	118.6(11)
C(90)-O(50)-K(1)	115.5(8)
C(100)-O(60)-C(110)	128.2(11)
C(100)-O(60)-K(1)	113.5(9)
C(110)-O(60)-K(1)	118.3(8)
O(10)-C(10)-C(20)	115.5(15)
O(10)-C(10)-H(10E)	108.4
C(20)-C(10)-H(10E)	108.4
O(10)-C(10)-H(10F)	108.4
C(20)-C(10)-H(10F)	108.4
H(10E)-C(10)-H(10F)	107.5
O(20)-C(20)-C(10)	124.5(16)
O(20)-C(20)-K(1)	45.3(8)
C(10)-C(20)-K(1)	80.3(10)
O(20)-C(20)-H(20A)	106.2
C(10)-C(20)-H(20A)	106.2
K(1)-C(20)-H(20A)	135.0

O(20)-C(20)-H(20B)	106.2
C(10)-C(20)-H(20B)	106.2
K(1)-C(20)-H(20B)	114.5
H(20A)-C(20)-H(20B)	106.4
O(20)-C(30)-C(40)	121.8(16)
O(20)-C(30)-H(30A)	106.9
C(40)-C(30)-H(30A)	106.9
O(20)-C(30)-H(30B)	106.9
C(40)-C(30)-H(30B)	106.9
H(30A)-C(30)-H(30B)	106.7
O(30)-C(40)-C(30)	118.9(16)
O(30)-C(40)-H(40A)	107.6
C(30)-C(40)-H(40A)	107.6
O(30)-C(40)-H(40B)	107.6
C(30)-C(40)-H(40B)	107.6
H(40A)-C(40)-H(40B)	107.0
O(30)-C(50)-C(60)	120.1(15)
O(30)-C(50)-H(50A)	107.3
C(60)-C(50)-H(50A)	107.3
O(30)-C(50)-H(50B)	107.3
C(60)-C(50)-H(50B)	107.3
H(50A)-C(50)-H(50B)	106.9
O(40)-C(60)-C(50)	119.1(15)
O(40)-C(60)-H(60A)	107.5
C(50)-C(60)-H(60A)	107.5
O(40)-C(60)-H(60B)	107.5
C(50)-C(60)-H(60B)	107.5
H(60A)-C(60)-H(60B)	107.0
O(40)-C(70)-C(80)	118.0(14)
O(40)-C(70)-H(70A)	107.8
C(80)-C(70)-H(70A)	107.8
O(40)-C(70)-H(70B)	107.8
C(80)-C(70)-H(70B)	107.8
H(70A)-C(70)-H(70B)	107.1
O(50)-C(80)-C(70)	118.8(16)
O(50)-C(80)-H(80A)	107.6

C(70)-C(80)-H(80A)	107.6
O(50)-C(80)-H(80B)	107.6
C(70)-C(80)-H(80B)	107.6
H(80A)-C(80)-H(80B)	107.0
O(50)-C(90)-C(100)	115.2(13)
O(50)-C(90)-H(90A)	108.5
C(100)-C(90)-H(90A)	108.5
O(50)-C(90)-H(90B)	108.5
C(100)-C(90)-H(90B)	108.5
H(90A)-C(90)-H(90B)	107.5
O(60)-C(100)-C(90)	130.6(16)
O(60)-C(100)-K(1)	46.7(7)
C(90)-C(100)-K(1)	84.1(9)
O(60)-C(100)-H(10G)	104.6
C(90)-C(100)-H(10G)	104.6
K(1)-C(100)-H(10G)	129.8
O(60)-C(100)-H(10H)	104.6
C(90)-C(100)-H(10H)	104.6
K(1)-C(100)-H(10H)	120.0
H(10G)-C(100)-H(10H)	105.7
O(60)-C(110)-C(120)	120.1(12)
O(60)-C(110)-H(11P)	107.3
C(120)-C(110)-H(11P)	107.3
O(60)-C(110)-H(11Q)	107.3
C(120)-C(110)-H(11Q)	107.3
H(11P)-C(110)-H(11Q)	106.9
O(10)-C(120)-C(110)	117.8(11)
O(10)-C(120)-H(12M)	107.9
C(110)-C(120)-H(12M)	107.9
O(10)-C(120)-H(12N)	107.9
C(110)-C(120)-H(12N)	107.9
H(12M)-C(120)-H(12N)	107.2

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,-z

Table S-16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. 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}
Fe(1)	37(1)	38(1)	37(1)	-6(1)	2(1)	-9(1)
C(1)	45(4)	36(4)	68(6)	2(4)	-2(4)	-13(3)
N(11)	50(4)	48(4)	32(3)	7(3)	-7(3)	-20(3)
N(21)	27(3)	38(3)	48(4)	-9(3)	-4(3)	-1(3)
C(11)	75(7)	49(5)	52(5)	4(4)	-14(5)	-29(5)
C(21)	52(5)	37(4)	42(5)	-2(4)	3(4)	-11(4)
C(31)	47(5)	35(4)	44(5)	2(3)	12(4)	-6(4)
C(41)	29(4)	38(4)	45(4)	-7(3)	4(3)	-6(3)
C(51)	32(4)	55(5)	61(5)	-1(4)	2(4)	-4(4)
C(1A)	25(9)	56(12)	48(10)	0(9)	-5(7)	-2(8)
C(2A)	47(9)	74(12)	41(9)	8(8)	-6(7)	24(8)
C(3A)	70(11)	210(30)	64(14)	-39(19)	-23(11)	62(14)
C(4A)	61(12)	240(30)	59(14)	-39(18)	-7(11)	38(15)
C(5A)	39(10)	190(30)	53(13)	-28(16)	3(9)	3(12)
C(6A)	42(9)	114(14)	50(10)	-27(10)	2(7)	-18(9)
C(7A)	63(11)	63(9)	45(9)	6(8)	-4(9)	15(8)
C(8A)	61(13)	50(11)	56(11)	7(9)	5(9)	22(9)
C(9A)	110(20)	68(10)	106(19)	21(10)	39(18)	33(10)
C(10A)	34(9)	118(14)	56(10)	-46(10)	-7(8)	-25(9)
C(11A)	35(12)	123(14)	81(16)	-45(11)	15(12)	-23(10)
C(12A)	73(16)	124(18)	69(11)	-52(11)	14(10)	-58(14)
C(1B)	71(12)	60(9)	36(8)	24(7)	-15(8)	-1(7)
C(2B)	67(11)	68(10)	84(13)	1(9)	-38(9)	4(8)
C(3B)	75(11)	77(11)	93(14)	-6(10)	-47(10)	-3(8)
C(4B)	69(12)	76(11)	79(14)	-1(10)	-41(11)	-11(9)
C(5B)	71(10)	79(10)	45(9)	15(8)	-30(8)	-12(7)
C(6B)	63(10)	80(9)	34(8)	14(6)	-11(7)	-13(7)
C(7B)	92(15)	91(11)	108(15)	-23(12)	-71(13)	43(10)
C(8B)	170(30)	103(19)	122(17)	-8(14)	-28(16)	81(18)
C(9B)	120(20)	95(12)	170(30)	-13(14)	-70(20)	48(12)
C(10B)	59(10)	86(9)	37(7)	-7(7)	-15(7)	-15(7)

C(11B)	66(13)	95(11)	58(11)	2(9)	-1(10)	-14(9)
C(12B)	105(17)	127(17)	52(9)	-26(10)	14(10)	-59(14)
C(1C)	27(4)	46(4)	29(8)	6(4)	-11(6)	-5(3)
C(2C)	53(10)	51(7)	36(9)	4(6)	-19(7)	1(6)
C(3C)	74(13)	48(8)	38(8)	3(6)	-27(8)	-8(7)
C(4C)	71(13)	54(8)	28(9)	-3(6)	-27(9)	-11(7)
C(5C)	46(10)	52(9)	33(8)	9(6)	-7(7)	-21(7)
C(6C)	34(9)	49(7)	26(7)	2(5)	-12(6)	-18(6)
C(7C)	55(10)	46(8)	23(9)	17(7)	1(7)	10(6)
C(8C)	103(18)	59(10)	55(15)	0(9)	19(14)	-13(9)
C(9C)	65(10)	36(10)	67(14)	-2(9)	26(9)	6(7)
C(10C)	52(9)	46(8)	23(8)	6(6)	6(6)	-17(6)
C(11C)	51(9)	51(12)	52(17)	-16(12)	2(7)	-14(7)
C(12C)	44(12)	75(15)	62(14)	-30(13)	0(10)	-8(9)
C(1D)	27(4)	46(4)	29(8)	6(4)	-11(6)	-5(3)
C(2D)	39(10)	48(7)	20(8)	12(6)	-1(7)	8(6)
C(3D)	56(13)	56(10)	23(9)	15(7)	0(9)	11(9)
C(4D)	77(16)	72(12)	39(10)	0(8)	2(9)	6(10)
C(5D)	52(13)	67(11)	33(9)	-5(7)	3(8)	-1(9)
C(6D)	69(16)	58(9)	36(8)	-3(6)	-1(7)	-10(8)
C(7D)	77(10)	53(8)	34(8)	6(6)	-11(7)	11(6)
C(8D)	90(14)	54(8)	63(13)	9(8)	-4(11)	10(7)
C(9D)	80(10)	47(9)	74(13)	11(9)	9(9)	18(7)
C(10D)	72(14)	52(10)	37(12)	-7(7)	-9(9)	-12(7)
C(11D)	79(13)	61(16)	37(17)	-3(12)	-6(9)	-7(9)
C(12D)	73(18)	43(12)	47(13)	-10(9)	-16(13)	-2(10)
K(1)	46(1)	38(1)	41(1)	2(1)	-6(1)	-8(1)
O(10)	154(9)	79(6)	173(9)	-43(6)	-98(8)	27(6)
O(20)	89(6)	142(8)	86(6)	19(6)	-22(5)	18(6)
O(30)	127(8)	163(8)	65(5)	-7(5)	-34(5)	-53(7)
O(40)	114(7)	138(9)	139(8)	-84(7)	-5(7)	-7(6)
O(50)	194(12)	77(5)	90(6)	4(5)	-38(7)	30(6)
O(60)	94(6)	74(4)	70(5)	-8(4)	-30(4)	4(4)
C(10)	58(6)	77(7)	128(9)	30(6)	3(6)	4(5)
C(20)	210(20)	110(10)	179(13)	2(9)	-84(14)	15(11)
C(30)	121(12)	178(12)	93(8)	24(8)	-49(8)	-30(10)

C(40)	240(20)	202(12)	143(17)	-19(10)	-135(19)	10(11)
C(50)	155(15)	167(11)	141(15)	-70(9)	-68(13)	-35(8)
C(60)	148(11)	122(10)	107(10)	-34(8)	-4(9)	-74(8)
C(70)	135(10)	77(8)	110(9)	-34(7)	30(7)	-10(7)
C(80)	140(13)	109(9)	153(11)	-45(8)	9(9)	-6(9)
C(90)	191(17)	89(8)	127(10)	-16(7)	-85(12)	74(9)
C(100)	227(18)	107(8)	98(11)	-23(7)	-37(12)	73(10)
C(110)	300(30)	133(10)	280(20)	-136(13)	-240(30)	112(14)
C(120)	71(7)	95(8)	85(7)	-22(6)	0(5)	-8(6)

Table S-17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	5529	7144	2284	75
H(1B)	6093	6959	3274	75
H(1C)	5358	7363	3493	75
H(11A)	4720	4879	5512	88
H(11B)	3764	4894	5605	88
H(11C)	4293	5332	6248	88
H(31)	3105	5270	4236	51
H(51A)	2147	6027	2625	74
H(51B)	2271	5388	2818	74
H(51C)	2590	5666	1719	74
H(3A)	7304	4918	4431	139
H(4A)	7749	5399	5989	144
H(5A)	6911	6023	6881	114
H(7A)	5378	5029	3248	68
H(8AA)	5999	5425	1878	83
H(8AB)	6743	5020	2016	83
H(8AC)	6727	5585	2665	83
H(9AA)	6771	4373	3614	140
H(9AB)	6124	4237	2689	140
H(9AC)	5874	4217	3951	140
H(10A)	4942	6389	5906	83
H(11D)	6423	6890	6490	120
H(11E)	5597	7162	6867	120
H(11F)	5791	7093	5595	120
H(12A)	4893	5856	7466	132
H(12B)	4980	6468	7899	132
H(12C)	5743	6074	7885	132
H(3B)	7195	5101	5097	98
H(4B)	7437	5679	6617	90
H(5B)	6542	6387	7014	78

H(7B)	5322	5010	3818	116
H(8BA)	5903	5380	2420	198
H(8BB)	6456	4848	2443	198
H(8BC)	6766	5401	2989	198
H(9BA)	6678	4335	4017	192
H(9BB)	5777	4169	3719	192
H(9BC)	6007	4321	4951	192
H(10B)	4653	6609	5597	72
H(11G)	5039	7460	6128	110
H(11H)	5884	7216	5754	110
H(11I)	5656	7237	7023	110
H(12D)	5006	6310	7788	142
H(12E)	4179	6237	7144	142
H(12F)	4433	6824	7594	142
H(3C)	3208	7725	838	64
H(4C)	3420	7293	-865	61
H(5C)	3580	6335	-903	52
H(7C)	3634	7200	3001	49
H(8CA)	3803	8026	1483	108
H(8CB)	4073	8037	2738	108
H(8CC)	3184	8216	2405	108
H(9CA)	2185	7696	2312	84
H(9CB)	2380	7422	3468	84
H(9CC)	2179	7048	2433	84
H(10C)	3821	5477	1322	48
H(11J)	5195	5698	64	76
H(11K)	5036	5149	731	76
H(11L)	5130	5714	1368	76
H(12G)	3128	5124	-84	91
H(12H)	3997	4848	-62	91
H(12I)	3794	5306	-950	91
H(3D)	3330	7597	206	54
H(4D)	3506	7042	-1309	75
H(5D)	3716	6087	-1118	61
H(7D)	3777	7205	3387	66
H(8DA)	3861	8067	2406	103

H(8DB)	3448	8109	3583	103
H(8DC)	2907	8108	2504	103
H(9DA)	2292	7515	3756	100
H(9DB)	2635	6923	4039	100
H(9DC)	2174	7024	2910	100
H(10D)	3920	5382	1475	65
H(11M)	4885	5814	-348	88
H(11N)	5146	5274	292	88
H(11O)	5162	5850	902	88
H(12J)	3217	5638	-593	81
H(12K)	3015	5109	119	81
H(12L)	3760	5104	-704	81
H(10E)	6822	9499	2516	105
H(10F)	6105	9184	3104	105
H(20A)	5614	9243	1557	200
H(20B)	6458	9285	969	200
H(30A)	6060	8714	-446	157
H(30B)	5190	8698	79	157
H(40A)	5034	7880	-223	234
H(40B)	5688	7995	-1141	234
H(50A)	5837	7060	-1055	186
H(50B)	5381	6960	68	186
H(60A)	6159	6313	159	151
H(60B)	6803	6586	-628	151
H(70A)	7967	6453	547	129
H(70B)	7350	6019	1024	129
H(80A)	7568	6238	2665	161
H(80B)	8430	6277	2114	161
H(90A)	8885	6841	3493	163
H(90B)	8034	6768	4068	163
H(10G)	8329	7473	4710	173
H(10H)	8934	7621	3765	173
H(11P)	8513	8568	4059	282
H(11Q)	7872	8369	4933	282
H(12M)	7015	8893	4365	100
H(12N)	7726	9184	3719	100

Table S-18. Torsion angles [°] for **4**.

C(1B)-N(11)-C(21)-C(31)	175.9(13)
C(1A)-N(11)-C(21)-C(31)	-162.1(11)
Fe(1)-N(11)-C(21)-C(31)	6.1(12)
C(1B)-N(11)-C(21)-C(11)	0.2(16)
C(1A)-N(11)-C(21)-C(11)	22.2(14)
Fe(1)-N(11)-C(21)-C(11)	-169.6(6)
N(11)-C(21)-C(31)-C(41)	3.0(14)
C(11)-C(21)-C(31)-C(41)	178.7(8)
C(1C)-N(21)-C(41)-C(31)	175.3(12)
C(1D)-N(21)-C(41)-C(31)	164.7(13)
Fe(1)-N(21)-C(41)-C(31)	0.1(10)
C(1C)-N(21)-C(41)-C(51)	-6.0(15)
C(1D)-N(21)-C(41)-C(51)	-16.6(15)
Fe(1)-N(21)-C(41)-C(51)	178.8(6)
C(21)-C(31)-C(41)-N(21)	-6.5(13)
C(21)-C(31)-C(41)-C(51)	174.8(8)
C(21)-N(11)-C(1A)-C(2A)	80(3)
Fe(1)-N(11)-C(1A)-C(2A)	-89(3)
C(21)-N(11)-C(1A)-C(6A)	-105(2)
Fe(1)-N(11)-C(1A)-C(6A)	87(3)
C(6A)-C(1A)-C(2A)-C(3A)	-5(4)
N(11)-C(1A)-C(2A)-C(3A)	171(3)
C(6A)-C(1A)-C(2A)-C(7A)	-172(2)
N(11)-C(1A)-C(2A)-C(7A)	4(4)
C(1A)-C(2A)-C(3A)-C(4A)	5(6)
C(7A)-C(2A)-C(3A)-C(4A)	172(3)
C(2A)-C(3A)-C(4A)-C(5A)	-1(6)
C(3A)-C(4A)-C(5A)-C(6A)	-2(6)
C(4A)-C(5A)-C(6A)-C(1A)	1(6)
C(4A)-C(5A)-C(6A)-C(10A)	-176(3)
C(2A)-C(1A)-C(6A)-C(5A)	2(5)
N(11)-C(1A)-C(6A)-C(5A)	-174(3)
C(2A)-C(1A)-C(6A)-C(10A)	180(2)
N(11)-C(1A)-C(6A)-C(10A)	4(4)

C(3A)-C(2A)-C(7A)-C(9A)	50(4)
C(1A)-C(2A)-C(7A)-C(9A)	-142(3)
C(3A)-C(2A)-C(7A)-C(8A)	-72(3)
C(1A)-C(2A)-C(7A)-C(8A)	97(3)
C(5A)-C(6A)-C(10A)-C(11A)	59(4)
C(1A)-C(6A)-C(10A)-C(11A)	-119(3)
C(5A)-C(6A)-C(10A)-C(12A)	-65(4)
C(1A)-C(6A)-C(10A)-C(12A)	117(3)
C(21)-N(11)-C(1B)-C(2B)	83(2)
Fe(1)-N(11)-C(1B)-C(2B)	-107(2)
C(21)-N(11)-C(1B)-C(6B)	-100(2)
Fe(1)-N(11)-C(1B)-C(6B)	70(3)
N(11)-C(1B)-C(2B)-C(3B)	169(3)
C(6B)-C(1B)-C(2B)-C(3B)	-8(4)
N(11)-C(1B)-C(2B)-C(7B)	-2(4)
C(6B)-C(1B)-C(2B)-C(7B)	-179(2)
C(1B)-C(2B)-C(3B)-C(4B)	10(4)
C(7B)-C(2B)-C(3B)-C(4B)	-179(2)
C(2B)-C(3B)-C(4B)-C(5B)	-7(4)
C(3B)-C(4B)-C(5B)-C(6B)	5(4)
C(4B)-C(5B)-C(6B)-C(1B)	-4(3)
C(4B)-C(5B)-C(6B)-C(10B)	179(2)
N(11)-C(1B)-C(6B)-C(5B)	-172(2)
C(2B)-C(1B)-C(6B)-C(5B)	5(3)
N(11)-C(1B)-C(6B)-C(10B)	6(3)
C(2B)-C(1B)-C(6B)-C(10B)	-177(2)
C(1B)-C(2B)-C(7B)-C(9B)	-138(3)
C(3B)-C(2B)-C(7B)-C(9B)	50(3)
C(1B)-C(2B)-C(7B)-C(8B)	92(3)
C(3B)-C(2B)-C(7B)-C(8B)	-80(3)
C(5B)-C(6B)-C(10B)-C(12B)	-74(2)
C(1B)-C(6B)-C(10B)-C(12B)	108(2)
C(5B)-C(6B)-C(10B)-C(11B)	47(2)
C(1B)-C(6B)-C(10B)-C(11B)	-130.8(19)
C(41)-N(21)-C(1C)-C(2C)	112(2)
Fe(1)-N(21)-C(1C)-C(2C)	-72(3)

C(41)-N(21)-C(1C)-C(6C)	-68(3)
Fe(1)-N(21)-C(1C)-C(6C)	108(2)
N(21)-C(1C)-C(2C)-C(3C)	177(2)
C(6C)-C(1C)-C(2C)-C(3C)	-3(4)
N(21)-C(1C)-C(2C)-C(7D)	-6(4)
C(6C)-C(1C)-C(2C)-C(7D)	174(2)
C(1C)-C(2C)-C(3C)-C(4C)	-1(3)
C(7D)-C(2C)-C(3C)-C(4C)	-178(2)
C(2C)-C(3C)-C(4C)-C(5C)	6(3)
C(2C)-C(3C)-C(4C)-K(1)#1	128.5(17)
C(3C)-C(4C)-C(5C)-C(6C)	-7(3)
K(1)#1-C(4C)-C(5C)-C(6C)	-135.2(18)
C(4C)-C(5C)-C(6C)-C(1C)	3(3)
C(4C)-C(5C)-C(6C)-C(10C)	-168.3(19)
N(21)-C(1C)-C(6C)-C(5C)	-178(2)
C(2C)-C(1C)-C(6C)-C(5C)	2(4)
N(21)-C(1C)-C(6C)-C(10C)	-8(4)
C(2C)-C(1C)-C(6C)-C(10C)	172(3)
C(5C)-C(6C)-C(10C)-C(12C)	-45(3)
C(1C)-C(6C)-C(10C)-C(12C)	145(3)
C(5C)-C(6C)-C(10C)-C(11C)	96(3)
C(1C)-C(6C)-C(10C)-C(11C)	-74(3)
C(41)-N(21)-C(1D)-C(2D)	119(3)
Fe(1)-N(21)-C(1D)-C(2D)	-75(3)
C(41)-N(21)-C(1D)-C(6D)	-65(3)
Fe(1)-N(21)-C(1D)-C(6D)	100(3)
C(6D)-C(1D)-C(2D)-C(3D)	-4(5)
N(21)-C(1D)-C(2D)-C(3D)	172(2)
C(6D)-C(1D)-C(2D)-C(7C)	178(3)
N(21)-C(1D)-C(2D)-C(7C)	-6(4)
C(9C)-C(7C)-C(2D)-C(1D)	-93(3)
C(8C)-C(7C)-C(2D)-C(1D)	146(3)
C(9C)-C(7C)-C(2D)-C(3D)	89(3)
C(8C)-C(7C)-C(2D)-C(3D)	-32(3)
C(1D)-C(2D)-C(3D)-C(4D)	3(4)
C(7C)-C(2D)-C(3D)-C(4D)	-179(2)

C(2D)-C(3D)-C(4D)-C(5D)	0(4)
C(2D)-C(3D)-C(4D)-K(1)#1	128(2)
C(3D)-C(4D)-C(5D)-C(6D)	-3(4)
K(1)#1-C(4D)-C(5D)-C(6D)	-123(3)
C(4D)-C(5D)-C(6D)-C(1D)	3(5)
C(4D)-C(5D)-C(6D)-C(10D)	-172(3)
C(2D)-C(1D)-C(6D)-C(5D)	1(6)
N(21)-C(1D)-C(6D)-C(5D)	-175(3)
C(2D)-C(1D)-C(6D)-C(10D)	175(4)
N(21)-C(1D)-C(6D)-C(10D)	0(5)
C(3C)-C(2C)-C(7D)-C(9D)	102(2)
C(1C)-C(2C)-C(7D)-C(9D)	-75(3)
C(3C)-C(2C)-C(7D)-C(8D)	-21(3)
C(1C)-C(2C)-C(7D)-C(8D)	162(2)
C(5D)-C(6D)-C(10D)-C(11D)	70(4)
C(1D)-C(6D)-C(10D)-C(11D)	-104(4)
C(5D)-C(6D)-C(10D)-C(12D)	-43(4)
C(1D)-C(6D)-C(10D)-C(12D)	142(4)
C(120)-O(10)-C(10)-C(20)	177.0(17)
K(1)-O(10)-C(10)-C(20)	-22(2)
C(30)-O(20)-C(20)-C(10)	-177(2)
K(1)-O(20)-C(20)-C(10)	-15(3)
C(30)-O(20)-C(20)-K(1)	-162(2)
O(10)-C(10)-C(20)-O(20)	25(3)
O(10)-C(10)-C(20)-K(1)	14.8(14)
C(20)-O(20)-C(30)-C(40)	-179(3)
K(1)-O(20)-C(30)-C(40)	19(3)
C(50)-O(30)-C(40)-C(30)	173(2)
K(1)-O(30)-C(40)-C(30)	14(3)
O(20)-C(30)-C(40)-O(30)	-24(4)
C(40)-O(30)-C(50)-C(60)	170(2)
K(1)-O(30)-C(50)-C(60)	-31(3)
C(70)-O(40)-C(60)-C(50)	-172(2)
K(1)-O(40)-C(60)-C(50)	-4(2)
O(30)-C(50)-C(60)-O(40)	24(3)
C(60)-O(40)-C(70)-C(80)	-165.9(17)

K(1)-O(40)-C(70)-C(80)	27(2)
C(90)-O(50)-C(80)-C(70)	-179.0(19)
K(1)-O(50)-C(80)-C(70)	30(2)
O(40)-C(70)-C(80)-O(50)	-39(3)
C(80)-O(50)-C(90)-C(100)	-177(2)
K(1)-O(50)-C(90)-C(100)	-25(3)
C(110)-O(60)-C(100)-C(90)	173(3)
K(1)-O(60)-C(100)-C(90)	-7(3)
C(110)-O(60)-C(100)-K(1)	180(3)
O(50)-C(90)-C(100)-O(60)	23(4)
O(50)-C(90)-C(100)-K(1)	18.2(18)
C(100)-O(60)-C(110)-C(120)	-178(2)
K(1)-O(60)-C(110)-C(120)	2(4)
C(10)-O(10)-C(120)-C(110)	179(2)
K(1)-O(10)-C(120)-C(110)	19(2)
O(60)-C(110)-C(120)-O(10)	-14(4)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,-z

[$L^{Me}FeCH_3$][K(18-crown-6)(12-crown-4)] (4') We also crystallographically characterized a crystal in which the potassium is bound by one 18-crown-6 and one 12-crown 4. Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å) for the structure of **4'**. The diffraction images were processed and scaled using Rigaku Oxford Diffraction software (CrysAlisPro; Rigaku OD: The Woodlands, TX, 2015). The structure was solved with SHELXT and was refined against F^2 on all data by full-matrix least squares with SHELXL (Sheldrick, G. M. Acta Cryst. 2008, A64, 112–122). All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups). One of the 12-crown-4 molecules was modeled as disordered. The site occupancies of the disordered atoms where fixed to 0.5. Chemically equivalent C-C and C-O bonds for the disordered atoms were restrained to be similar. The disordered atoms thermal parameters were also restrained to behave as a rigid group. Restraints were also applied to "non-disordered" atoms of the other 18-crown-6/12-crown-4 potassium complexes. These sites are likely disordered, and generate a number of checkCIF alerts. However, the weak, twinned data did not strongly support additional parameters. Restraints and constraints were used to obtain a stable model that converged. Atom C310 is likely an average position of two disordered positions. Its close proximity to the crystallographic special position also caused the thermal parameters to be large. Its thermal parameters were subsequently constrained to the value of its neighbor, C320. The program SQUEEZE was used to compensate for the contribution of disordered solvents contained in voids within the crystal lattice from the diffraction intensities. This procedure was applied to the data file and the submitted model is based on the solvent removed data. Based on the total electron density found in the voids (175 e/$Å^3$), it is likely that ~4 ether molecules are present in the unit cell. See "_platon_squeeze_details" in this .cif for more information. The full numbering scheme of compound **4'** can be found in the full details of the X-ray structure determination (CIF), which is included as Supporting Information.

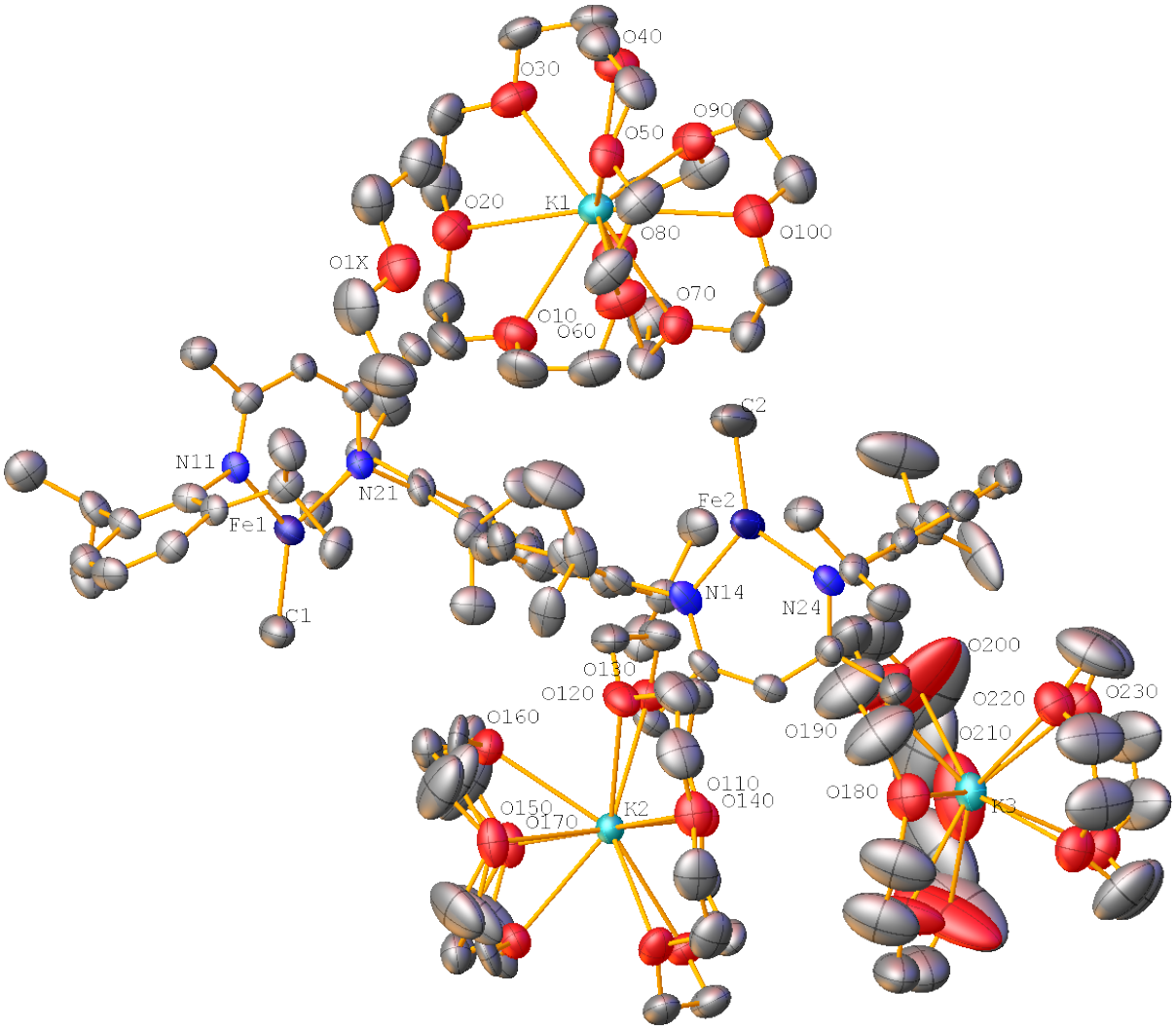

Figure S-27: A partial numbering scheme of **4'** with 50% thermal ellipsoid probability levels. The hydrogen atoms are shown as circles for clarity.

Table S-19. Crystal data and structure refinement for **4'**.

Identification code	007-16130	
CSD Deposition Number	1944811	
Empirical formula	$C_{52}H_{89}FeKN_2O_{10.5}$	
Formula weight	1005.20	
Temperature	93(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/m$	
Unit cell dimensions	a = 12.8093(4) Å	α= 90°.
	b = 49.1255(11) Å	β= 90.131(2)°.
	c = 18.9290(4) Å	γ = 90°.
Volume	11911.3(5) $Å^3$	
Z	8	
Density (calculated)	1.121 g/cm^3	
Absorption coefficient	3.067 mm^{-1}	
F(000)	4352	
Crystal size	0.050 x 0.050 x 0.020 mm^3	
Crystal color and habit	Red Plate	
Diffractometer	Rigaku Saturn 944+ CCD	
Theta range for data collection	1.799 to 67.369°.	
Index ranges	-14<=h<=14, -58<=k<=58, 0<=l<=22	
Reflections collected	21384	
Independent reflections	21384 [R(int) = 0.1394]	
Observed reflections (I > 2sigma(I))	17694	
Completeness to theta = 67.369°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.62537	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	21384 / 196 / 1265	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.0992, wR2 = 0.2324	
R indices (all data)	R1 = 0.1147, wR2 = 0.2420	
Largest diff. peak and hole	0.956 and -0.866 $e.Å^{-3}$	

Table S-20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4'**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	-1012(1)	3900(1)	4792(1)	34(1)
C(1)	-1314(6)	3513(1)	4498(4)	57(2)
N(11)	-1864(4)	4169(1)	5274(2)	31(1)
N(21)	238(4)	4120(1)	4713(2)	32(1)
C(11)	-2327(6)	4630(1)	5679(4)	50(2)
C(21)	-1563(5)	4432(1)	5362(3)	35(1)
C(31)	-573(4)	4524(1)	5175(3)	32(1)
C(41)	286(5)	4385(1)	4897(3)	34(1)
C(51)	1291(5)	4540(1)	4816(3)	44(2)
C(12)	-2751(5)	4070(1)	5639(3)	37(1)
C(22)	-2657(5)	4003(1)	6374(3)	33(1)
C(32)	-3491(5)	3881(1)	6707(3)	38(1)
C(42)	-4385(5)	3811(1)	6350(3)	46(2)
C(52)	-4482(6)	3878(1)	5641(3)	45(2)
C(62)	-3682(5)	4009(1)	5284(3)	38(1)
C(72)	-1639(6)	4058(1)	6767(3)	44(2)
C(82)	-1031(6)	3789(2)	6852(4)	57(2)
C(92)	-1787(6)	4193(2)	7481(4)	61(2)
C(102)	-3846(5)	4086(1)	4517(3)	45(2)
C(112)	-3950(6)	3833(2)	4052(4)	59(2)
C(122)	-4801(7)	4272(2)	4414(4)	64(2)
C(13)	1172(4)	3988(1)	4467(3)	33(1)
C(23)	1764(5)	3823(1)	4945(3)	37(1)
C(33)	2641(5)	3693(2)	4675(3)	47(2)
C(43)	2940(5)	3718(2)	3999(4)	47(2)
C(53)	2364(5)	3877(1)	3537(3)	42(2)
C(63)	1468(5)	4012(1)	3758(3)	36(1)
C(73)	1465(6)	3797(1)	5710(3)	45(2)
C(83)	1262(7)	3499(2)	5913(4)	61(2)
C(93)	2246(8)	3930(2)	6196(4)	68(2)
C(103)	815(5)	4173(1)	3241(3)	41(2)

C(113)	115(6)	3981(2)	2811(3)	49(2)
C(123)	1476(7)	4352(2)	2751(4)	68(2)
Fe(2)	4201(1)	3637(1)	10205(1)	52(1)
C(2)	4149(9)	4047(2)	10366(7)	108(4)
N(14)	3240(4)	3385(1)	9770(2)	40(1)
N(24)	5215(4)	3372(1)	10531(2)	36(1)
C(14)	2551(6)	2927(1)	9458(4)	51(2)
C(24)	3375(5)	3110(1)	9783(3)	36(1)
C(34)	4231(5)	2986(1)	10091(3)	37(1)
C(44)	5099(5)	3097(1)	10441(3)	38(1)
C(54)	5940(6)	2913(1)	10730(5)	59(2)
C(15)	2386(5)	3492(1)	9378(3)	42(2)
C(25)	2441(5)	3497(1)	8623(3)	38(1)
C(35)	1586(6)	3597(1)	8259(3)	44(2)
C(45)	700(6)	3692(1)	8579(4)	47(2)
C(55)	685(5)	3705(2)	9324(4)	49(2)
C(65)	1507(5)	3604(1)	9716(3)	46(2)
C(75)	3418(6)	3417(1)	8247(3)	44(2)
C(85)	4119(7)	3669(2)	8158(5)	64(2)
C(95)	3243(7)	3269(2)	7553(4)	70(2)
C(105)	1467(6)	3613(2)	10515(3)	61(2)
C(115)	1106(11)	3888(2)	10790(5)	103(4)
C(125)	735(6)	3395(2)	10789(4)	67(2)
C(16)	6100(5)	3468(1)	10902(3)	35(1)
C(26)	6983(6)	3562(2)	10545(4)	50(2)
C(36)	7803(5)	3666(1)	10920(4)	53(2)
C(46)	7812(6)	3675(2)	11644(5)	56(2)
C(56)	6943(6)	3580(1)	12011(4)	49(2)
C(66)	6082(5)	3479(1)	11651(3)	35(1)
C(76)	6993(7)	3551(2)	9745(4)	70(2)
C(86)	7951(7)	3397(3)	9475(6)	122(5)
C(96)	6917(15)	3834(3)	9410(7)	156(7)
C(106)	5112(5)	3389(1)	12046(3)	40(1)
C(116)	4401(6)	3629(2)	12213(4)	56(2)
C(126)	5337(7)	3235(2)	12737(4)	67(2)
K(1)	3340(1)	4968(1)	7858(1)	43(1)

O(10)	1852(5)	4516(1)	7800(3)	70(2)
O(20)	1398(4)	4966(1)	6945(3)	62(1)
O(30)	2599(5)	5444(1)	7021(3)	70(2)
O(40)	3821(5)	5513(1)	8287(3)	65(2)
O(50)	3116(4)	5155(1)	9351(3)	59(1)
O(60)	3131(5)	4590(1)	9037(3)	74(2)
O(70)	4389(4)	4473(1)	7662(2)	53(1)
O(80)	4003(5)	4791(1)	6455(3)	66(1)
O(90)	5203(5)	5185(1)	7201(3)	66(2)
O(100)	5552(5)	4852(1)	8427(3)	69(2)
C(10)	946(8)	4534(2)	7372(6)	84(3)
C(20)	1179(8)	4694(2)	6764(5)	83(3)
C(30)	1516(8)	5146(2)	6371(4)	73(2)
C(40)	1664(7)	5424(2)	6626(4)	63(2)
C(50)	2727(7)	5696(2)	7339(5)	67(2)
C(60)	3763(7)	5707(2)	7717(5)	68(2)
C(70)	3378(8)	5609(2)	8916(5)	72(2)
C(80)	3656(7)	5404(2)	9475(4)	68(2)
C(90)	3369(8)	4954(2)	9831(4)	76(3)
C(100)	2782(8)	4701(2)	9674(4)	71(3)
C(110)	2649(9)	4338(2)	8836(5)	81(3)
C(120)	1674(9)	4377(2)	8452(5)	83(3)
C(130)	4074(7)	4358(2)	7003(4)	60(2)
C(140)	4445(8)	4527(2)	6391(4)	69(2)
C(150)	4602(8)	4999(2)	6124(5)	76(3)
C(160)	5541(8)	5084(2)	6546(5)	81(3)
C(170)	5991(7)	5234(2)	7708(5)	76(3)
C(180)	6397(8)	4974(2)	8049(5)	84(3)
C(190)	5668(7)	4568(2)	8513(4)	66(2)
C(200)	5406(6)	4407(2)	7851(4)	61(2)
K(2)	544(1)	2500	12844(1)	36(1)
O(110)	1350(6)	2500	14325(3)	59(2)
O(120)	713(4)	2992(1)	13688(3)	58(1)
O(130)	1605(4)	3005(1)	12325(3)	53(1)
O(140)	2326(5)	2500	11834(3)	45(2)
O(150)	-1527(5)	2500	13552(3)	59(2)

O(160)	-1045(4)	2886(1)	12498(2)	52(1)
C(210)	1125(8)	2740(2)	14712(4)	79(3)
C(220)	1373(8)	2981(2)	14280(5)	77(3)
C(230)	801(7)	3236(2)	13285(5)	65(2)
C(240)	1728(7)	3227(2)	12811(5)	63(2)
C(250)	2464(6)	2979(2)	11881(4)	56(2)
C(260)	2317(6)	2741(2)	11401(4)	57(2)
C(8X)	-2202(17)	2745(2)	13517(16)	123(10)
C(7Y)	-2068(9)	2911(3)	12777(8)	54(3)
C(6X)	-1707(12)	2892(3)	11892(7)	56(3)
C(5Y)	-1205(19)	2736(2)	11245(11)	86(7)
O(170)	-572(5)	2500	11448(3)	56(2)
K(3)	8000(2)	2500	7411(1)	45(1)
O(180)	6620(7)	2500	8621(4)	73(2)
O(190)	6619(9)	2950(2)	7694(4)	131(4)
O(200)	7698(13)	2967(3)	6479(6)	265(9)
O(220)	9078(5)	2788(1)	8573(3)	70(2)
O(230)	9941(5)	2786(1)	7205(3)	68(2)
C(310)	6260(14)	2757(2)	8764(7)	144(4)
C(320)	6048(14)	2958(3)	8297(7)	144(4)
C(330)	6524(9)	3166(2)	7258(7)	103(3)
C(360)	8062(16)	2711(3)	5446(9)	254(8)
C(370)	9358(13)	2630(2)	9132(5)	129(5)
C(380)	9811(12)	2972(3)	8364(6)	126(5)
C(390)	10220(11)	2970(3)	7713(6)	115(4)
O(1X)	-223(5)	4828(1)	9069(3)	80(2)
C(3X)	-418(8)	5110(2)	8910(6)	86(3)
C(4X)	501(8)	5233(2)	8609(5)	82(3)
C(1X)	-789(10)	4411(2)	9575(7)	109(4)
C(2X)	-1060(8)	4699(2)	9376(6)	93(3)
C(400)	10725(10)	2634(2)	6929(8)	144(6)
O(210)	8342(12)	2500	5842(7)	167(6)
C(340)	7097(12)	3158(3)	6658(7)	125(4)
C(350)	8191(16)	2950(4)	5813(7)	229(8)
C(5X)	-1020(20)	2777(4)	11421(10)	87(6)
C(6Y)	-1053(15)	2934(3)	11718(6)	63(4)

C(7X)	-1698(11)	2928(4)	13143(7)	59(3)
C(8Y)	-1920(20)	2778(4)	13411(10)	103(8)

Table S-21. Bond lengths [Å] and angles [°] for **4'**.

Fe(1)-N(21)	1.938(5)
Fe(1)-N(11)	1.942(5)
Fe(1)-C(1)	2.016(7)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
N(11)-C(21)	1.361(7)
N(11)-C(12)	1.417(7)
N(21)-C(41)	1.349(7)
N(21)-C(13)	1.438(7)
C(11)-C(21)	1.505(9)
C(11)-H(11G)	0.9800
C(11)-H(11H)	0.9800
C(11)-H(11I)	0.9800
C(21)-C(31)	1.393(8)
C(31)-C(41)	1.401(8)
C(31)-H(31)	0.9500
C(41)-C(51)	1.503(8)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(12)-C(62)	1.399(9)
C(12)-C(22)	1.434(8)
C(22)-C(32)	1.380(8)
C(22)-C(72)	1.523(9)
C(32)-C(42)	1.372(10)
C(32)-H(32)	0.9500
C(42)-C(52)	1.389(9)
C(42)-H(42)	0.9500
C(52)-C(62)	1.386(9)
C(52)-H(52)	0.9500
C(62)-C(102)	1.514(9)
C(72)-C(92)	1.519(9)
C(72)-C(82)	1.543(10)

C(72)-H(72)	1.0000
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(92)-H(92A)	0.9800
C(92)-H(92B)	0.9800
C(92)-H(92C)	0.9800
C(102)-C(112)	1.529(9)
C(102)-C(122)	1.538(11)
C(102)-H(102)	1.0000
C(112)-H(11J)	0.9800
C(112)-H(11K)	0.9800
C(112)-H(11L)	0.9800
C(122)-H(12G)	0.9800
C(122)-H(12H)	0.9800
C(122)-H(12I)	0.9800
C(13)-C(63)	1.401(8)
C(13)-C(23)	1.433(8)
C(23)-C(33)	1.389(9)
C(23)-C(73)	1.505(8)
C(33)-C(43)	1.343(10)
C(33)-H(33)	0.9500
C(43)-C(53)	1.384(10)
C(43)-H(43)	0.9500
C(53)-C(63)	1.390(9)
C(53)-H(53)	0.9500
C(63)-C(103)	1.508(9)
C(73)-C(93)	1.504(10)
C(73)-C(83)	1.534(10)
C(73)-H(73)	1.0000
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800
C(93)-H(93A)	0.9800
C(93)-H(93B)	0.9800
C(93)-H(93C)	0.9800

C(103)-C(113)	1.532(9)
C(103)-C(123)	1.536(9)
C(103)-H(103)	1.0000
C(113)-H(11M)	0.9800
C(113)-H(11N)	0.9800
C(113)-H(11O)	0.9800
C(123)-H(12J)	0.9800
C(123)-H(12K)	0.9800
C(123)-H(12L)	0.9800
Fe(2)-N(14)	1.929(5)
Fe(2)-N(24)	1.938(5)
Fe(2)-C(2)	2.038(9)
C(2)-H(0AA)	0.9800
C(2)-H(0AB)	0.9800
C(2)-H(0AC)	0.9800
N(14)-C(24)	1.359(8)
N(14)-C(15)	1.422(8)
N(24)-C(44)	1.370(8)
N(24)-C(16)	1.414(8)
C(14)-C(24)	1.516(8)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(24)-C(34)	1.383(9)
C(34)-C(44)	1.403(9)
C(34)-H(34)	0.9500
C(44)-C(54)	1.507(9)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(15)-C(65)	1.409(10)
C(15)-C(25)	1.431(8)
C(25)-C(35)	1.381(9)
C(25)-C(75)	1.495(9)
C(35)-C(45)	1.370(10)
C(35)-H(35)	0.9500

C(45)-C(55)	1.412(10)
C(45)-H(45)	0.9500
C(55)-C(65)	1.378(10)
C(55)-H(55)	0.9500
C(65)-C(105)	1.515(9)
C(75)-C(95)	1.516(10)
C(75)-C(85)	1.543(10)
C(75)-H(75)	1.0000
C(85)-H(85A)	0.9800
C(85)-H(85B)	0.9800
C(85)-H(85C)	0.9800
C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(105)-C(125)	1.517(11)
C(105)-C(115)	1.519(14)
C(105)-H(105)	1.0000
C(115)-H(11A)	0.9800
C(115)-H(11B)	0.9800
C(115)-H(11C)	0.9800
C(125)-H(12A)	0.9800
C(125)-H(12B)	0.9800
C(125)-H(12C)	0.9800
C(16)-C(26)	1.398(9)
C(16)-C(66)	1.419(9)
C(26)-C(36)	1.367(10)
C(26)-C(76)	1.514(11)
C(36)-C(46)	1.371(11)
C(36)-H(36)	0.9500
C(46)-C(56)	1.394(11)
C(46)-H(46)	0.9500
C(56)-C(66)	1.387(9)
C(56)-H(56)	0.9500
C(66)-C(106)	1.518(9)
C(76)-C(86)	1.530(13)
C(76)-C(96)	1.533(15)

C(76)-H(76)	1.0000
C(86)-H(86A)	0.9800
C(86)-H(86B)	0.9800
C(86)-H(86C)	0.9800
C(96)-H(96A)	0.9800
C(96)-H(96B)	0.9800
C(96)-H(96C)	0.9800
C(106)-C(116)	1.525(9)
C(106)-C(126)	1.537(10)
C(106)-H(106)	1.0000
C(116)-H(11D)	0.9800
C(116)-H(11E)	0.9800
C(116)-H(11F)	0.9800
C(126)-H(12D)	0.9800
C(126)-H(12E)	0.9800
C(126)-H(12F)	0.9800
K(1)-O(70)	2.802(5)
K(1)-O(40)	2.866(5)
K(1)-O(90)	2.897(6)
K(1)-O(60)	2.915(5)
K(1)-O(80)	2.920(5)
K(1)-O(10)	2.926(6)
K(1)-O(30)	2.981(6)
K(1)-O(50)	2.986(5)
K(1)-O(20)	3.025(6)
K(1)-O(100)	3.082(6)
K(1)-C(130)	3.531(7)
O(10)-C(10)	1.416(11)
O(10)-C(120)	1.431(10)
O(20)-C(30)	1.408(10)
O(20)-C(20)	1.410(11)
O(30)-C(50)	1.385(10)
O(30)-C(40)	1.413(10)
O(40)-C(70)	1.401(10)
O(40)-C(60)	1.440(9)
O(50)-C(90)	1.377(10)

O(50)-C(80)	1.427(10)
O(60)-C(100)	1.397(9)
O(60)-C(110)	1.435(11)
O(70)-C(200)	1.389(9)
O(70)-C(130)	1.426(8)
O(80)-C(140)	1.422(9)
O(80)-C(150)	1.423(10)
O(90)-C(160)	1.405(10)
O(90)-C(170)	1.413(11)
O(100)-C(190)	1.415(10)
O(100)-C(180)	1.431(11)
C(10)-C(20)	1.427(14)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(30)-C(40)	1.460(12)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(40)-H(40C)	0.9900
C(40)-H(40D)	0.9900
C(50)-C(60)	1.507(12)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(70)-C(80)	1.502(12)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(90)-C(100)	1.485(13)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(100)-H(10C)	0.9900
C(100)-H(10D)	0.9900

C(110)-C(120)	1.457(14)
C(110)-H(11P)	0.9900
C(110)-H(11Q)	0.9900
C(120)-H(12M)	0.9900
C(120)-H(12N)	0.9900
C(130)-C(140)	1.502(11)
C(130)-H(13A)	0.9900
C(130)-H(13B)	0.9900
C(140)-H(14D)	0.9900
C(140)-H(14E)	0.9900
C(150)-C(160)	1.501(14)
C(150)-H(15A)	0.9900
C(150)-H(15B)	0.9900
C(160)-H(16A)	0.9900
C(160)-H(16B)	0.9900
C(170)-C(180)	1.521(14)
C(170)-H(17A)	0.9900
C(170)-H(17B)	0.9900
C(180)-H(18A)	0.9900
C(180)-H(18B)	0.9900
C(190)-C(200)	1.519(11)
C(190)-H(19A)	0.9900
C(190)-H(19B)	0.9900
C(200)-H(20C)	0.9900
C(200)-H(20D)	0.9900
K(2)-O(160)	2.854(5)
K(2)-O(160)#1	2.854(5)
K(2)-O(120)#1	2.904(5)
K(2)-O(120)	2.904(5)
K(2)-O(150)	2.974(7)
K(2)-O(140)	2.981(6)
K(2)-O(110)	2.986(7)
K(2)-O(130)#1	2.996(5)
K(2)-O(130)	2.996(5)
K(2)-O(170)	3.001(7)
O(110)-C(210)	1.419(9)

O(110)-C(210)#1	1.419(9)
O(120)-C(220)	1.402(10)
O(120)-C(230)	1.426(9)
O(130)-C(250)	1.392(9)
O(130)-C(240)	1.437(9)
O(140)-C(260)	1.439(8)
O(140)-C(260)#1	1.439(8)
O(150)-C(8Y)#1	1.481(13)
O(150)-C(8Y)	1.481(13)
O(150)-C(8X)#1	1.482(13)
O(150)-C(8X)	1.482(13)
O(160)-C(7Y)	1.420(11)
O(160)-C(6X)	1.427(11)
O(160)-C(7X)	1.495(11)
O(160)-C(6Y)	1.496(11)
C(210)-C(220)	1.473(13)
C(210)-H(21A)	0.9900
C(210)-H(21B)	0.9900
C(220)-H(22A)	0.9900
C(220)-H(22B)	0.9900
C(230)-C(240)	1.490(12)
C(230)-H(23A)	0.9900
C(230)-H(23B)	0.9900
C(240)-H(24A)	0.9900
C(240)-H(24B)	0.9900
C(250)-C(260)	1.492(11)
C(250)-H(25A)	0.9900
C(250)-H(25B)	0.9900
C(260)-H(26A)	0.9900
C(260)-H(26B)	0.9900
C(8X)-C(7X)	1.316(15)
C(8X)-H(8XA)	0.9900
C(8X)-H(8XB)	0.9900
C(7Y)-C(8Y)	1.376(15)
C(7Y)-H(7YA)	0.9900
C(7Y)-H(7YB)	0.9900

C(6X)-C(5X)	1.378(16)
C(6X)-H(6XA)	0.9900
C(6X)-H(6XB)	0.9900
C(5Y)-C(6Y)	1.336(15)
C(5Y)-O(170)	1.466(12)
C(5Y)-H(5YA)	0.9900
C(5Y)-H(5YB)	0.9900
O(170)-C(5Y)#1	1.466(12)
O(170)-C(5X)	1.477(12)
O(170)-C(5X)#1	1.477(13)
K(3)-O(230)#1	2.883(6)
K(3)-O(230)	2.883(6)
K(3)-O(190)	2.884(7)
K(3)-O(190)#1	2.884(7)
K(3)-O(180)	2.896(8)
K(3)-O(200)#1	2.919(9)
K(3)-O(200)	2.919(9)
K(3)-O(220)	2.956(6)
K(3)-O(220)#1	2.956(6)
K(3)-O(210)	3.003(13)
O(180)-C(310)#1	1.371(10)
O(180)-C(310)	1.371(10)
O(190)-C(330)	1.348(10)
O(190)-C(320)	1.357(14)
O(200)-C(340)	1.262(10)
O(200)-C(350)	1.414(11)
O(220)-C(370)	1.361(12)
O(220)-C(380)	1.364(12)
O(230)-C(400)	1.356(12)
O(230)-C(390)	1.369(11)
C(310)-C(320)	1.352(13)
C(310)-H(31A)	0.9900
C(310)-H(31B)	0.9900
C(320)-H(32A)	0.9900
C(320)-H(32B)	0.9900
C(330)-C(340)	1.356(13)

C(330)-H(33A)	0.9900
C(330)-H(33B)	0.9900
C(360)-O(210)	1.326(13)
C(360)-C(350)	1.377(17)
C(360)-H(36A)	0.9900
C(360)-H(36B)	0.9900
C(370)-C(370)#1	1.28(2)
C(370)-H(37A)	0.9900
C(370)-H(37B)	0.9900
C(380)-C(390)	1.340(14)
C(380)-H(38A)	0.9900
C(380)-H(38B)	0.9900
C(390)-H(39A)	0.9900
C(390)-H(39B)	0.9900
O(1X)-C(2X)	1.375(11)
O(1X)-C(3X)	1.439(12)
C(3X)-C(4X)	1.444(13)
C(3X)-H(3XA)	0.9900
C(3X)-H(3XB)	0.9900
C(4X)-H(4XA)	0.9800
C(4X)-H(4XB)	0.9800
C(4X)-H(4XC)	0.9800
C(1X)-C(2X)	1.500(15)
C(1X)-H(1XA)	0.9800
C(1X)-H(1XB)	0.9800
C(1X)-H(1XC)	0.9800
C(2X)-H(2XA)	0.9900
C(2X)-H(2XB)	0.9900
C(400)-C(400)#1	1.32(2)
C(400)-H(40A)	0.9900
C(400)-H(40B)	0.9900
O(210)-C(360)#1	1.326(13)
C(340)-H(34A)	0.9900
C(340)-H(34B)	0.9900
C(350)-H(35A)	0.9900
C(350)-H(35B)	0.9900

C(5X)-H(5XA)	0.9900
C(5X)-H(5XB)	0.9900
C(6Y)-H(6YA)	0.9900
C(6Y)-H(6YB)	0.9900
C(7X)-H(7XA)	0.9900
C(7X)-H(7XB)	0.9900
C(8Y)-H(8YA)	0.9900
C(8Y)-H(8YB)	0.9900

N(21)-Fe(1)-N(11)	97.0(2)
N(21)-Fe(1)-C(1)	131.5(3)
N(11)-Fe(1)-C(1)	131.5(3)
Fe(1)-C(1)-H(1A)	109.5
Fe(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Fe(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(21)-N(11)-C(12)	119.6(5)
C(21)-N(11)-Fe(1)	123.1(4)
C(12)-N(11)-Fe(1)	116.6(4)
C(41)-N(21)-C(13)	118.6(5)
C(41)-N(21)-Fe(1)	123.8(4)
C(13)-N(21)-Fe(1)	117.5(4)
C(21)-C(11)-H(11G)	109.5
C(21)-C(11)-H(11H)	109.5
H(11G)-C(11)-H(11H)	109.5
C(21)-C(11)-H(11I)	109.5
H(11G)-C(11)-H(11I)	109.5
H(11H)-C(11)-H(11I)	109.5
N(11)-C(21)-C(31)	122.4(5)
N(11)-C(21)-C(11)	118.6(5)
C(31)-C(21)-C(11)	119.0(5)
C(21)-C(31)-C(41)	130.8(5)
C(21)-C(31)-H(31)	114.6
C(41)-C(31)-H(31)	114.6

N(21)-C(41)-C(31)	122.2(5)
N(21)-C(41)-C(51)	120.1(5)
C(31)-C(41)-C(51)	117.6(5)
C(41)-C(51)-H(51A)	109.5
C(41)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(41)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(62)-C(12)-N(11)	121.5(5)
C(62)-C(12)-C(22)	119.2(5)
N(11)-C(12)-C(22)	119.0(6)
C(32)-C(22)-C(12)	118.6(6)
C(32)-C(22)-C(72)	121.1(5)
C(12)-C(22)-C(72)	120.3(5)
C(42)-C(32)-C(22)	122.0(6)
C(42)-C(32)-H(32)	119.0
C(22)-C(32)-H(32)	119.0
C(32)-C(42)-C(52)	119.3(6)
C(32)-C(42)-H(42)	120.4
C(52)-C(42)-H(42)	120.4
C(62)-C(52)-C(42)	121.1(6)
C(62)-C(52)-H(52)	119.4
C(42)-C(52)-H(52)	119.4
C(52)-C(62)-C(12)	119.7(6)
C(52)-C(62)-C(102)	118.8(6)
C(12)-C(62)-C(102)	121.5(5)
C(92)-C(72)-C(22)	113.8(6)
C(92)-C(72)-C(82)	110.2(6)
C(22)-C(72)-C(82)	109.3(6)
C(92)-C(72)-H(72)	107.7
C(22)-C(72)-H(72)	107.7
C(82)-C(72)-H(72)	107.7
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
H(82B)-C(82)-H(82C)	109.5
C(72)-C(92)-H(92A)	109.5
C(72)-C(92)-H(92B)	109.5
H(92A)-C(92)-H(92B)	109.5
C(72)-C(92)-H(92C)	109.5
H(92A)-C(92)-H(92C)	109.5
H(92B)-C(92)-H(92C)	109.5
C(62)-C(102)-C(112)	111.1(6)
C(62)-C(102)-C(122)	112.2(6)
C(112)-C(102)-C(122)	109.9(6)
C(62)-C(102)-H(102)	107.8
C(112)-C(102)-H(102)	107.8
C(122)-C(102)-H(102)	107.8
C(102)-C(112)-H(11J)	109.5
C(102)-C(112)-H(11K)	109.5
H(11J)-C(112)-H(11K)	109.5
C(102)-C(112)-H(11L)	109.5
H(11J)-C(112)-H(11L)	109.5
H(11K)-C(112)-H(11L)	109.5
C(102)-C(122)-H(12G)	109.5
C(102)-C(122)-H(12H)	109.5
H(12G)-C(122)-H(12H)	109.5
C(102)-C(122)-H(12I)	109.5
H(12G)-C(122)-H(12I)	109.5
H(12H)-C(122)-H(12I)	109.5
C(63)-C(13)-C(23)	120.5(5)
C(63)-C(13)-N(21)	120.0(5)
C(23)-C(13)-N(21)	119.4(5)
C(33)-C(23)-C(13)	117.2(5)
C(33)-C(23)-C(73)	121.5(6)
C(13)-C(23)-C(73)	121.3(6)
C(43)-C(33)-C(23)	122.7(7)
C(43)-C(33)-H(33)	118.7
C(23)-C(33)-H(33)	118.7

C(33)-C(43)-C(53)	120.1(6)
C(33)-C(43)-H(43)	119.9
C(53)-C(43)-H(43)	119.9
C(43)-C(53)-C(63)	121.2(6)
C(43)-C(53)-H(53)	119.4
C(63)-C(53)-H(53)	119.4
C(53)-C(63)-C(13)	118.3(6)
C(53)-C(63)-C(103)	120.7(5)
C(13)-C(63)-C(103)	121.0(5)
C(93)-C(73)-C(23)	112.5(6)
C(93)-C(73)-C(83)	111.9(6)
C(23)-C(73)-C(83)	111.3(5)
C(93)-C(73)-H(73)	106.9
C(23)-C(73)-H(73)	106.9
C(83)-C(73)-H(73)	106.9
C(73)-C(83)-H(83A)	109.5
C(73)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(73)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
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(63)-C(103)-C(113)	110.4(5)
C(63)-C(103)-C(123)	112.7(6)
C(113)-C(103)-C(123)	110.8(6)
C(63)-C(103)-H(103)	107.6
C(113)-C(103)-H(103)	107.6
C(123)-C(103)-H(103)	107.6
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
N(14)-Fe(2)-N(24)	97.5(2)
N(14)-Fe(2)-C(2)	132.7(4)
N(24)-Fe(2)-C(2)	129.6(3)
Fe(2)-C(2)-H(0AA)	109.5
Fe(2)-C(2)-H(0AB)	109.5
H(0AA)-C(2)-H(0AB)	109.5
Fe(2)-C(2)-H(0AC)	109.5
H(0AA)-C(2)-H(0AC)	109.5
H(0AB)-C(2)-H(0AC)	109.5
C(24)-N(14)-C(15)	118.3(5)
C(24)-N(14)-Fe(2)	123.3(4)
C(15)-N(14)-Fe(2)	118.4(4)
C(44)-N(24)-C(16)	118.6(5)
C(44)-N(24)-Fe(2)	123.4(4)
C(16)-N(24)-Fe(2)	118.0(4)
C(24)-C(14)-H(14A)	109.5
C(24)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(24)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(14)-C(24)-C(34)	123.1(5)
N(14)-C(24)-C(14)	119.5(6)
C(34)-C(24)-C(14)	117.4(6)
C(24)-C(34)-C(44)	130.9(6)
C(24)-C(34)-H(34)	114.5
C(44)-C(34)-H(34)	114.5

N(24)-C(44)-C(34)	121.8(6)
N(24)-C(44)-C(54)	118.0(6)
C(34)-C(44)-C(54)	120.2(6)
C(44)-C(54)-H(54A)	109.5
C(44)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(44)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(65)-C(15)-N(14)	121.5(6)
C(65)-C(15)-C(25)	119.1(6)
N(14)-C(15)-C(25)	119.3(6)
C(35)-C(25)-C(15)	117.6(6)
C(35)-C(25)-C(75)	121.3(5)
C(15)-C(25)-C(75)	120.9(6)
C(45)-C(35)-C(25)	123.9(6)
C(45)-C(35)-H(35)	118.1
C(25)-C(35)-H(35)	118.1
C(35)-C(45)-C(55)	117.9(7)
C(35)-C(45)-H(45)	121.0
C(55)-C(45)-H(45)	121.0
C(65)-C(55)-C(45)	120.7(7)
C(65)-C(55)-H(55)	119.6
C(45)-C(55)-H(55)	119.6
C(55)-C(65)-C(15)	120.4(6)
C(55)-C(65)-C(105)	120.0(7)
C(15)-C(65)-C(105)	119.6(7)
C(25)-C(75)-C(95)	114.7(6)
C(25)-C(75)-C(85)	109.1(6)
C(95)-C(75)-C(85)	112.0(6)
C(25)-C(75)-H(75)	106.9
C(95)-C(75)-H(75)	106.9
C(85)-C(75)-H(75)	106.9
C(75)-C(85)-H(85A)	109.5
C(75)-C(85)-H(85B)	109.5
H(85A)-C(85)-H(85B)	109.5

C(75)-C(85)-H(85C)	109.5
H(85A)-C(85)-H(85C)	109.5
H(85B)-C(85)-H(85C)	109.5
C(75)-C(95)-H(95A)	109.5
C(75)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(75)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
C(65)-C(105)-C(125)	110.0(7)
C(65)-C(105)-C(115)	112.3(7)
C(125)-C(105)-C(115)	108.7(7)
C(65)-C(105)-H(105)	108.6
C(125)-C(105)-H(105)	108.6
C(115)-C(105)-H(105)	108.6
C(105)-C(115)-H(11A)	109.5
C(105)-C(115)-H(11B)	109.5
H(11A)-C(115)-H(11B)	109.5
C(105)-C(115)-H(11C)	109.5
H(11A)-C(115)-H(11C)	109.5
H(11B)-C(115)-H(11C)	109.5
C(105)-C(125)-H(12A)	109.5
C(105)-C(125)-H(12B)	109.5
H(12A)-C(125)-H(12B)	109.5
C(105)-C(125)-H(12C)	109.5
H(12A)-C(125)-H(12C)	109.5
H(12B)-C(125)-H(12C)	109.5
C(26)-C(16)-N(24)	121.2(6)
C(26)-C(16)-C(66)	119.1(6)
N(24)-C(16)-C(66)	119.7(5)
C(36)-C(26)-C(16)	119.5(7)
C(36)-C(26)-C(76)	121.7(7)
C(16)-C(26)-C(76)	118.7(7)
C(26)-C(36)-C(46)	122.4(7)
C(26)-C(36)-H(36)	118.8
C(46)-C(36)-H(36)	118.8

C(36)-C(46)-C(56)	118.9(7)
C(36)-C(46)-H(46)	120.6
C(56)-C(46)-H(46)	120.6
C(66)-C(56)-C(46)	120.7(7)
C(66)-C(56)-H(56)	119.7
C(46)-C(56)-H(56)	119.7
C(56)-C(66)-C(16)	119.3(6)
C(56)-C(66)-C(106)	120.9(6)
C(16)-C(66)-C(106)	119.7(5)
C(26)-C(76)-C(86)	111.1(9)
C(26)-C(76)-C(96)	112.3(8)
C(86)-C(76)-C(96)	111.1(10)
C(26)-C(76)-H(76)	107.4
C(86)-C(76)-H(76)	107.4
C(96)-C(76)-H(76)	107.4
C(76)-C(86)-H(86A)	109.5
C(76)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	109.5
C(76)-C(86)-H(86C)	109.5
H(86A)-C(86)-H(86C)	109.5
H(86B)-C(86)-H(86C)	109.5
C(76)-C(96)-H(96A)	109.5
C(76)-C(96)-H(96B)	109.5
H(96A)-C(96)-H(96B)	109.5
C(76)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5
H(96B)-C(96)-H(96C)	109.5
C(66)-C(106)-C(116)	111.4(5)
C(66)-C(106)-C(126)	114.3(6)
C(116)-C(106)-C(126)	108.4(6)
C(66)-C(106)-H(106)	107.5
C(116)-C(106)-H(106)	107.5
C(126)-C(106)-H(106)	107.5
C(106)-C(116)-H(11D)	109.5
C(106)-C(116)-H(11E)	109.5
H(11D)-C(116)-H(11E)	109.5

C(106)-C(116)-H(11F)	109.5
H(11D)-C(116)-H(11F)	109.5
H(11E)-C(116)-H(11F)	109.5
C(106)-C(126)-H(12D)	109.5
C(106)-C(126)-H(12E)	109.5
H(12D)-C(126)-H(12E)	109.5
C(106)-C(126)-H(12F)	109.5
H(12D)-C(126)-H(12F)	109.5
H(12E)-C(126)-H(12F)	109.5
O(70)-K(1)-O(40)	138.17(17)
O(70)-K(1)-O(90)	82.38(15)
O(40)-K(1)-O(90)	66.44(16)
O(70)-K(1)-O(60)	66.07(15)
O(40)-K(1)-O(60)	113.40(17)
O(90)-K(1)-O(60)	129.82(19)
O(70)-K(1)-O(80)	58.80(14)
O(40)-K(1)-O(80)	118.19(17)
O(90)-K(1)-O(80)	58.52(17)
O(60)-K(1)-O(80)	122.33(16)
O(70)-K(1)-O(10)	69.53(16)
O(40)-K(1)-O(10)	149.16(18)
O(90)-K(1)-O(10)	143.17(16)
O(60)-K(1)-O(10)	59.05(18)
O(80)-K(1)-O(10)	86.09(17)
O(70)-K(1)-O(30)	139.75(16)
O(40)-K(1)-O(30)	58.97(16)
O(90)-K(1)-O(30)	75.14(17)
O(60)-K(1)-O(30)	151.29(18)
O(80)-K(1)-O(30)	80.97(16)
O(10)-K(1)-O(30)	111.66(18)
O(70)-K(1)-O(50)	116.03(15)
O(40)-K(1)-O(50)	57.66(16)
O(90)-K(1)-O(50)	111.94(17)
O(60)-K(1)-O(50)	57.42(16)
O(80)-K(1)-O(50)	168.59(17)
O(10)-K(1)-O(50)	101.81(16)

O(30)-K(1)-O(50)	103.31(15)
O(70)-K(1)-O(20)	108.47(15)
O(40)-K(1)-O(20)	109.88(16)
O(90)-K(1)-O(20)	115.63(17)
O(60)-K(1)-O(20)	111.06(18)
O(80)-K(1)-O(20)	73.79(16)
O(10)-K(1)-O(20)	56.11(16)
O(30)-K(1)-O(20)	55.81(16)
O(50)-K(1)-O(20)	117.43(15)
O(70)-K(1)-O(100)	56.34(15)
O(40)-K(1)-O(100)	82.86(17)
O(90)-K(1)-O(100)	57.34(17)
O(60)-K(1)-O(100)	72.61(18)
O(80)-K(1)-O(100)	89.67(16)
O(10)-K(1)-O(100)	118.16(17)
O(30)-K(1)-O(100)	128.42(18)
O(50)-K(1)-O(100)	79.38(15)
O(20)-K(1)-O(100)	162.44(15)
O(70)-K(1)-C(130)	22.47(16)
O(40)-K(1)-C(130)	149.9(2)
O(90)-K(1)-C(130)	83.99(18)
O(60)-K(1)-C(130)	80.61(17)
O(80)-K(1)-C(130)	41.72(17)
O(10)-K(1)-C(130)	60.97(18)
O(30)-K(1)-C(130)	120.47(17)
O(50)-K(1)-C(130)	136.11(17)
O(20)-K(1)-C(130)	87.49(17)
O(100)-K(1)-C(130)	76.03(17)
C(10)-O(10)-C(120)	112.9(7)
C(10)-O(10)-K(1)	120.6(5)
C(120)-O(10)-K(1)	115.8(5)
C(30)-O(20)-C(20)	115.5(7)
C(30)-O(20)-K(1)	110.4(5)
C(20)-O(20)-K(1)	107.6(5)
C(50)-O(30)-C(40)	113.1(6)
C(50)-O(30)-K(1)	115.7(5)

C(40)-O(30)-K(1)	119.5(5)
C(70)-O(40)-C(60)	113.2(6)
C(70)-O(40)-K(1)	117.9(5)
C(60)-O(40)-K(1)	113.2(4)
C(90)-O(50)-C(80)	113.1(7)
C(90)-O(50)-K(1)	112.5(5)
C(80)-O(50)-K(1)	111.9(4)
C(100)-O(60)-C(110)	115.2(7)
C(100)-O(60)-K(1)	116.4(4)
C(110)-O(60)-K(1)	112.7(5)
C(200)-O(70)-C(130)	113.3(6)
C(200)-O(70)-K(1)	128.2(4)
C(130)-O(70)-K(1)	108.9(4)
C(140)-O(80)-C(150)	113.7(7)
C(140)-O(80)-K(1)	117.8(4)
C(150)-O(80)-K(1)	110.2(5)
C(160)-O(90)-C(170)	116.0(7)
C(160)-O(90)-K(1)	120.2(5)
C(170)-O(90)-K(1)	111.1(5)
C(190)-O(100)-C(180)	113.1(7)
C(190)-O(100)-K(1)	108.6(5)
C(180)-O(100)-K(1)	116.4(5)
O(10)-C(10)-C(20)	108.8(8)
O(10)-C(10)-H(10A)	109.9
C(20)-C(10)-H(10A)	109.9
O(10)-C(10)-H(10B)	109.9
C(20)-C(10)-H(10B)	109.9
H(10A)-C(10)-H(10B)	108.3
O(20)-C(20)-C(10)	111.7(8)
O(20)-C(20)-H(20A)	109.3
C(10)-C(20)-H(20A)	109.3
O(20)-C(20)-H(20B)	109.3
C(10)-C(20)-H(20B)	109.3
H(20A)-C(20)-H(20B)	107.9
O(20)-C(30)-C(40)	110.2(7)
O(20)-C(30)-H(30A)	109.6

C(40)-C(30)-H(30A)	109.6
O(20)-C(30)-H(30B)	109.6
C(40)-C(30)-H(30B)	109.6
H(30A)-C(30)-H(30B)	108.1
O(30)-C(40)-C(30)	110.5(7)
O(30)-C(40)-H(40C)	109.5
C(30)-C(40)-H(40C)	109.5
O(30)-C(40)-H(40D)	109.5
C(30)-C(40)-H(40D)	109.5
H(40C)-C(40)-H(40D)	108.1
O(30)-C(50)-C(60)	109.9(7)
O(30)-C(50)-H(50A)	109.7
C(60)-C(50)-H(50A)	109.7
O(30)-C(50)-H(50B)	109.7
C(60)-C(50)-H(50B)	109.7
H(50A)-C(50)-H(50B)	108.2
O(40)-C(60)-C(50)	112.2(7)
O(40)-C(60)-H(60A)	109.2
C(50)-C(60)-H(60A)	109.2
O(40)-C(60)-H(60B)	109.2
C(50)-C(60)-H(60B)	109.2
H(60A)-C(60)-H(60B)	107.9
O(40)-C(70)-C(80)	106.1(7)
O(40)-C(70)-H(70A)	110.5
C(80)-C(70)-H(70A)	110.5
O(40)-C(70)-H(70B)	110.5
C(80)-C(70)-H(70B)	110.5
H(70A)-C(70)-H(70B)	108.7
O(50)-C(80)-C(70)	110.2(6)
O(50)-C(80)-H(80A)	109.6
C(70)-C(80)-H(80A)	109.6
O(50)-C(80)-H(80B)	109.6
C(70)-C(80)-H(80B)	109.6
H(80A)-C(80)-H(80B)	108.1
O(50)-C(90)-C(100)	110.4(8)
O(50)-C(90)-H(90A)	109.6

C(100)-C(90)-H(90A)	109.6
O(50)-C(90)-H(90B)	109.6
C(100)-C(90)-H(90B)	109.6
H(90A)-C(90)-H(90B)	108.1
O(60)-C(100)-C(90)	109.7(7)
O(60)-C(100)-H(10C)	109.7
C(90)-C(100)-H(10C)	109.7
O(60)-C(100)-H(10D)	109.7
C(90)-C(100)-H(10D)	109.7
H(10C)-C(100)-H(10D)	108.2
O(60)-C(110)-C(120)	112.8(8)
O(60)-C(110)-H(11P)	109.0
C(120)-C(110)-H(11P)	109.0
O(60)-C(110)-H(11Q)	109.0
C(120)-C(110)-H(11Q)	109.0
H(11P)-C(110)-H(11Q)	107.8
O(10)-C(120)-C(110)	110.8(8)
O(10)-C(120)-H(12M)	109.5
C(110)-C(120)-H(12M)	109.5
O(10)-C(120)-H(12N)	109.5
C(110)-C(120)-H(12N)	109.5
H(12M)-C(120)-H(12N)	108.1
O(70)-C(130)-C(140)	111.6(7)
O(70)-C(130)-K(1)	48.7(3)
C(140)-C(130)-K(1)	88.4(4)
O(70)-C(130)-H(13A)	109.3
C(140)-C(130)-H(13A)	109.3
K(1)-C(130)-H(13A)	78.5
O(70)-C(130)-H(13B)	109.3
C(140)-C(130)-H(13B)	109.3
K(1)-C(130)-H(13B)	156.9
H(13A)-C(130)-H(13B)	108.0
O(80)-C(140)-C(130)	108.1(6)
O(80)-C(140)-H(14D)	110.1
C(130)-C(140)-H(14D)	110.1
O(80)-C(140)-H(14E)	110.1

C(130)-C(140)-H(14E)	110.1
H(14D)-C(140)-H(14E)	108.4
O(80)-C(150)-C(160)	113.4(7)
O(80)-C(150)-H(15A)	108.9
C(160)-C(150)-H(15A)	108.9
O(80)-C(150)-H(15B)	108.9
C(160)-C(150)-H(15B)	108.9
H(15A)-C(150)-H(15B)	107.7
O(90)-C(160)-C(150)	108.6(7)
O(90)-C(160)-H(16A)	110.0
C(150)-C(160)-H(16A)	110.0
O(90)-C(160)-H(16B)	110.0
C(150)-C(160)-H(16B)	110.0
H(16A)-C(160)-H(16B)	108.4
O(90)-C(170)-C(180)	112.9(7)
O(90)-C(170)-H(17A)	109.0
C(180)-C(170)-H(17A)	109.0
O(90)-C(170)-H(17B)	109.0
C(180)-C(170)-H(17B)	109.0
H(17A)-C(170)-H(17B)	107.8
O(100)-C(180)-C(170)	107.8(8)
O(100)-C(180)-H(18A)	110.2
C(170)-C(180)-H(18A)	110.2
O(100)-C(180)-H(18B)	110.2
C(170)-C(180)-H(18B)	110.2
H(18A)-C(180)-H(18B)	108.5
O(100)-C(190)-C(200)	113.3(7)
O(100)-C(190)-H(19A)	108.9
C(200)-C(190)-H(19A)	108.9
O(100)-C(190)-H(19B)	108.9
C(200)-C(190)-H(19B)	108.9
H(19A)-C(190)-H(19B)	107.7
O(70)-C(200)-C(190)	107.2(6)
O(70)-C(200)-H(20C)	110.3
C(190)-C(200)-H(20C)	110.3
O(70)-C(200)-H(20D)	110.3

C(190)-C(200)-H(20D)	110.3
H(20C)-C(200)-H(20D)	108.5
O(160)-K(2)-O(160)#1	83.1(2)
O(160)-K(2)-O(120)#1	136.91(16)
O(160)#1-K(2)-O(120)#1	68.06(14)
O(160)-K(2)-O(120)	68.07(14)
O(160)#1-K(2)-O(120)	136.91(16)
O(120)#1-K(2)-O(120)	112.6(2)
O(160)-K(2)-O(150)	57.82(13)
O(160)#1-K(2)-O(150)	57.82(13)
O(120)#1-K(2)-O(150)	79.50(13)
O(120)-K(2)-O(150)	79.50(13)
O(160)-K(2)-O(140)	113.56(14)
O(160)#1-K(2)-O(140)	113.56(13)
O(120)#1-K(2)-O(140)	107.24(13)
O(120)-K(2)-O(140)	107.24(13)
O(150)-K(2)-O(140)	166.90(19)
O(160)-K(2)-O(110)	117.38(14)
O(160)#1-K(2)-O(110)	117.38(14)
O(120)#1-K(2)-O(110)	57.19(12)
O(120)-K(2)-O(110)	57.19(12)
O(150)-K(2)-O(110)	83.32(19)
O(140)-K(2)-O(110)	109.78(19)
O(160)-K(2)-O(130)#1	142.95(15)
O(160)#1-K(2)-O(130)#1	72.48(14)
O(120)#1-K(2)-O(130)#1	57.18(14)
O(120)-K(2)-O(130)#1	146.71(16)
O(150)-K(2)-O(130)#1	123.60(10)
O(140)-K(2)-O(130)#1	56.02(10)
O(110)-K(2)-O(130)#1	98.72(13)
O(160)-K(2)-O(130)	72.48(14)
O(160)#1-K(2)-O(130)	142.95(15)
O(120)#1-K(2)-O(130)	146.71(16)
O(120)-K(2)-O(130)	57.18(14)
O(150)-K(2)-O(130)	123.60(10)
O(140)-K(2)-O(130)	56.02(10)

O(110)-K(2)-O(130)	98.72(13)
O(130)#1-K(2)-O(130)	111.8(2)
O(160)-K(2)-O(170)	57.36(13)
O(160)#1-K(2)-O(170)	57.36(13)
O(120)#1-K(2)-O(170)	121.28(12)
O(120)-K(2)-O(170)	121.28(12)
O(150)-K(2)-O(170)	88.48(19)
O(140)-K(2)-O(170)	78.41(18)
O(110)-K(2)-O(170)	171.8(2)
O(130)#1-K(2)-O(170)	85.80(13)
O(130)-K(2)-O(170)	85.80(13)
C(210)-O(110)-C(210)#1	112.6(9)
C(210)-O(110)-K(2)	114.5(5)
C(210)#1-O(110)-K(2)	114.5(5)
C(220)-O(120)-C(230)	114.3(6)
C(220)-O(120)-K(2)	116.8(5)
C(230)-O(120)-K(2)	114.3(4)
C(250)-O(130)-C(240)	111.7(6)
C(250)-O(130)-K(2)	118.8(4)
C(240)-O(130)-K(2)	118.0(4)
C(260)-O(140)-C(260)#1	110.7(7)
C(260)-O(140)-K(2)	111.1(4)
C(260)#1-O(140)-K(2)	111.1(4)
C(8Y)#1-O(150)-C(8Y)	135(3)
C(8X)#1-O(150)-C(8X)	108.5(17)
C(8Y)#1-O(150)-K(2)	102.9(10)
C(8Y)-O(150)-K(2)	102.9(10)
C(8X)#1-O(150)-K(2)	120.0(7)
C(8X)-O(150)-K(2)	120.0(8)
C(6X)-O(160)-C(7X)	108.7(9)
C(7Y)-O(160)-C(6Y)	110.4(10)
C(7Y)-O(160)-K(2)	129.1(7)
C(6X)-O(160)-K(2)	128.5(7)
C(7X)-O(160)-K(2)	107.8(7)
C(6Y)-O(160)-K(2)	109.5(7)
O(110)-C(210)-C(220)	109.6(7)

O(110)-C(210)-H(21A)	109.7
C(220)-C(210)-H(21A)	109.7
O(110)-C(210)-H(21B)	109.7
C(220)-C(210)-H(21B)	109.7
H(21A)-C(210)-H(21B)	108.2
O(120)-C(220)-C(210)	110.2(7)
O(120)-C(220)-H(22A)	109.6
C(210)-C(220)-H(22A)	109.6
O(120)-C(220)-H(22B)	109.6
C(210)-C(220)-H(22B)	109.6
H(22A)-C(220)-H(22B)	108.1
O(120)-C(230)-C(240)	111.3(6)
O(120)-C(230)-H(23A)	109.4
C(240)-C(230)-H(23A)	109.4
O(120)-C(230)-H(23B)	109.4
C(240)-C(230)-H(23B)	109.4
H(23A)-C(230)-H(23B)	108.0
O(130)-C(240)-C(230)	108.7(6)
O(130)-C(240)-H(24A)	110.0
C(230)-C(240)-H(24A)	110.0
O(130)-C(240)-H(24B)	110.0
C(230)-C(240)-H(24B)	110.0
H(24A)-C(240)-H(24B)	108.3
O(130)-C(250)-C(260)	109.9(6)
O(130)-C(250)-H(25A)	109.7
C(260)-C(250)-H(25A)	109.7
O(130)-C(250)-H(25B)	109.7
C(260)-C(250)-H(25B)	109.7
H(25A)-C(250)-H(25B)	108.2
O(140)-C(260)-C(250)	107.4(6)
O(140)-C(260)-H(26A)	110.2
C(250)-C(260)-H(26A)	110.2
O(140)-C(260)-H(26B)	110.2
C(250)-C(260)-H(26B)	110.2
H(26A)-C(260)-H(26B)	108.5
C(7X)-C(8X)-O(150)	106.9(15)

C(7X)-C(8X)-H(8XA)	110.3
O(150)-C(8X)-H(8XA)	110.3
C(7X)-C(8X)-H(8XB)	110.3
O(150)-C(8X)-H(8XB)	110.3
H(8XA)-C(8X)-H(8XB)	108.6
C(8Y)-C(7Y)-O(160)	99.1(14)
C(8Y)-C(7Y)-H(7YA)	111.9
O(160)-C(7Y)-H(7YA)	111.9
C(8Y)-C(7Y)-H(7YB)	111.9
O(160)-C(7Y)-H(7YB)	111.9
H(7YA)-C(7Y)-H(7YB)	109.6
C(5X)-C(6X)-O(160)	97.4(13)
C(5X)-C(6X)-H(6XA)	112.3
O(160)-C(6X)-H(6XA)	112.3
C(5X)-C(6X)-H(6XB)	112.3
O(160)-C(6X)-H(6XB)	112.3
H(6XA)-C(6X)-H(6XB)	109.9
C(6Y)-C(5Y)-O(170)	108.6(14)
C(6Y)-C(5Y)-H(5YA)	110.0
O(170)-C(5Y)-H(5YA)	110.0
C(6Y)-C(5Y)-H(5YB)	110.0
O(170)-C(5Y)-H(5YB)	110.0
H(5YA)-C(5Y)-H(5YB)	108.3
C(5Y)#1-O(170)-C(5Y)	104.5(15)
C(5X)-O(170)-C(5X)#1	134(2)
C(5Y)#1-O(170)-K(2)	119.5(7)
C(5Y)-O(170)-K(2)	119.5(7)
C(5X)-O(170)-K(2)	102.3(10)
C(5X)#1-O(170)-K(2)	102.3(10)
O(230)#1-K(3)-O(230)	58.3(2)
O(230)#1-K(3)-O(190)	158.2(3)
O(230)-K(3)-O(190)	100.4(3)
O(230)#1-K(3)-O(190)#1	100.4(3)
O(230)-K(3)-O(190)#1	158.2(3)
O(190)-K(3)-O(190)#1	100.2(4)
O(230)#1-K(3)-O(180)	129.46(18)

O(230)-K(3)-O(180)	129.46(19)
O(190)-K(3)-O(180)	58.50(17)
O(190)#1-K(3)-O(180)	58.50(17)
O(230)#1-K(3)-O(200)#1	69.4(4)
O(230)-K(3)-O(200)#1	114.4(3)
O(190)-K(3)-O(200)#1	129.4(5)
O(190)#1-K(3)-O(200)#1	55.2(2)
O(180)-K(3)-O(200)#1	113.4(2)
O(230)#1-K(3)-O(200)	114.4(3)
O(230)-K(3)-O(200)	69.4(4)
O(190)-K(3)-O(200)	55.2(2)
O(190)#1-K(3)-O(200)	129.4(5)
O(180)-K(3)-O(200)	113.4(2)
O(200)#1-K(3)-O(200)	103.5(7)
O(230)#1-K(3)-O(220)	86.15(18)
O(230)-K(3)-O(220)	57.74(16)
O(190)-K(3)-O(220)	77.3(2)
O(190)#1-K(3)-O(220)	121.0(2)
O(180)-K(3)-O(220)	72.3(2)
O(200)#1-K(3)-O(220)	152.6(4)
O(200)-K(3)-O(220)	97.7(4)
O(230)#1-K(3)-O(220)#1	57.74(16)
O(230)-K(3)-O(220)#1	86.15(18)
O(190)-K(3)-O(220)#1	121.0(2)
O(190)#1-K(3)-O(220)#1	77.3(2)
O(180)-K(3)-O(220)#1	72.3(2)
O(200)#1-K(3)-O(220)#1	97.7(4)
O(200)-K(3)-O(220)#1	152.6(4)
O(220)-K(3)-O(220)#1	57.3(2)
O(230)#1-K(3)-O(210)	74.8(3)
O(230)-K(3)-O(210)	74.8(3)
O(190)-K(3)-O(210)	105.9(2)
O(190)#1-K(3)-O(210)	105.9(2)
O(180)-K(3)-O(210)	150.8(4)
O(200)#1-K(3)-O(210)	54.7(3)
O(200)-K(3)-O(210)	54.7(3)

O(220)-K(3)-O(210)	131.8(3)
O(220)#1-K(3)-O(210)	131.8(3)
C(310)#1-O(180)-C(310)	134.0(15)
C(310)#1-O(180)-K(3)	111.3(7)
C(310)-O(180)-K(3)	111.3(7)
C(330)-O(190)-C(320)	116.4(9)
C(330)-O(190)-K(3)	123.0(7)
C(320)-O(190)-K(3)	120.5(7)
C(340)-O(200)-C(350)	123.7(11)
C(340)-O(200)-K(3)	120.2(8)
C(350)-O(200)-K(3)	115.8(8)
C(370)-O(220)-C(380)	115.1(11)
C(370)-O(220)-K(3)	115.3(6)
C(380)-O(220)-K(3)	115.0(6)
C(400)-O(230)-C(390)	116.2(9)
C(400)-O(230)-K(3)	115.1(6)
C(390)-O(230)-K(3)	116.8(6)
C(320)-C(310)-O(180)	127.5(11)
C(320)-C(310)-H(31A)	105.4
O(180)-C(310)-H(31A)	105.4
C(320)-C(310)-H(31B)	105.4
O(180)-C(310)-H(31B)	105.4
H(31A)-C(310)-H(31B)	106.0
C(310)-C(320)-O(190)	115.1(11)
C(310)-C(320)-H(32A)	108.5
O(190)-C(320)-H(32A)	108.5
C(310)-C(320)-H(32B)	108.5
O(190)-C(320)-H(32B)	108.5
H(32A)-C(320)-H(32B)	107.5
O(190)-C(330)-C(340)	116.2(10)
O(190)-C(330)-H(33A)	108.2
C(340)-C(330)-H(33A)	108.2
O(190)-C(330)-H(33B)	108.2
C(340)-C(330)-H(33B)	108.2
H(33A)-C(330)-H(33B)	107.4
O(210)-C(360)-C(350)	110.5(15)

O(210)-C(360)-H(36A)	109.5
C(350)-C(360)-H(36A)	109.5
O(210)-C(360)-H(36B)	109.5
C(350)-C(360)-H(36B)	109.5
H(36A)-C(360)-H(36B)	108.1
C(370)#1-C(370)-O(220)	124.9(5)
C(370)#1-C(370)-H(37A)	106.1
O(220)-C(370)-H(37A)	106.1
C(370)#1-C(370)-H(37B)	106.1
O(220)-C(370)-H(37B)	106.1
H(37A)-C(370)-H(37B)	106.3
C(390)-C(380)-O(220)	122.3(10)
C(390)-C(380)-H(38A)	106.8
O(220)-C(380)-H(38A)	106.8
C(390)-C(380)-H(38B)	106.8
O(220)-C(380)-H(38B)	106.8
H(38A)-C(380)-H(38B)	106.6
C(380)-C(390)-O(230)	123.3(10)
C(380)-C(390)-H(39A)	106.5
O(230)-C(390)-H(39A)	106.5
C(380)-C(390)-H(39B)	106.5
O(230)-C(390)-H(39B)	106.5
H(39A)-C(390)-H(39B)	106.5
C(2X)-O(1X)-C(3X)	113.5(8)
O(1X)-C(3X)-C(4X)	110.2(9)
O(1X)-C(3X)-H(3XA)	109.6
C(4X)-C(3X)-H(3XA)	109.6
O(1X)-C(3X)-H(3XB)	109.6
C(4X)-C(3X)-H(3XB)	109.6
H(3XA)-C(3X)-H(3XB)	108.1
C(3X)-C(4X)-H(4XA)	109.5
C(3X)-C(4X)-H(4XB)	109.5
H(4XA)-C(4X)-H(4XB)	109.5
C(3X)-C(4X)-H(4XC)	109.5
H(4XA)-C(4X)-H(4XC)	109.5
H(4XB)-C(4X)-H(4XC)	109.5

C(2X)-C(1X)-H(1XA)	109.5
C(2X)-C(1X)-H(1XB)	109.5
H(1XA)-C(1X)-H(1XB)	109.5
C(2X)-C(1X)-H(1XC)	109.5
H(1XA)-C(1X)-H(1XC)	109.5
H(1XB)-C(1X)-H(1XC)	109.5
O(1X)-C(2X)-C(1X)	111.1(9)
O(1X)-C(2X)-H(2XA)	109.4
C(1X)-C(2X)-H(2XA)	109.4
O(1X)-C(2X)-H(2XB)	109.4
C(1X)-C(2X)-H(2XB)	109.4
H(2XA)-C(2X)-H(2XB)	108.0
C(400)#1-C(400)-O(230)	123.4(5)
C(400)#1-C(400)-H(40A)	106.5
O(230)-C(400)-H(40A)	106.5
C(400)#1-C(400)-H(40B)	106.5
O(230)-C(400)-H(40B)	106.5
H(40A)-C(400)-H(40B)	106.5
C(360)#1-O(210)-C(360)	102(2)
C(360)#1-O(210)-K(3)	121.3(9)
C(360)-O(210)-K(3)	121.3(9)
O(200)-C(340)-C(330)	125.3(11)
O(200)-C(340)-H(34A)	106.0
C(330)-C(340)-H(34A)	106.0
O(200)-C(340)-H(34B)	106.0
C(330)-C(340)-H(34B)	106.0
H(34A)-C(340)-H(34B)	106.3
C(360)-C(350)-O(200)	116.4(16)
C(360)-C(350)-H(35A)	108.2
O(200)-C(350)-H(35A)	108.2
C(360)-C(350)-H(35B)	108.2
O(200)-C(350)-H(35B)	108.2
H(35A)-C(350)-H(35B)	107.3
C(6X)-C(5X)-O(170)	127.3(16)
C(6X)-C(5X)-H(5XA)	105.5
O(170)-C(5X)-H(5XA)	105.5

C(6X)-C(5X)-H(5XB)	105.5
O(170)-C(5X)-H(5XB)	105.5
H(5XA)-C(5X)-H(5XB)	106.1
C(5Y)-C(6Y)-O(160)	123.2(16)
C(5Y)-C(6Y)-H(6YA)	106.5
O(160)-C(6Y)-H(6YA)	106.5
C(5Y)-C(6Y)-H(6YB)	106.5
O(160)-C(6Y)-H(6YB)	106.5
H(6YA)-C(6Y)-H(6YB)	106.5
C(8X)-C(7X)-O(160)	128.4(17)
C(8X)-C(7X)-H(7XA)	105.2
O(160)-C(7X)-H(7XA)	105.2
C(8X)-C(7X)-H(7XB)	105.2
O(160)-C(7X)-H(7XB)	105.2
H(7XA)-C(7X)-H(7XB)	105.9
C(7Y)-C(8Y)-O(150)	129.7(16)
C(7Y)-C(8Y)-H(8YA)	104.8
O(150)-C(8Y)-H(8YA)	104.8
C(7Y)-C(8Y)-H(8YB)	104.8
O(150)-C(8Y)-H(8YB)	104.8
H(8YA)-C(8Y)-H(8YB)	105.8

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table S-21. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4'**. 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}
Fe(1)	35(1)	39(1)	28(1)	-3(1)	7(1)	-6(1)
C(1)	49(5)	48(4)	72(5)	-10(4)	5(4)	-3(3)
N(11)	29(3)	42(3)	22(2)	-1(2)	9(2)	-2(2)
N(21)	29(3)	39(3)	27(2)	-4(2)	2(2)	-1(2)
C(11)	53(4)	47(4)	50(4)	-2(3)	9(3)	1(3)
C(21)	41(4)	40(3)	24(3)	-2(2)	3(2)	4(3)
C(31)	31(3)	36(3)	29(3)	-4(2)	-5(2)	-3(2)
C(41)	38(3)	41(3)	23(3)	1(2)	1(2)	-5(3)
C(51)	39(4)	51(4)	41(3)	-10(3)	3(3)	-13(3)
C(12)	46(4)	38(3)	28(3)	-5(2)	16(3)	-3(3)
C(22)	28(3)	41(3)	30(3)	-2(2)	12(2)	2(2)
C(32)	41(4)	45(3)	29(3)	0(2)	10(3)	5(3)
C(42)	44(4)	47(4)	47(4)	0(3)	24(3)	-6(3)
C(52)	43(4)	50(4)	41(4)	-7(3)	2(3)	-2(3)
C(62)	37(4)	42(3)	34(3)	-8(3)	13(3)	-6(3)
C(72)	51(4)	51(4)	28(3)	5(3)	11(3)	3(3)
C(82)	54(5)	74(5)	44(4)	-2(3)	-8(3)	15(4)
C(92)	56(5)	81(5)	44(4)	-15(4)	3(3)	-6(4)
C(102)	42(4)	60(4)	33(3)	-6(3)	-3(3)	-14(3)
C(112)	49(4)	90(6)	38(4)	-22(4)	-1(3)	-3(4)
C(122)	77(6)	71(5)	45(4)	10(4)	2(4)	1(4)
C(13)	23(3)	45(3)	30(3)	-6(2)	-2(2)	-5(2)
C(23)	35(3)	54(4)	21(3)	-4(2)	0(2)	-6(3)
C(33)	42(4)	62(4)	38(3)	-9(3)	-7(3)	0(3)
C(43)	25(3)	64(4)	52(4)	-9(3)	0(3)	2(3)
C(53)	31(3)	58(4)	37(3)	-13(3)	13(3)	-11(3)
C(63)	26(3)	53(4)	27(3)	-4(3)	9(2)	-5(3)
C(73)	53(4)	54(4)	29(3)	-4(3)	-7(3)	5(3)
C(83)	84(6)	64(5)	33(4)	0(3)	3(4)	-5(4)
C(93)	97(7)	73(5)	35(4)	-5(4)	-26(4)	-15(5)
C(103)	50(4)	47(4)	27(3)	1(3)	4(3)	-6(3)

C(113)	50(4)	61(4)	36(3)	-7(3)	-11(3)	0(3)
C(123)	72(6)	75(6)	58(5)	20(4)	6(4)	-12(4)
Fe(2)	61(1)	39(1)	56(1)	8(1)	-28(1)	-9(1)
C(2)	107(8)	48(5)	170(12)	18(6)	-56(8)	-16(5)
N(14)	46(3)	53(3)	23(2)	10(2)	-6(2)	-13(2)
N(24)	38(3)	41(3)	30(2)	0(2)	-1(2)	-11(2)
C(14)	57(5)	51(4)	46(4)	-3(3)	-8(3)	-18(3)
C(24)	37(3)	47(3)	26(3)	2(3)	-1(2)	-18(3)
C(34)	44(4)	37(3)	30(3)	-1(2)	4(3)	-8(3)
C(44)	32(3)	41(3)	40(3)	4(3)	5(3)	-1(3)
C(54)	48(4)	42(4)	87(6)	-11(4)	-10(4)	6(3)
C(15)	48(4)	42(3)	35(3)	7(3)	-9(3)	-19(3)
C(25)	46(4)	42(3)	25(3)	7(2)	-4(3)	-10(3)
C(35)	58(5)	41(3)	34(3)	9(3)	-9(3)	-9(3)
C(45)	45(4)	46(4)	50(4)	6(3)	0(3)	-8(3)
C(55)	33(4)	63(4)	50(4)	3(3)	-2(3)	-5(3)
C(65)	46(4)	67(4)	26(3)	5(3)	13(3)	-18(3)
C(75)	53(4)	48(4)	32(3)	6(3)	2(3)	-1(3)
C(85)	57(5)	63(5)	73(5)	5(4)	27(4)	-6(4)
C(95)	77(6)	90(6)	44(4)	-16(4)	6(4)	12(5)
C(105)	50(5)	108(7)	25(3)	6(4)	-1(3)	-11(4)
C(115)	143(11)	111(8)	54(5)	-20(5)	15(6)	-38(8)
C(125)	51(5)	101(6)	49(4)	35(4)	19(4)	5(4)
C(16)	24(3)	35(3)	47(3)	-5(3)	2(3)	0(2)
C(26)	44(4)	51(4)	56(4)	-11(3)	6(3)	-4(3)
C(36)	28(4)	49(4)	82(6)	-12(4)	9(3)	-1(3)
C(46)	32(4)	52(4)	83(6)	-22(4)	-10(4)	3(3)
C(56)	46(4)	43(4)	56(4)	-10(3)	-13(3)	6(3)
C(66)	32(3)	31(3)	42(3)	-6(2)	-3(3)	3(2)
C(76)	66(5)	82(6)	61(5)	-15(4)	34(4)	-31(4)
C(86)	49(6)	219(14)	98(8)	-84(9)	43(5)	-38(7)
C(96)	280(20)	108(10)	79(8)	21(7)	-11(11)	-70(12)
C(106)	40(4)	45(4)	34(3)	-6(3)	-6(3)	0(3)
C(116)	61(5)	53(4)	54(4)	-4(3)	12(4)	1(4)
C(126)	85(6)	62(5)	54(5)	10(4)	-10(4)	-6(4)
K(1)	51(1)	40(1)	38(1)	-2(1)	6(1)	2(1)

O(10)	72(4)	62(3)	75(4)	0(3)	10(3)	-10(3)
O(20)	70(4)	66(3)	50(3)	-7(2)	-7(3)	5(3)
O(30)	95(5)	53(3)	62(3)	2(3)	-4(3)	12(3)
O(40)	87(4)	51(3)	57(3)	-10(2)	-5(3)	0(3)
O(50)	57(3)	78(4)	43(3)	-7(2)	-9(2)	8(3)
O(60)	106(5)	61(3)	56(3)	9(3)	23(3)	12(3)
O(70)	50(3)	61(3)	48(3)	-6(2)	-4(2)	6(2)
O(80)	83(4)	66(3)	49(3)	3(2)	10(3)	11(3)
O(90)	67(4)	60(3)	73(4)	-4(3)	21(3)	2(3)
O(100)	64(4)	80(4)	63(3)	-12(3)	3(3)	-2(3)
C(10)	61(6)	67(6)	123(9)	-18(6)	-10(6)	-15(5)
C(20)	80(7)	84(7)	85(7)	-11(5)	-25(5)	-3(5)
C(30)	80(6)	94(7)	44(4)	9(4)	-11(4)	7(5)
C(40)	65(5)	70(5)	53(4)	12(4)	-9(4)	12(4)
C(50)	76(6)	41(4)	84(6)	14(4)	13(5)	10(4)
C(60)	89(7)	38(4)	76(5)	5(4)	5(5)	-6(4)
C(70)	76(6)	66(5)	73(6)	-21(4)	3(5)	-2(5)
C(80)	73(6)	83(6)	48(4)	-24(4)	-4(4)	-7(5)
C(90)	98(7)	79(6)	50(5)	4(4)	10(5)	22(5)
C(100)	98(7)	77(6)	39(4)	15(4)	20(4)	31(5)
C(110)	111(8)	55(5)	76(6)	12(4)	16(6)	5(5)
C(120)	93(7)	66(6)	90(7)	13(5)	25(6)	-27(5)
C(130)	64(5)	63(5)	51(4)	-19(4)	-9(4)	10(4)
C(140)	89(6)	70(5)	48(4)	-12(4)	12(4)	13(5)
C(150)	95(7)	80(6)	53(5)	16(4)	-1(5)	9(5)
C(160)	87(7)	77(6)	78(6)	17(5)	43(5)	12(5)
C(170)	52(5)	76(6)	101(7)	-16(5)	16(5)	-13(4)
C(180)	70(6)	101(8)	81(6)	-7(6)	4(5)	-8(6)
C(190)	71(6)	67(5)	58(5)	-6(4)	-17(4)	3(4)
C(200)	53(5)	69(5)	61(5)	-9(4)	-2(4)	12(4)
K(2)	34(1)	38(1)	34(1)	0	-1(1)	0
O(110)	56(5)	86(5)	35(3)	0	6(3)	0
O(120)	55(3)	56(3)	65(3)	-22(2)	0(3)	-7(2)
O(130)	59(3)	43(3)	56(3)	-4(2)	2(2)	-6(2)
O(140)	44(4)	58(4)	34(3)	0	4(3)	0
O(150)	39(4)	103(5)	36(3)	0	2(3)	0

O(160)	43(3)	53(3)	61(3)	-3(2)	-2(2)	4(2)
C(210)	83(7)	109(7)	43(4)	-25(5)	3(4)	-3(5)
C(220)	80(7)	87(6)	65(5)	-26(5)	0(5)	-15(5)
C(230)	59(5)	39(4)	99(6)	-11(4)	-2(5)	-2(3)
C(240)	67(5)	43(4)	77(5)	-3(4)	6(4)	-10(4)
C(250)	47(4)	56(4)	67(5)	19(4)	9(4)	-12(3)
C(260)	59(5)	66(5)	46(4)	13(4)	14(3)	-4(4)
C(8X)	80(12)	152(10)	138(19)	50(11)	54(13)	47(9)
C(7Y)	39(6)	65(8)	58(7)	3(6)	-4(5)	0(5)
C(6X)	47(7)	67(8)	55(6)	1(5)	-4(5)	4(6)
C(5Y)	97(14)	120(9)	42(8)	-7(6)	-14(8)	43(9)
O(170)	42(4)	84(4)	42(4)	0	4(3)	0
K(3)	40(1)	60(1)	36(1)	0	4(1)	0
O(180)	69(5)	93(5)	57(5)	0	20(4)	0
O(190)	235(10)	81(4)	78(4)	6(3)	44(5)	76(5)
O(200)	336(17)	246(11)	214(9)	178(8)	167(11)	190(12)
O(220)	69(4)	85(4)	57(3)	-7(3)	-5(3)	-8(3)
O(230)	65(4)	79(4)	61(3)	-4(3)	8(3)	-14(3)
C(310)	201(10)	131(6)	99(6)	7(4)	54(6)	66(6)
C(320)	201(10)	131(6)	99(6)	7(4)	54(6)	66(6)
C(330)	86(7)	73(6)	149(8)	32(5)	-4(6)	4(5)
C(360)	162(14)	409(18)	192(13)	101(10)	100(11)	101(12)
C(370)	215(14)	111(7)	60(5)	-12(5)	-36(7)	-7(7)
C(380)	164(11)	120(8)	94(6)	-36(5)	37(6)	-70(8)
C(390)	137(9)	131(8)	77(5)	-25(5)	18(5)	-64(7)
O(1X)	70(4)	95(5)	74(4)	-11(3)	13(3)	6(4)
C(3X)	76(7)	106(8)	77(6)	13(6)	-1(5)	-1(6)
C(4X)	81(7)	99(7)	65(6)	4(5)	-2(5)	10(6)
C(1X)	112(9)	89(8)	125(10)	-20(7)	46(8)	-20(7)
C(2X)	68(6)	134(10)	77(6)	6(6)	31(5)	-3(6)
C(400)	115(8)	112(8)	204(13)	11(7)	101(9)	-6(6)
O(210)	103(10)	321(17)	77(8)	0	8(8)	0
C(340)	142(11)	96(8)	137(8)	44(6)	2(7)	4(7)
C(350)	228(17)	306(15)	152(10)	150(9)	92(11)	110(11)
C(5X)	102(14)	124(9)	34(7)	16(6)	-2(7)	52(9)
C(6Y)	54(9)	85(8)	50(6)	9(5)	-4(5)	24(7)

C(7X)	28(7)	90(8)	58(6)	-3(5)	-14(5)	22(6)
C(8Y)	94(15)	152(10)	62(8)	33(7)	46(9)	68(10)

Table S-22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4'**.

	x	y	z	U(eq)
H(1A)	-1957	3451	4726	85
H(1B)	-733	3396	4641	85
H(1C)	-1400	3505	3984	85
H(11G)	-2955	4639	5382	75
H(11H)	-2007	4811	5705	75
H(11I)	-2518	4570	6155	75
H(31)	-463	4714	5248	38
H(51A)	1859	4438	5042	65
H(51B)	1223	4719	5041	65
H(51C)	1445	4564	4313	65
H(32)	-3445	3844	7199	46
H(42)	-4930	3717	6586	55
H(52)	-5108	3834	5396	54
H(72)	-1209	4183	6469	52
H(82A)	-1412	3668	7170	86
H(82B)	-338	3827	7049	86
H(82C)	-955	3702	6389	86
H(92A)	-2124	4371	7417	91
H(92B)	-1106	4219	7708	91
H(92C)	-2227	4078	7780	91
H(102)	-3215	4189	4357	54
H(11J)	-3312	3724	4087	88
H(11K)	-4058	3889	3560	88
H(11L)	-4548	3725	4210	88
H(12G)	-5439	4170	4522	97
H(12H)	-4827	4335	3923	97
H(12I)	-4747	4429	4731	97
H(33)	3045	3582	4982	57
H(43)	3549	3628	3838	56
H(53)	2584	3894	3060	50

H(73)	791	3897	5771	54
H(83A)	781	3418	5570	91
H(83B)	951	3492	6385	91
H(83C)	1922	3399	5913	91
H(93A)	2892	3823	6200	103
H(93B)	1959	3938	6675	103
H(93C)	2395	4114	6029	103
H(103)	350	4295	3520	50
H(11M)	550	3857	2532	74
H(11N)	-328	4089	2493	74
H(11O)	-326	3876	3132	74
H(12J)	1935	4468	3036	103
H(12K)	1014	4467	2462	103
H(12L)	1899	4237	2442	103
H(0AA)	3440	4100	10500	163
H(0AB)	4348	4141	9931	163
H(0AC)	4636	4096	10746	163
H(14A)	1870	2968	9669	77
H(14B)	2732	2736	9547	77
H(14C)	2518	2959	8947	77
H(34)	4232	2793	10060	44
H(54A)	6611	2960	10514	88
H(54B)	5768	2723	10620	88
H(54C)	5988	2936	11243	88
H(35)	1614	3599	7758	53
H(45)	113	3748	8307	57
H(55)	103	3783	9557	58
H(75)	3800	3288	8564	53
H(85A)	3755	3805	7870	96
H(85B)	4771	3617	7924	96
H(85C)	4278	3747	8623	96
H(95A)	2820	3106	7635	105
H(95B)	3918	3216	7352	105
H(95C)	2878	3390	7222	105
H(105)	2184	3576	10704	73
H(11A)	1541	4032	10588	154

H(11B)	1167	3891	11307	154
H(11C)	376	3917	10655	154
H(12A)	46	3417	10571	100
H(12B)	672	3411	11303	100
H(12C)	1014	3215	10670	100
H(36)	8390	3735	10671	64
H(46)	8401	3745	11892	67
H(56)	6941	3584	12513	58
H(76)	6362	3446	9593	84
H(86A)	7920	3385	8959	183
H(86B)	7962	3214	9678	183
H(86C)	8585	3495	9616	183
H(96A)	6278	3924	9571	233
H(96B)	6901	3817	8894	233
H(96C)	7525	3943	9550	233
H(106)	4715	3263	11729	48
H(11D)	4752	3751	12548	84
H(11E)	3750	3562	12422	84
H(11F)	4244	3729	11777	84
H(12D)	5776	3076	12636	101
H(12E)	4677	3174	12946	101
H(12F)	5701	3355	13068	101
H(10A)	371	4618	7642	101
H(10B)	723	4349	7226	101
H(20A)	1789	4615	6518	99
H(20B)	578	4689	6435	99
H(30A)	887	5138	6066	87
H(30B)	2126	5091	6085	87
H(40C)	1691	5551	6220	75
H(40D)	1066	5477	6927	75
H(50A)	2155	5728	7680	81
H(50B)	2698	5841	6976	81
H(60A)	4329	5669	7376	81
H(60B)	3873	5892	7907	81
H(70A)	2610	5624	8867	86
H(70B)	3663	5790	9038	86

H(80A)	4418	5371	9470	81
H(80B)	3465	5476	9946	81
H(90A)	3198	5017	10314	91
H(90B)	4128	4917	9811	91
H(10C)	2888	4568	10060	85
H(10D)	2027	4741	9640	85
H(11P)	2511	4229	9266	97
H(11Q)	3139	4234	8536	97
H(12M)	1350	4198	8356	100
H(12N)	1184	4484	8746	100
H(13A)	3303	4345	6987	72
H(13B)	4362	4172	6961	72
H(14D)	5217	4539	6395	83
H(14E)	4223	4443	5940	83
H(15A)	4151	5160	6046	91
H(15B)	4835	4933	5656	91
H(16A)	6009	4926	6620	97
H(16B)	5934	5226	6289	97
H(17A)	5710	5355	8080	91
H(17B)	6579	5330	7478	91
H(18A)	6658	4848	7682	101
H(18B)	6979	5017	8376	101
H(19A)	5209	4506	8902	79
H(19B)	6398	4528	8652	79
H(20C)	5893	4455	7465	73
H(20D)	5465	4209	7945	73
H(21A)	1545	2744	15152	94
H(21B)	378	2743	14843	94
H(22A)	1285	3148	14566	93
H(22B)	2109	2971	14123	93
H(23A)	863	3393	13609	78
H(23B)	162	3261	12997	78
H(24A)	1788	3401	12549	75
H(24B)	2371	3202	13095	75
H(25A)	3105	2954	12166	68
H(25B)	2546	3147	11597	68

H(26A)	1644	2756	11146	68
H(26B)	2887	2733	11050	68
H(8XA)	-2877	2700	13291	148
H(8XB)	-2340	2815	13999	148
H(7YA)	-2271	3103	12846	65
H(7YB)	-2593	2818	12478	65
H(6XA)	-2344	2781	11954	68
H(6XB)	-1902	3080	11757	68
H(5YA)	-1001	2800	10769	104
H(5YB)	-1953	2685	11231	104
H(31A)	5607	2730	9034	173
H(31B)	6769	2836	9100	173
H(32A)	6168	3135	8532	173
H(32B)	5299	2948	8169	173
H(33A)	6720	3332	7525	123
H(33B)	5779	3184	7125	123
H(36A)	7322	2691	5304	305
H(36B)	8492	2715	5012	305
H(37A)	10076	2686	9262	155
H(37B)	8905	2686	9530	155
H(38A)	9505	3155	8435	151
H(38B)	10403	2957	8699	151
H(39A)	10986	2954	7773	138
H(39B)	10090	3153	7510	138
H(3XA)	-614	5208	9348	104
H(3XB)	-1007	5124	8573	104
H(4XA)	1076	5225	8950	123
H(4XB)	354	5424	8493	123
H(4XC)	697	5135	8178	123
H(1XA)	-759	4299	9148	163
H(1XB)	-1322	4339	9894	163
H(1XC)	-108	4409	9811	163
H(2XA)	-1655	4697	9041	112
H(2XB)	-1276	4800	9803	112
H(40A)	10800	2691	6431	172
H(40B)	11372	2691	7175	172

H(34A)	6594	3180	6264	150
H(34B)	7532	3325	6662	150
H(35A)	7927	3101	5515	274
H(35B)	8949	2981	5883	274
H(5XA)	-411	2902	11407	104
H(5XB)	-1359	2792	10953	104
H(6YA)	-1596	3073	11627	76
H(6YB)	-375	3019	11601	76
H(7XA)	-1236	3022	13483	71
H(7XB)	-2233	3063	13002	71
H(8YA)	-2609	2786	13647	123
H(8YB)	-1457	2899	13687	123

Table S-23. Torsion angles [°] for **4'**.

C(12)-N(11)-C(21)-C(31)	163.1(5)
Fe(1)-N(11)-C(21)-C(31)	-6.4(8)
C(12)-N(11)-C(21)-C(11)	-16.5(8)
Fe(1)-N(11)-C(21)-C(11)	174.0(4)
N(11)-C(21)-C(31)-C(41)	-1.9(10)
C(11)-C(21)-C(31)-C(41)	177.7(6)
C(13)-N(21)-C(41)-C(31)	-176.7(5)
Fe(1)-N(21)-C(41)-C(31)	1.0(8)
C(13)-N(21)-C(41)-C(51)	2.4(8)
Fe(1)-N(21)-C(41)-C(51)	-179.9(4)
C(21)-C(31)-C(41)-N(21)	5.0(10)
C(21)-C(31)-C(41)-C(51)	-174.2(6)
C(21)-N(11)-C(12)-C(62)	109.2(7)
Fe(1)-N(11)-C(12)-C(62)	-80.6(6)
C(21)-N(11)-C(12)-C(22)	-77.4(7)
Fe(1)-N(11)-C(12)-C(22)	92.8(5)
C(62)-C(12)-C(22)-C(32)	0.1(9)
N(11)-C(12)-C(22)-C(32)	-173.4(5)
C(62)-C(12)-C(22)-C(72)	177.9(6)
N(11)-C(12)-C(22)-C(72)	4.4(8)
C(12)-C(22)-C(32)-C(42)	2.9(9)
C(72)-C(22)-C(32)-C(42)	-174.9(6)
C(22)-C(32)-C(42)-C(52)	-3.8(10)
C(32)-C(42)-C(52)-C(62)	1.7(10)
C(42)-C(52)-C(62)-C(12)	1.2(10)
C(42)-C(52)-C(62)-C(102)	-178.0(6)
N(11)-C(12)-C(62)-C(52)	171.3(6)
C(22)-C(12)-C(62)-C(52)	-2.1(9)
N(11)-C(12)-C(62)-C(102)	-9.5(9)
C(22)-C(12)-C(62)-C(102)	177.1(6)
C(32)-C(22)-C(72)-C(92)	-48.1(8)
C(12)-C(22)-C(72)-C(92)	134.2(6)
C(32)-C(22)-C(72)-C(82)	75.7(7)
C(12)-C(22)-C(72)-C(82)	-102.1(7)

C(52)-C(62)-C(102)-C(112)	-65.9(8)
C(12)-C(62)-C(102)-C(112)	114.9(7)
C(52)-C(62)-C(102)-C(122)	57.5(8)
C(12)-C(62)-C(102)-C(122)	-121.7(7)
C(41)-N(21)-C(13)-C(63)	-83.6(7)
Fe(1)-N(21)-C(13)-C(63)	98.6(6)
C(41)-N(21)-C(13)-C(23)	99.5(6)
Fe(1)-N(21)-C(13)-C(23)	-78.3(6)
C(63)-C(13)-C(23)-C(33)	1.1(9)
N(21)-C(13)-C(23)-C(33)	178.0(5)
C(63)-C(13)-C(23)-C(73)	179.3(6)
N(21)-C(13)-C(23)-C(73)	-3.8(9)
C(13)-C(23)-C(33)-C(43)	0.1(10)
C(73)-C(23)-C(33)-C(43)	-178.1(7)
C(23)-C(33)-C(43)-C(53)	-0.5(11)
C(33)-C(43)-C(53)-C(63)	-0.2(10)
C(43)-C(53)-C(63)-C(13)	1.3(9)
C(43)-C(53)-C(63)-C(103)	-176.8(6)
C(23)-C(13)-C(63)-C(53)	-1.8(9)
N(21)-C(13)-C(63)-C(53)	-178.7(5)
C(23)-C(13)-C(63)-C(103)	176.3(5)
N(21)-C(13)-C(63)-C(103)	-0.5(9)
C(33)-C(23)-C(73)-C(93)	66.4(9)
C(13)-C(23)-C(73)-C(93)	-111.7(7)
C(33)-C(23)-C(73)-C(83)	-60.0(9)
C(13)-C(23)-C(73)-C(83)	121.9(7)
C(53)-C(63)-C(103)-C(113)	79.5(7)
C(13)-C(63)-C(103)-C(113)	-98.6(7)
C(53)-C(63)-C(103)-C(123)	-45.0(8)
C(13)-C(63)-C(103)-C(123)	137.0(7)
C(15)-N(14)-C(24)-C(34)	173.7(6)
Fe(2)-N(14)-C(24)-C(34)	-2.0(8)
C(15)-N(14)-C(24)-C(14)	-7.2(8)
Fe(2)-N(14)-C(24)-C(14)	177.0(4)
N(14)-C(24)-C(34)-C(44)	0.5(10)
C(14)-C(24)-C(34)-C(44)	-178.6(6)

C(16)-N(24)-C(44)-C(34)	178.7(5)
Fe(2)-N(24)-C(44)-C(34)	1.1(8)
C(16)-N(24)-C(44)-C(54)	-1.6(8)
Fe(2)-N(24)-C(44)-C(54)	-179.1(5)
C(24)-C(34)-C(44)-N(24)	0.0(10)
C(24)-C(34)-C(44)-C(54)	-179.7(7)
C(24)-N(14)-C(15)-C(65)	108.2(7)
Fe(2)-N(14)-C(15)-C(65)	-75.8(7)
C(24)-N(14)-C(15)-C(25)	-74.8(7)
Fe(2)-N(14)-C(15)-C(25)	101.2(6)
C(65)-C(15)-C(25)-C(35)	-4.5(9)
N(14)-C(15)-C(25)-C(35)	178.5(5)
C(65)-C(15)-C(25)-C(75)	171.3(6)
N(14)-C(15)-C(25)-C(75)	-5.7(9)
C(15)-C(25)-C(35)-C(45)	0.7(10)
C(75)-C(25)-C(35)-C(45)	-175.1(6)
C(25)-C(35)-C(45)-C(55)	3.9(10)
C(35)-C(45)-C(55)-C(65)	-4.9(10)
C(45)-C(55)-C(65)-C(15)	1.3(10)
C(45)-C(55)-C(65)-C(105)	-178.6(7)
N(14)-C(15)-C(65)-C(55)	-179.5(6)
C(25)-C(15)-C(65)-C(55)	3.5(10)
N(14)-C(15)-C(65)-C(105)	0.3(10)
C(25)-C(15)-C(65)-C(105)	-176.7(6)
C(35)-C(25)-C(75)-C(95)	-39.9(9)
C(15)-C(25)-C(75)-C(95)	144.4(7)
C(35)-C(25)-C(75)-C(85)	86.6(8)
C(15)-C(25)-C(75)-C(85)	-89.1(7)
C(55)-C(65)-C(105)-C(125)	75.3(9)
C(15)-C(65)-C(105)-C(125)	-104.5(8)
C(55)-C(65)-C(105)-C(115)	-45.9(10)
C(15)-C(65)-C(105)-C(115)	134.2(8)
C(44)-N(24)-C(16)-C(26)	98.1(7)
Fe(2)-N(24)-C(16)-C(26)	-84.2(6)
C(44)-N(24)-C(16)-C(66)	-84.0(7)
Fe(2)-N(24)-C(16)-C(66)	93.6(6)

N(24)-C(16)-C(26)-C(36)	176.9(6)
C(66)-C(16)-C(26)-C(36)	-1.0(10)
N(24)-C(16)-C(26)-C(76)	-1.9(10)
C(66)-C(16)-C(26)-C(76)	-179.8(7)
C(16)-C(26)-C(36)-C(46)	2.0(11)
C(76)-C(26)-C(36)-C(46)	-179.2(8)
C(26)-C(36)-C(46)-C(56)	-1.4(11)
C(36)-C(46)-C(56)-C(66)	-0.3(10)
C(46)-C(56)-C(66)-C(16)	1.2(9)
C(46)-C(56)-C(66)-C(106)	-176.9(6)
C(26)-C(16)-C(66)-C(56)	-0.6(9)
N(24)-C(16)-C(66)-C(56)	-178.5(5)
C(26)-C(16)-C(66)-C(106)	177.5(6)
N(24)-C(16)-C(66)-C(106)	-0.4(8)
C(36)-C(26)-C(76)-C(86)	55.6(11)
C(16)-C(26)-C(76)-C(86)	-125.7(8)
C(36)-C(26)-C(76)-C(96)	-69.5(13)
C(16)-C(26)-C(76)-C(96)	109.3(11)
C(56)-C(66)-C(106)-C(116)	83.4(7)
C(16)-C(66)-C(106)-C(116)	-94.6(7)
C(56)-C(66)-C(106)-C(126)	-39.9(8)
C(16)-C(66)-C(106)-C(126)	142.0(6)
C(120)-O(10)-C(10)-C(20)	175.4(8)
K(1)-O(10)-C(10)-C(20)	32.3(10)
C(30)-O(20)-C(20)-C(10)	-172.8(8)
K(1)-O(20)-C(20)-C(10)	63.2(9)
O(10)-C(10)-C(20)-O(20)	-65.6(11)
C(20)-O(20)-C(30)-C(40)	176.0(8)
K(1)-O(20)-C(30)-C(40)	-61.6(8)
C(50)-O(30)-C(40)-C(30)	-173.6(7)
K(1)-O(30)-C(40)-C(30)	-32.1(8)
O(20)-C(30)-C(40)-O(30)	63.6(10)
C(40)-O(30)-C(50)-C(60)	-177.2(7)
K(1)-O(30)-C(50)-C(60)	39.7(8)
C(70)-O(40)-C(60)-C(50)	-83.8(9)
K(1)-O(40)-C(60)-C(50)	53.7(8)

O(30)-C(50)-C(60)-O(40)	-63.6(9)
C(60)-O(40)-C(70)-C(80)	-171.1(7)
K(1)-O(40)-C(70)-C(80)	53.5(8)
C(90)-O(50)-C(80)-C(70)	177.7(7)
K(1)-O(50)-C(80)-C(70)	49.4(8)
O(40)-C(70)-C(80)-O(50)	-68.7(9)
C(80)-O(50)-C(90)-C(100)	179.9(7)
K(1)-O(50)-C(90)-C(100)	-52.1(8)
C(110)-O(60)-C(100)-C(90)	177.9(8)
K(1)-O(60)-C(100)-C(90)	-46.8(9)
O(50)-C(90)-C(100)-O(60)	67.7(9)
C(100)-O(60)-C(110)-C(120)	85.8(9)
K(1)-O(60)-C(110)-C(120)	-51.0(9)
C(10)-O(10)-C(120)-C(110)	173.7(8)
K(1)-O(10)-C(120)-C(110)	-41.3(9)
O(60)-C(110)-C(120)-O(10)	63.0(11)
C(200)-O(70)-C(130)-C(140)	-82.2(8)
K(1)-O(70)-C(130)-C(140)	67.1(7)
C(200)-O(70)-C(130)-K(1)	-149.3(7)
C(150)-O(80)-C(140)-C(130)	153.9(7)
K(1)-O(80)-C(140)-C(130)	22.8(9)
O(70)-C(130)-C(140)-O(80)	-60.3(9)
K(1)-C(130)-C(140)-O(80)	-16.5(6)
C(140)-O(80)-C(150)-C(160)	-77.7(9)
K(1)-O(80)-C(150)-C(160)	57.0(8)
C(170)-O(90)-C(160)-C(150)	170.3(7)
K(1)-O(90)-C(160)-C(150)	32.0(9)
O(80)-C(150)-C(160)-O(90)	-60.5(10)
C(160)-O(90)-C(170)-C(180)	-76.0(9)
K(1)-O(90)-C(170)-C(180)	66.0(8)
C(190)-O(100)-C(180)-C(170)	155.0(7)
K(1)-O(100)-C(180)-C(170)	28.2(9)
O(90)-C(170)-C(180)-O(100)	-63.5(10)
C(180)-O(100)-C(190)-C(200)	-77.4(9)
K(1)-O(100)-C(190)-C(200)	53.3(8)
C(130)-O(70)-C(200)-C(190)	173.6(7)

K(1)-O(70)-C(200)-C(190)	31.6(9)
O(100)-C(190)-C(200)-O(70)	-57.1(10)
C(210)#1-O(110)-C(210)-C(220)	-179.8(5)
K(2)-O(110)-C(210)-C(220)	-46.7(9)
C(230)-O(120)-C(220)-C(210)	172.3(7)
K(2)-O(120)-C(220)-C(210)	-50.5(9)
O(110)-C(210)-C(220)-O(120)	65.0(10)
C(220)-O(120)-C(230)-C(240)	79.8(9)
K(2)-O(120)-C(230)-C(240)	-58.5(7)
C(250)-O(130)-C(240)-C(230)	-177.9(6)
K(2)-O(130)-C(240)-C(230)	-34.8(8)
O(120)-C(230)-C(240)-O(130)	61.5(9)
C(240)-O(130)-C(250)-C(260)	178.2(6)
K(2)-O(130)-C(250)-C(260)	35.5(7)
C(260)#1-O(140)-C(260)-C(250)	-172.9(4)
K(2)-O(140)-C(260)-C(250)	63.2(7)
O(130)-C(250)-C(260)-O(140)	-66.0(8)
C(8X)#1-O(150)-C(8X)-C(7X)	-143.1(10)
K(2)-O(150)-C(8X)-C(7X)	0(3)
C(6Y)-O(160)-C(7Y)-C(8Y)	162.0(15)
K(2)-O(160)-C(7Y)-C(8Y)	22.3(19)
C(7X)-O(160)-C(6X)-C(5X)	-164.2(14)
K(2)-O(160)-C(6X)-C(5X)	-31.3(17)
C(6Y)-C(5Y)-O(170)-C(5Y)#1	145.0(11)
C(6Y)-C(5Y)-O(170)-K(2)	8(2)
C(310)#1-O(180)-C(310)-C(320)	-123.0(17)
K(3)-O(180)-C(310)-C(320)	33(2)
O(180)-C(310)-C(320)-O(190)	-29(3)
C(330)-O(190)-C(320)-C(310)	-171.8(16)
K(3)-O(190)-C(320)-C(310)	6(2)
C(320)-O(190)-C(330)-C(340)	179.9(15)
K(3)-O(190)-C(330)-C(340)	1.8(17)
C(380)-O(220)-C(370)-C(370)#1	-124.5(8)
K(3)-O(220)-C(370)-C(370)#1	13.0(9)
C(370)-O(220)-C(380)-C(390)	119.9(16)
K(3)-O(220)-C(380)-C(390)	-18(2)

O(220)-C(380)-C(390)-O(230)	0(3)
C(400)-O(230)-C(390)-C(380)	-122.8(16)
K(3)-O(230)-C(390)-C(380)	18.3(19)
C(2X)-O(1X)-C(3X)-C(4X)	178.5(9)
C(3X)-O(1X)-C(2X)-C(1X)	-176.1(9)
C(390)-O(230)-C(400)-C(400)#1	124.0(8)
K(3)-O(230)-C(400)-C(400)#1	-17.8(9)
C(350)-C(360)-O(210)-C(360)#1	173.3(10)
C(350)-C(360)-O(210)-K(3)	34(2)
C(350)-O(200)-C(340)-C(330)	172.4(18)
K(3)-O(200)-C(340)-C(330)	-2(3)
O(190)-C(330)-C(340)-O(200)	0(3)
O(210)-C(360)-C(350)-O(200)	-54(3)
C(340)-O(200)-C(350)-C(360)	-127(2)
K(3)-O(200)-C(350)-C(360)	47(2)
O(160)-C(6X)-C(5X)-O(170)	63(3)
C(5X)#1-O(170)-C(5X)-C(6X)	62(4)
K(2)-O(170)-C(5X)-C(6X)	-60(3)
O(170)-C(5Y)-C(6Y)-O(160)	-45(3)
C(7Y)-O(160)-C(6Y)-C(5Y)	-89(2)
K(2)-O(160)-C(6Y)-C(5Y)	59(2)
O(150)-C(8X)-C(7X)-O(160)	39(3)
C(6X)-O(160)-C(7X)-C(8X)	87(2)
K(2)-O(160)-C(7X)-C(8X)	-56(2)
O(160)-C(7Y)-C(8Y)-O(150)	-56(3)
C(8Y)#1-O(150)-C(8Y)-C(7Y)	-67(4)
K(2)-O(150)-C(8Y)-C(7Y)	56(3)

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

$L^{Me}Fe(OCPh_2CHCPh)$ (6). Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å) for the structure of **6**. The diffraction images were processed and scaled using Rigaku Oxford Diffraction software (CrysAlisPro; Rigaku OD: The Woodlands, TX, 2015). The structure was solved with SHELXT and was refined against F^2 on all data by full-matrix least squares with SHELXL (Sheldrick, G. M. Acta Cryst. 2008, A64, 112–122). All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups.

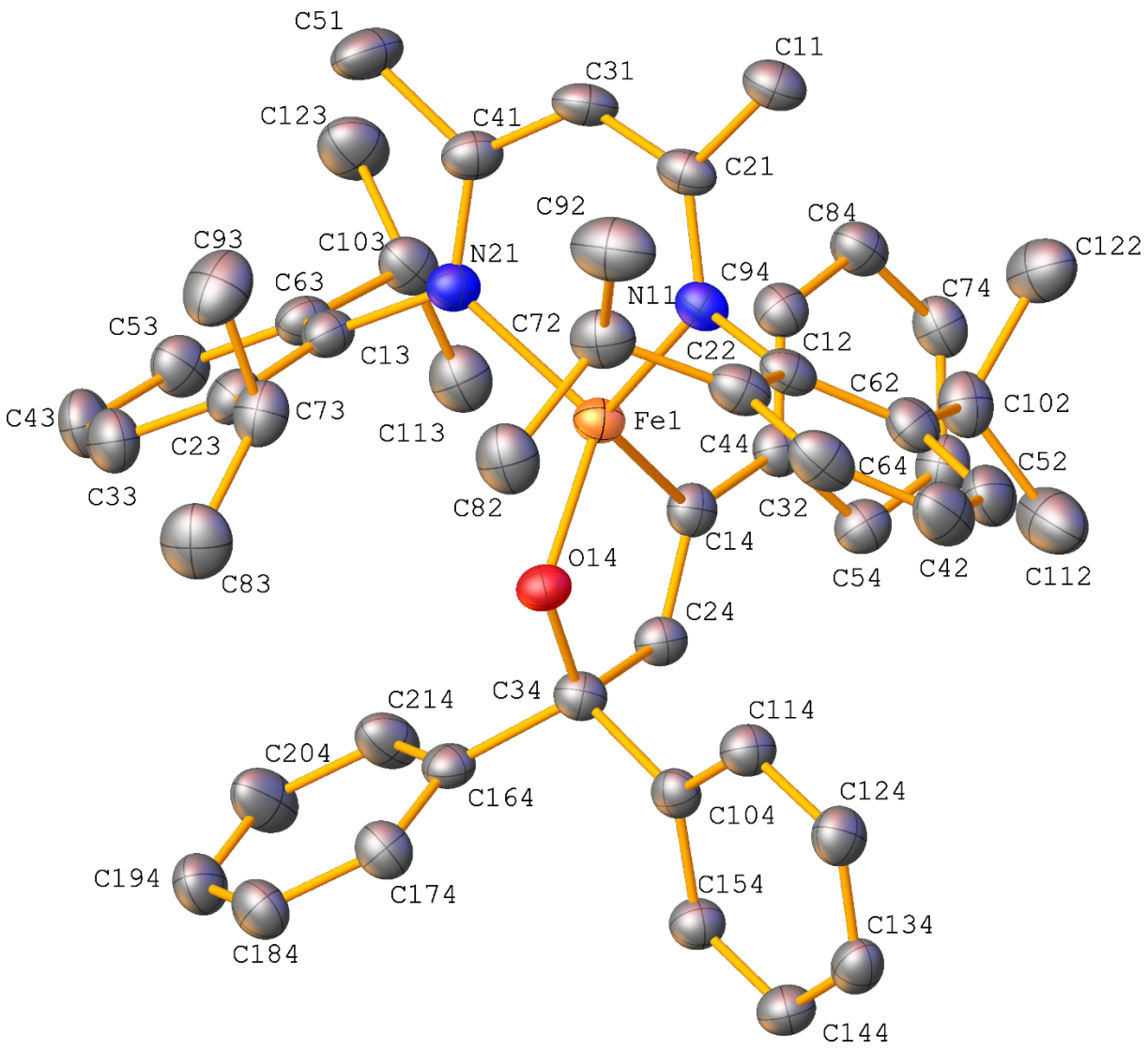

Figure S-28: The complete numbering scheme of **L^{Me}Fe(OCPh$_2$CHCPh) (6)** with 50% thermal ellipsoid probability levels. The hydrogen atoms are omitted for clarity.

Table S-24. Crystal data and structure refinement for **6**.

Identification code	007b-18035	
CSD Deposition Number	1944812	
Empirical formula	C50 H57 Fe N2 O	
Formula weight	757.82	
Temperature	93(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 13.1153(3) Å	α= 90°.
	b = 11.5562(3) Å	β= 97.040(2)°.
	c = 14.0967(4) Å	γ = 90°.
Volume	2120.43(10) $Å^3$	
Z	2	
Density (calculated)	1.187 g/cm^3	
Absorption coefficient	3.130 mm^{-1}	
F(000)	810	
Crystal size	0.200 x 0.200 x 0.030 mm^3	
Crystal color and habit	Green Plate	
Diffractometer	Rigaku Saturn 944+ CCD	
Theta range for data collection	3.159 to 66.600°.	
Index ranges	-15<=h<=15, -13<=k<=13, -16<=l<=16	
Reflections collected	76162	
Independent reflections	7495 [R(int) = 0.0861]	
Observed reflections (I > 2sigma(I))	6924	
Completeness to theta = 66.600°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86231	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	7495 / 1 / 497	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0799	
R indices (all data)	R1 = 0.0396, wR2 = 0.0827	
Absolute structure parameter	-0.007(2)	
Largest diff. peak and hole	0.353 and -0.252 $e.Å^{-3}$	

Table S-25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(01)	7500(1)	5547(1)	7097(1)	24(1)
N(11)	8237(2)	7054(2)	7193(2)	26(1)
N(21)	6160(2)	6169(2)	7384(2)	27(1)
C(11)	8287(3)	9187(3)	7072(3)	34(1)
C(21)	7724(3)	8054(3)	7096(2)	27(1)
C(31)	6649(3)	8129(3)	7065(3)	33(1)
C(41)	5937(3)	7298(3)	7267(3)	31(1)
C(51)	4869(3)	7727(4)	7371(3)	45(1)
C(12)	9344(2)	7049(3)	7425(2)	27(1)
C(22)	9763(3)	7273(3)	8377(2)	32(1)
C(32)	10831(3)	7195(3)	8597(3)	38(1)
C(42)	11455(3)	6894(4)	7921(3)	41(1)
C(52)	11025(3)	6675(3)	6990(3)	39(1)
C(62)	9968(3)	6746(3)	6724(2)	31(1)
C(72)	9104(3)	7552(3)	9159(2)	36(1)
C(82)	9127(3)	6535(4)	9861(3)	42(1)
C(92)	9437(4)	8684(4)	9676(3)	51(1)
C(102)	9514(3)	6518(3)	5694(3)	36(1)
C(112)	10111(3)	5628(4)	5195(3)	52(1)
C(122)	9398(3)	7641(4)	5118(3)	45(1)
C(13)	5411(2)	5378(3)	7684(2)	27(1)
C(23)	5528(3)	5005(3)	8638(2)	31(1)
C(33)	4806(3)	4250(3)	8932(3)	38(1)
C(43)	3983(3)	3867(4)	8300(3)	40(1)
C(53)	3897(3)	4203(3)	7356(3)	36(1)
C(63)	4604(2)	4955(3)	7021(2)	30(1)
C(73)	6417(2)	5442(4)	9357(2)	35(1)
C(83)	6784(3)	4545(4)	10128(3)	49(1)
C(93)	6143(3)	6586(4)	9810(3)	51(1)
C(103)	4504(3)	5240(3)	5957(2)	34(1)
C(113)	4724(3)	4167(4)	5379(3)	40(1)
C(123)	3436(3)	5736(4)	5580(3)	47(1)

O(14)	8047(2)	4367(2)	7879(2)	26(1)
C(14)	7541(2)	4500(3)	5945(2)	27(1)
C(24)	7868(2)	3476(3)	6310(2)	26(1)
C(34)	8193(2)	3315(3)	7388(2)	26(1)
C(44)	7293(2)	4762(3)	4915(2)	26(1)
C(54)	7595(3)	4057(3)	4187(2)	31(1)
C(64)	7355(3)	4342(3)	3233(2)	33(1)
C(74)	6804(2)	5342(3)	2974(2)	32(1)
C(84)	6515(3)	6064(3)	3677(3)	33(1)
C(94)	6768(2)	5780(3)	4630(2)	30(1)
C(104)	9345(2)	3008(3)	7494(2)	26(1)
C(114)	10086(3)	3860(3)	7732(2)	30(1)
C(124)	11123(3)	3592(3)	7779(3)	34(1)
C(134)	11433(3)	2474(3)	7615(2)	32(1)
C(144)	10705(3)	1624(3)	7384(2)	33(1)
C(154)	9670(3)	1893(3)	7316(2)	30(1)
C(164)	7561(2)	2385(3)	7832(2)	27(1)
C(174)	7925(3)	1927(3)	8715(2)	32(1)
C(184)	7352(3)	1135(3)	9171(3)	37(1)
C(194)	6395(3)	790(3)	8738(3)	40(1)
C(204)	6029(3)	1246(4)	7858(3)	46(1)
C(214)	6601(3)	2043(3)	7408(3)	39(1)

Table S-26. Bond lengths [Å] and angles [°] for **6**.

Fe(01)-O(14)	1.843(2)
Fe(01)-N(21)	1.986(3)
Fe(01)-N(11)	1.988(3)
Fe(01)-C(14)	2.031(3)
N(11)-C(21)	1.336(4)
N(11)-C(12)	1.449(4)
N(21)-C(41)	1.342(4)
N(21)-C(13)	1.443(4)
C(11)-C(21)	1.505(5)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(21)-C(31)	1.408(5)
C(31)-C(41)	1.393(5)
C(31)-H(31)	0.9500
C(41)-C(51)	1.509(5)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(12)-C(62)	1.402(5)
C(12)-C(22)	1.410(5)
C(22)-C(32)	1.400(5)
C(22)-C(72)	1.516(5)
C(32)-C(42)	1.375(6)
C(32)-H(32)	0.9500
C(42)-C(52)	1.386(6)
C(42)-H(42)	0.9500
C(52)-C(62)	1.393(5)
C(52)-H(52)	0.9500
C(62)-C(102)	1.523(5)
C(72)-C(82)	1.534(5)
C(72)-C(92)	1.535(6)
C(72)-H(72)	1.0000
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800

C(82)-H(82C)	0.9800
C(92)-H(92A)	0.9800
C(92)-H(92B)	0.9800
C(92)-H(92C)	0.9800
C(102)-C(112)	1.517(6)
C(102)-C(122)	1.529(6)
C(102)-H(102)	1.0000
C(112)-H(11D)	0.9800
C(112)-H(11E)	0.9800
C(112)-H(11F)	0.9800
C(122)-H(12A)	0.9800
C(122)-H(12B)	0.9800
C(122)-H(12C)	0.9800
C(13)-C(23)	1.404(5)
C(13)-C(63)	1.411(5)
C(23)-C(33)	1.387(5)
C(23)-C(73)	1.534(5)
C(33)-C(43)	1.385(5)
C(33)-H(33)	0.9500
C(43)-C(53)	1.378(5)
C(43)-H(43)	0.9500
C(53)-C(63)	1.394(5)
C(53)-H(53)	0.9500
C(63)-C(103)	1.525(5)
C(73)-C(93)	1.529(6)
C(73)-C(83)	1.536(6)
C(73)-H(73)	1.0000
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800
C(93)-H(93A)	0.9800
C(93)-H(93B)	0.9800
C(93)-H(93C)	0.9800
C(103)-C(113)	1.531(5)
C(103)-C(123)	1.545(5)
C(103)-H(103)	1.0000
C(113)-H(11G)	0.9800

C(113)-H(11H)	0.9800
C(113)-H(11I)	0.9800
C(123)-H(12D)	0.9800
C(123)-H(12E)	0.9800
C(123)-H(12F)	0.9800
O(14)-C(34)	1.423(4)
C(14)-C(24)	1.341(5)
C(14)-C(44)	1.479(5)
C(24)-C(34)	1.538(4)
C(24)-H(24)	0.9500
C(34)-C(164)	1.536(5)
C(34)-C(104)	1.542(4)
C(44)-C(94)	1.397(5)
C(44)-C(54)	1.405(5)
C(54)-C(64)	1.383(5)
C(54)-H(54)	0.9500
C(64)-C(74)	1.387(5)
C(64)-H(64)	0.9500
C(74)-C(84)	1.384(5)
C(74)-H(74)	0.9500
C(84)-C(94)	1.382(5)
C(84)-H(84)	0.9500
C(94)-H(94)	0.9500
C(104)-C(154)	1.389(5)
C(104)-C(114)	1.395(5)
C(114)-C(124)	1.388(5)
C(114)-H(114)	0.9500
C(124)-C(134)	1.383(5)
C(124)-H(124)	0.9500
C(134)-C(144)	1.380(5)
C(134)-H(134)	0.9500
C(144)-C(154)	1.385(5)
C(144)-H(144)	0.9500
C(154)-H(154)	0.9500
C(164)-C(174)	1.383(5)
C(164)-C(214)	1.384(5)
C(174)-C(184)	1.391(5)

C(174)-H(174)	0.9500
C(184)-C(194)	1.385(5)
C(184)-H(184)	0.9500
C(194)-C(204)	1.379(6)
C(194)-H(194)	0.9500
C(204)-C(214)	1.388(5)
C(204)-H(204)	0.9500
C(214)-H(214)	0.9500

O(14)-Fe(01)-N(21)	115.80(11)
O(14)-Fe(01)-N(11)	117.21(10)
N(21)-Fe(01)-N(11)	95.94(11)
O(14)-Fe(01)-C(14)	89.50(12)
N(21)-Fe(01)-C(14)	119.27(12)
N(11)-Fe(01)-C(14)	121.11(12)
C(21)-N(11)-C(12)	120.3(3)
C(21)-N(11)-Fe(01)	121.1(2)
C(12)-N(11)-Fe(01)	118.5(2)
C(41)-N(21)-C(13)	120.3(3)
C(41)-N(21)-Fe(01)	120.8(2)
C(13)-N(21)-Fe(01)	118.8(2)
C(21)-C(11)-H(11A)	109.5
C(21)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(21)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(11)-C(21)-C(31)	123.1(3)
N(11)-C(21)-C(11)	120.8(3)
C(31)-C(21)-C(11)	116.0(3)
C(41)-C(31)-C(21)	130.2(3)
C(41)-C(31)-H(31)	114.9
C(21)-C(31)-H(31)	114.9
N(21)-C(41)-C(31)	123.6(3)
N(21)-C(41)-C(51)	119.9(3)
C(31)-C(41)-C(51)	116.5(3)
C(41)-C(51)-H(51A)	109.5

C(41)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(41)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(62)-C(12)-C(22)	121.6(3)
C(62)-C(12)-N(11)	119.9(3)
C(22)-C(12)-N(11)	118.4(3)
C(32)-C(22)-C(12)	117.5(3)
C(32)-C(22)-C(72)	119.7(3)
C(12)-C(22)-C(72)	122.7(3)
C(42)-C(32)-C(22)	121.8(3)
C(42)-C(32)-H(32)	119.1
C(22)-C(32)-H(32)	119.1
C(32)-C(42)-C(52)	119.7(3)
C(32)-C(42)-H(42)	120.2
C(52)-C(42)-H(42)	120.2
C(42)-C(52)-C(62)	121.3(3)
C(42)-C(52)-H(52)	119.3
C(62)-C(52)-H(52)	119.3
C(52)-C(62)-C(12)	118.2(3)
C(52)-C(62)-C(102)	120.4(3)
C(12)-C(62)-C(102)	121.4(3)
C(22)-C(72)-C(82)	109.8(3)
C(22)-C(72)-C(92)	111.9(3)
C(82)-C(72)-C(92)	111.4(3)
C(22)-C(72)-H(72)	107.9
C(82)-C(72)-H(72)	107.9
C(92)-C(72)-H(72)	107.9
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
H(82B)-C(82)-H(82C)	109.5
C(72)-C(92)-H(92A)	109.5
C(72)-C(92)-H(92B)	109.5

H(92A)-C(92)-H(92B)	109.5
C(72)-C(92)-H(92C)	109.5
H(92A)-C(92)-H(92C)	109.5
H(92B)-C(92)-H(92C)	109.5
C(112)-C(102)-C(62)	113.3(3)
C(112)-C(102)-C(122)	110.6(3)
C(62)-C(102)-C(122)	111.2(3)
C(112)-C(102)-H(102)	107.1
C(62)-C(102)-H(102)	107.1
C(122)-C(102)-H(102)	107.1
C(102)-C(112)-H(11D)	109.5
C(102)-C(112)-H(11E)	109.5
H(11D)-C(112)-H(11E)	109.5
C(102)-C(112)-H(11F)	109.5
H(11D)-C(112)-H(11F)	109.5
H(11E)-C(112)-H(11F)	109.5
C(102)-C(122)-H(12A)	109.5
C(102)-C(122)-H(12B)	109.5
H(12A)-C(122)-H(12B)	109.5
C(102)-C(122)-H(12C)	109.5
H(12A)-C(122)-H(12C)	109.5
H(12B)-C(122)-H(12C)	109.5
C(23)-C(13)-C(63)	120.9(3)
C(23)-C(13)-N(21)	118.5(3)
C(63)-C(13)-N(21)	120.6(3)
C(33)-C(23)-C(13)	118.7(3)
C(33)-C(23)-C(73)	120.1(3)
C(13)-C(23)-C(73)	121.1(3)
C(43)-C(33)-C(23)	121.1(3)
C(43)-C(33)-H(33)	119.5
C(23)-C(33)-H(33)	119.5
C(53)-C(43)-C(33)	119.8(3)
C(53)-C(43)-H(43)	120.1
C(33)-C(43)-H(43)	120.1
C(43)-C(53)-C(63)	121.6(3)
C(43)-C(53)-H(53)	119.2
C(63)-C(53)-H(53)	119.2

C(53)-C(63)-C(13)	117.9(3)
C(53)-C(63)-C(103)	119.2(3)
C(13)-C(63)-C(103)	122.9(3)
C(93)-C(73)-C(23)	111.2(3)
C(93)-C(73)-C(83)	111.0(3)
C(23)-C(73)-C(83)	113.1(3)
C(93)-C(73)-H(73)	107.1
C(23)-C(73)-H(73)	107.1
C(83)-C(73)-H(73)	107.1
C(73)-C(83)-H(83A)	109.5
C(73)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(73)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
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(63)-C(103)-C(113)	110.4(3)
C(63)-C(103)-C(123)	112.6(3)
C(113)-C(103)-C(123)	109.8(3)
C(63)-C(103)-H(103)	108.0
C(113)-C(103)-H(103)	108.0
C(123)-C(103)-H(103)	108.0
C(103)-C(113)-H(11G)	109.5
C(103)-C(113)-H(11H)	109.5
H(11G)-C(113)-H(11H)	109.5
C(103)-C(113)-H(11I)	109.5
H(11G)-C(113)-H(11I)	109.5
H(11H)-C(113)-H(11I)	109.5
C(103)-C(123)-H(12D)	109.5
C(103)-C(123)-H(12E)	109.5
H(12D)-C(123)-H(12E)	109.5
C(103)-C(123)-H(12F)	109.5

H(12D)-C(123)-H(12F)	109.5
H(12E)-C(123)-H(12F)	109.5
C(34)-O(14)-Fe(01)	114.01(19)
C(24)-C(14)-C(44)	125.4(3)
C(24)-C(14)-Fe(01)	104.9(2)
C(44)-C(14)-Fe(01)	129.7(2)
C(14)-C(24)-C(34)	121.5(3)
C(14)-C(24)-H(24)	119.2
C(34)-C(24)-H(24)	119.2
O(14)-C(34)-C(164)	106.7(2)
O(14)-C(34)-C(24)	109.9(3)
C(164)-C(34)-C(24)	112.9(3)
O(14)-C(34)-C(104)	109.8(3)
C(164)-C(34)-C(104)	111.8(3)
C(24)-C(34)-C(104)	105.9(2)
C(94)-C(44)-C(54)	116.8(3)
C(94)-C(44)-C(14)	119.7(3)
C(54)-C(44)-C(14)	123.4(3)
C(64)-C(54)-C(44)	121.5(3)
C(64)-C(54)-H(54)	119.3
C(44)-C(54)-H(54)	119.3
C(54)-C(64)-C(74)	120.2(3)
C(54)-C(64)-H(64)	119.9
C(74)-C(64)-H(64)	119.9
C(84)-C(74)-C(64)	119.5(3)
C(84)-C(74)-H(74)	120.2
C(64)-C(74)-H(74)	120.2
C(94)-C(84)-C(74)	119.9(3)
C(94)-C(84)-H(84)	120.0
C(74)-C(84)-H(84)	120.0
C(84)-C(94)-C(44)	122.0(3)
C(84)-C(94)-H(94)	119.0
C(44)-C(94)-H(94)	119.0
C(154)-C(104)-C(114)	118.6(3)
C(154)-C(104)-C(34)	121.0(3)
C(114)-C(104)-C(34)	120.4(3)
C(124)-C(114)-C(104)	120.2(3)

C(124)-C(114)-H(114)	119.9
C(104)-C(114)-H(114)	119.9
C(134)-C(124)-C(114)	120.5(3)
C(134)-C(124)-H(124)	119.8
C(114)-C(124)-H(124)	119.8
C(144)-C(134)-C(124)	119.7(3)
C(144)-C(134)-H(134)	120.2
C(124)-C(134)-H(134)	120.2
C(134)-C(144)-C(154)	120.0(3)
C(134)-C(144)-H(144)	120.0
C(154)-C(144)-H(144)	120.0
C(144)-C(154)-C(104)	121.0(3)
C(144)-C(154)-H(154)	119.5
C(104)-C(154)-H(154)	119.5
C(174)-C(164)-C(214)	118.3(3)
C(174)-C(164)-C(34)	119.4(3)
C(214)-C(164)-C(34)	122.2(3)
C(164)-C(174)-C(184)	121.4(3)
C(164)-C(174)-H(174)	119.3
C(184)-C(174)-H(174)	119.3
C(194)-C(184)-C(174)	119.8(3)
C(194)-C(184)-H(184)	120.1
C(174)-C(184)-H(184)	120.1
C(204)-C(194)-C(184)	118.9(3)
C(204)-C(194)-H(194)	120.5
C(184)-C(194)-H(194)	120.5
C(194)-C(204)-C(214)	121.1(3)
C(194)-C(204)-H(204)	119.5
C(214)-C(204)-H(204)	119.5
C(164)-C(214)-C(204)	120.5(3)
C(164)-C(214)-H(214)	119.8
C(204)-C(214)-H(214)	119.8

Table S-27. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. 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}
Fe(01)	24(1)	21(1)	26(1)	-1(1)	0(1)	-1(1)
N(11)	28(1)	24(2)	23(1)	1(1)	-2(1)	-2(1)
N(21)	26(1)	25(2)	31(2)	0(1)	0(1)	1(1)
C(11)	39(2)	25(2)	36(2)	3(2)	-2(2)	-1(2)
C(21)	36(2)	22(2)	23(2)	0(1)	-4(1)	0(1)
C(31)	36(2)	22(2)	38(2)	4(1)	-5(2)	5(1)
C(41)	29(2)	28(2)	36(2)	-1(1)	-3(1)	3(1)
C(51)	33(2)	33(2)	69(3)	-3(2)	4(2)	8(2)
C(12)	29(2)	20(2)	31(2)	3(1)	-3(1)	-4(1)
C(22)	34(2)	27(2)	34(2)	4(1)	-5(2)	-2(1)
C(32)	34(2)	39(2)	36(2)	7(2)	-10(2)	-7(2)
C(42)	28(2)	44(2)	50(2)	9(2)	-2(2)	-6(2)
C(52)	36(2)	37(2)	44(2)	5(2)	9(2)	-5(2)
C(62)	34(2)	26(2)	32(2)	1(2)	3(1)	-7(2)
C(72)	40(2)	40(2)	28(2)	-2(2)	-5(2)	2(2)
C(82)	41(2)	52(3)	33(2)	1(2)	-2(2)	-5(2)
C(92)	69(3)	43(2)	38(2)	-7(2)	-11(2)	5(2)
C(102)	37(2)	38(2)	34(2)	-4(2)	5(2)	-10(2)
C(112)	77(3)	40(2)	39(2)	-1(2)	10(2)	0(2)
C(122)	53(2)	50(2)	33(2)	-4(2)	1(2)	10(2)
C(13)	24(2)	24(2)	34(2)	-2(1)	3(1)	1(1)
C(23)	29(2)	34(2)	31(2)	-6(2)	4(1)	2(1)
C(33)	40(2)	43(2)	32(2)	2(2)	8(2)	-3(2)
C(43)	35(2)	44(2)	44(2)	3(2)	9(2)	-11(2)
C(53)	28(2)	39(2)	41(2)	1(2)	-1(2)	-6(2)
C(63)	24(2)	28(2)	37(2)	-1(1)	0(1)	1(1)
C(73)	33(2)	42(2)	30(2)	-9(2)	4(1)	-6(2)
C(83)	49(2)	62(3)	33(2)	-2(2)	-7(2)	-3(2)
C(93)	50(2)	53(3)	50(2)	-20(2)	9(2)	-6(2)
C(103)	28(2)	37(2)	37(2)	5(2)	-4(1)	-4(1)
C(113)	39(2)	46(2)	32(2)	0(2)	-3(2)	-5(2)
C(123)	37(2)	50(3)	50(2)	10(2)	-7(2)	2(2)

O(14)	27(1)	23(1)	27(1)	-4(1)	0(1)	2(1)
C(14)	22(2)	28(2)	28(2)	-2(1)	1(1)	-5(1)
C(24)	24(2)	25(2)	28(2)	-2(1)	0(1)	-1(1)
C(34)	26(2)	24(2)	26(2)	-2(1)	-1(1)	-2(1)
C(44)	25(2)	26(2)	28(2)	-2(1)	1(1)	-5(1)
C(54)	29(2)	30(2)	32(2)	-4(1)	1(1)	-1(1)
C(64)	32(2)	38(2)	28(2)	-7(2)	3(1)	-5(2)
C(74)	33(2)	36(2)	25(2)	0(1)	-1(1)	-8(2)
C(84)	32(2)	32(2)	35(2)	5(2)	0(1)	-2(2)
C(94)	32(2)	28(2)	29(2)	-2(1)	3(1)	-3(1)
C(104)	27(2)	28(2)	22(2)	3(1)	1(1)	0(1)
C(114)	28(2)	28(2)	33(2)	-1(1)	1(1)	-1(1)
C(124)	29(2)	35(2)	37(2)	-1(2)	3(2)	-5(2)
C(134)	28(2)	38(2)	31(2)	2(2)	4(1)	4(2)
C(144)	34(2)	29(2)	36(2)	-2(2)	4(2)	4(2)
C(154)	30(2)	27(2)	32(2)	-2(1)	2(1)	-1(1)
C(164)	28(2)	21(2)	32(2)	-2(1)	4(1)	2(1)
C(174)	33(2)	32(2)	29(2)	-2(2)	-1(1)	-5(2)
C(184)	42(2)	37(2)	30(2)	4(2)	4(2)	-2(2)
C(194)	34(2)	38(2)	49(2)	7(2)	10(2)	-5(2)
C(204)	28(2)	44(2)	63(3)	13(2)	-5(2)	-9(2)
C(214)	29(2)	37(2)	48(2)	11(2)	-5(2)	-1(2)

Table S-28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(11A)	8314	9566	7697	51
H(11B)	7926	9687	6580	51
H(11C)	8987	9044	6925	51
H(31)	6364	8862	6877	39
H(51A)	4422	7606	6770	68
H(51B)	4897	8555	7525	68
H(51C)	4597	7301	7886	68
H(32)	11133	7356	9231	45
H(42)	12176	6835	8090	49
H(52)	11459	6472	6524	47
H(72)	8380	7650	8854	44
H(82A)	8856	5840	9520	64
H(82B)	8703	6721	10367	64
H(82C)	9836	6394	10145	64
H(92A)	10134	8596	10009	77
H(92B)	8963	8866	10141	77
H(92C)	9427	9313	9209	77
H(102)	8808	6199	5713	43
H(11D)	10772	5958	5076	78
H(11E)	9716	5410	4586	78
H(11F)	10231	4941	5601	78
H(12A)	8983	8192	5435	68
H(12B)	9057	7478	4473	68
H(12C)	10078	7974	5075	68
H(33)	4877	3991	9576	46
H(43)	3480	3375	8517	49
H(53)	3343	3915	6923	43
H(73)	7008	5600	8991	42
H(83A)	6251	4434	10550	73
H(83B)	7416	4821	10503	73
H(83C)	6919	3808	9823	73

H(93A)	5985	7169	9308	77
H(93B)	6726	6849	10260	77
H(93C)	5543	6473	10151	77
H(103)	5031	5840	5859	41
H(11G)	5395	3846	5630	60
H(11H)	4730	4382	4707	60
H(11I)	4189	3586	5428	60
H(12D)	2911	5142	5624	70
H(12E)	3431	5971	4911	70
H(12F)	3290	6408	5965	70
H(24)	7899	2834	5893	31
H(54)	7973	3370	4354	37
H(64)	7567	3852	2753	39
H(74)	6626	5529	2318	38
H(84)	6143	6753	3506	40
H(94)	6579	6294	5105	36
H(114)	9880	4627	7861	36
H(124)	11623	4180	7926	41
H(134)	12143	2291	7661	39
H(144)	10915	854	7272	39
H(154)	9174	1306	7144	36
H(174)	8581	2159	9017	38
H(184)	7616	831	9778	44
H(194)	5998	248	9042	48
H(204)	5375	1011	7554	55
H(214)	6331	2355	6806	47

Table S-29. Torsion angles [°] for [$L^{Me}Fe(OCPh_2CHCPh)$] (**6**).

C(12)-N(11)-C(21)-C(31)	-166.8(3)
Fe(01)-N(11)-C(21)-C(31)	9.9(4)
C(12)-N(11)-C(21)-C(11)	9.5(4)
Fe(01)-N(11)-C(21)-C(11)	-173.9(2)
N(11)-C(21)-C(31)-C(41)	11.1(6)
C(11)-C(21)-C(31)-C(41)	-165.3(4)
C(13)-N(21)-C(41)-C(31)	173.9(3)
Fe(01)-N(21)-C(41)-C(31)	-8.7(5)
C(13)-N(21)-C(41)-C(51)	-5.0(5)
Fe(01)-N(21)-C(41)-C(51)	172.5(3)
C(21)-C(31)-C(41)-N(21)	-11.8(6)
C(21)-C(31)-C(41)-C(51)	167.1(4)
C(21)-N(11)-C(12)-C(62)	-107.3(4)
Fe(01)-N(11)-C(12)-C(62)	76.0(3)
C(21)-N(11)-C(12)-C(22)	77.2(4)
Fe(01)-N(11)-C(12)-C(22)	-99.5(3)
C(62)-C(12)-C(22)-C(32)	0.8(5)
N(11)-C(12)-C(22)-C(32)	176.2(3)
C(62)-C(12)-C(22)-C(72)	-177.3(3)
N(11)-C(12)-C(22)-C(72)	-1.9(5)
C(12)-C(22)-C(32)-C(42)	-1.2(5)
C(72)-C(22)-C(32)-C(42)	177.0(4)
C(22)-C(32)-C(42)-C(52)	1.0(6)
C(32)-C(42)-C(52)-C(62)	-0.5(6)
C(42)-C(52)-C(62)-C(12)	0.2(5)
C(42)-C(52)-C(62)-C(102)	179.2(3)
C(22)-C(12)-C(62)-C(52)	-0.4(5)
N(11)-C(12)-C(62)-C(52)	-175.7(3)
C(22)-C(12)-C(62)-C(102)	-179.4(3)
N(11)-C(12)-C(62)-C(102)	5.3(5)
C(32)-C(22)-C(72)-C(82)	-68.5(4)
C(12)-C(22)-C(72)-C(82)	109.6(4)
C(32)-C(22)-C(72)-C(92)	55.7(4)
C(12)-C(22)-C(72)-C(92)	-126.2(4)
C(52)-C(62)-C(102)-C(112)	32.4(5)

C(12)-C(62)-C(102)-C(112)	-148.6(3)
C(52)-C(62)-C(102)-C(122)	-92.9(4)
C(12)-C(62)-C(102)-C(122)	86.1(4)
C(41)-N(21)-C(13)-C(23)	-103.1(4)
Fe(01)-N(21)-C(13)-C(23)	79.4(3)
C(41)-N(21)-C(13)-C(63)	79.5(4)
Fe(01)-N(21)-C(13)-C(63)	-98.0(3)
C(63)-C(13)-C(23)-C(33)	-3.0(5)
N(21)-C(13)-C(23)-C(33)	179.6(3)
C(63)-C(13)-C(23)-C(73)	178.7(3)
N(21)-C(13)-C(23)-C(73)	1.2(5)
C(13)-C(23)-C(33)-C(43)	0.0(5)
C(73)-C(23)-C(33)-C(43)	178.4(4)
C(23)-C(33)-C(43)-C(53)	2.6(6)
C(33)-C(43)-C(53)-C(63)	-2.1(6)
C(43)-C(53)-C(63)-C(13)	-0.8(5)
C(43)-C(53)-C(63)-C(103)	176.5(3)
C(23)-C(13)-C(63)-C(53)	3.3(5)
N(21)-C(13)-C(63)-C(53)	-179.3(3)
C(23)-C(13)-C(63)-C(103)	-173.9(3)
N(21)-C(13)-C(63)-C(103)	3.5(5)
C(33)-C(23)-C(73)-C(93)	-92.4(4)
C(13)-C(23)-C(73)-C(93)	85.9(4)
C(33)-C(23)-C(73)-C(83)	33.2(5)
C(13)-C(23)-C(73)-C(83)	-148.5(3)
C(53)-C(63)-C(103)-C(113)	-67.1(4)
C(13)-C(63)-C(103)-C(113)	110.0(4)
C(53)-C(63)-C(103)-C(123)	56.0(4)
C(13)-C(63)-C(103)-C(123)	-126.9(4)
N(21)-Fe(01)-O(14)-C(34)	119.6(2)
N(11)-Fe(01)-O(14)-C(34)	-128.2(2)
C(14)-Fe(01)-O(14)-C(34)	-3.0(2)
C(44)-C(14)-C(24)-C(34)	174.8(3)
Fe(01)-C(14)-C(24)-C(34)	-4.3(4)
Fe(01)-O(14)-C(34)-C(164)	-121.3(2)
Fe(01)-O(14)-C(34)-C(24)	1.4(3)
Fe(01)-O(14)-C(34)-C(104)	117.4(2)

C(14)-C(24)-C(34)-O(14)	2.3(4)
C(14)-C(24)-C(34)-C(164)	121.3(3)
C(14)-C(24)-C(34)-C(104)	-116.2(3)
C(24)-C(14)-C(44)-C(94)	167.2(3)
Fe(01)-C(14)-C(44)-C(94)	-14.0(4)
C(24)-C(14)-C(44)-C(54)	-15.5(5)
Fe(01)-C(14)-C(44)-C(54)	163.3(3)
C(94)-C(44)-C(54)-C(64)	-2.0(5)
C(14)-C(44)-C(54)-C(64)	-179.4(3)
C(44)-C(54)-C(64)-C(74)	0.0(5)
C(54)-C(64)-C(74)-C(84)	1.3(5)
C(64)-C(74)-C(84)-C(94)	-0.6(5)
C(74)-C(84)-C(94)-C(44)	-1.5(5)
C(54)-C(44)-C(94)-C(84)	2.7(5)
C(14)-C(44)-C(94)-C(84)	-179.8(3)
O(14)-C(34)-C(104)-C(154)	162.2(3)
C(164)-C(34)-C(104)-C(154)	44.0(4)
C(24)-C(34)-C(104)-C(154)	-79.3(4)
O(14)-C(34)-C(104)-C(114)	-20.6(4)
C(164)-C(34)-C(104)-C(114)	-138.8(3)
C(24)-C(34)-C(104)-C(114)	97.9(3)
C(154)-C(104)-C(114)-C(124)	0.5(5)
C(34)-C(104)-C(114)-C(124)	-176.8(3)
C(104)-C(114)-C(124)-C(134)	-1.6(5)
C(114)-C(124)-C(134)-C(144)	1.2(5)
C(124)-C(134)-C(144)-C(154)	0.1(5)
C(134)-C(144)-C(154)-C(104)	-1.2(5)
C(114)-C(104)-C(154)-C(144)	0.9(5)
C(34)-C(104)-C(154)-C(144)	178.1(3)
O(14)-C(34)-C(164)-C(174)	-76.1(4)
C(24)-C(34)-C(164)-C(174)	163.1(3)
C(104)-C(34)-C(164)-C(174)	43.9(4)
O(14)-C(34)-C(164)-C(214)	99.3(4)
C(24)-C(34)-C(164)-C(214)	-21.4(4)
C(104)-C(34)-C(164)-C(214)	-140.7(3)
C(214)-C(164)-C(174)-C(184)	0.5(5)
C(34)-C(164)-C(174)-C(184)	176.1(3)

C(164)-C(174)-C(184)-C(194)	0.0(6)
C(174)-C(184)-C(194)-C(204)	-0.1(6)
C(184)-C(194)-C(204)-C(214)	-0.3(6)
C(174)-C(164)-C(214)-C(204)	-0.9(6)
C(34)-C(164)-C(214)-C(204)	-176.4(3)
C(194)-C(204)-C(214)-C(164)	0.9(6)

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