Journal of Helmintology

Supplementary material

# *In vitro* nematicidal activity of two ferrocenyl chalcones against larvae of *Haemonchus contortus* ($L_3$) and *Nacobbus aberrans* ($J_2$)

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## 1. Chemical characterization

$^{1}H$ NMR and $^{13}C$ NMR spectra were recorded at 500 MHz and 125 MHz, respectively, in $CDCl_3$ using a Bruker Avance III Spectrometer. Chemical shifts (δ) are given in ppm and reported to the residual solvent peak ($CHCl_3$, 7.26 ppm and 77.16 ppm, respectively for $^{1}H$ and $^{13}C$). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (*J*, Hz) and integration. Analytical TLC was performed on silica gel 60 $F_{254}$ plates. Column chromatography was carried out on silica gel 60 (63-200 μm). IR spectra were obtained using an FT–IR spectrometer, Spectrum One, Perkin Elmer. X-ray diffraction analysis was performed on a diffractometer STOE Stadivari using Ag-$K\alpha$ radiation (λ = 0.56083 Å) and equipped with a Pilatus-100 K detector. Melting points were measured using a Mel-Temp II apparatus and are uncorrected. Elemental analyses were recorded from a Euro EA elemental analyzer (C and H only). All reagents were purchased from Sigma-Aldrich (Toluca, MEXICO) and used without further purification.

## 2. General procedure for the preparation of FcC's 1 and 2.

A solution of acetylferrocene (0.99 g, 4.38 mmol), NaOH (0.35 g, 8.76 mmol) and the corresponding benzaldehyde derivative (4.38 mmol) was refluxed during 4-5 h in 25 mL of EtOH. After cooling, the solvent was evaporated under reduced pressure to give the crude product as a red solid. This crude product was dissolved in 22 mL of AcOEt and transferred to a separatory funnel; then 25 mL of distilled water was added and the mixture was shaken vigorously. The mixture was allowed to stand undisturbed for ten minutes and the organic layer was separated. The extraction from the aqueous solution was repeated twice with 12 mL of AcOEt and the light red organic extracts were collected, dried over $Na_2SO_4$ and rotaevaporated under reduced pressure. Finally, the crude product was purified by column chromatography using Silica-gel (grade 60, 70–230 mesh) and a mixture of 9:1 hexanes–ethyl acetate as mobile phase. FcC's **1** and **2** were obtained in almost quantitative yields.

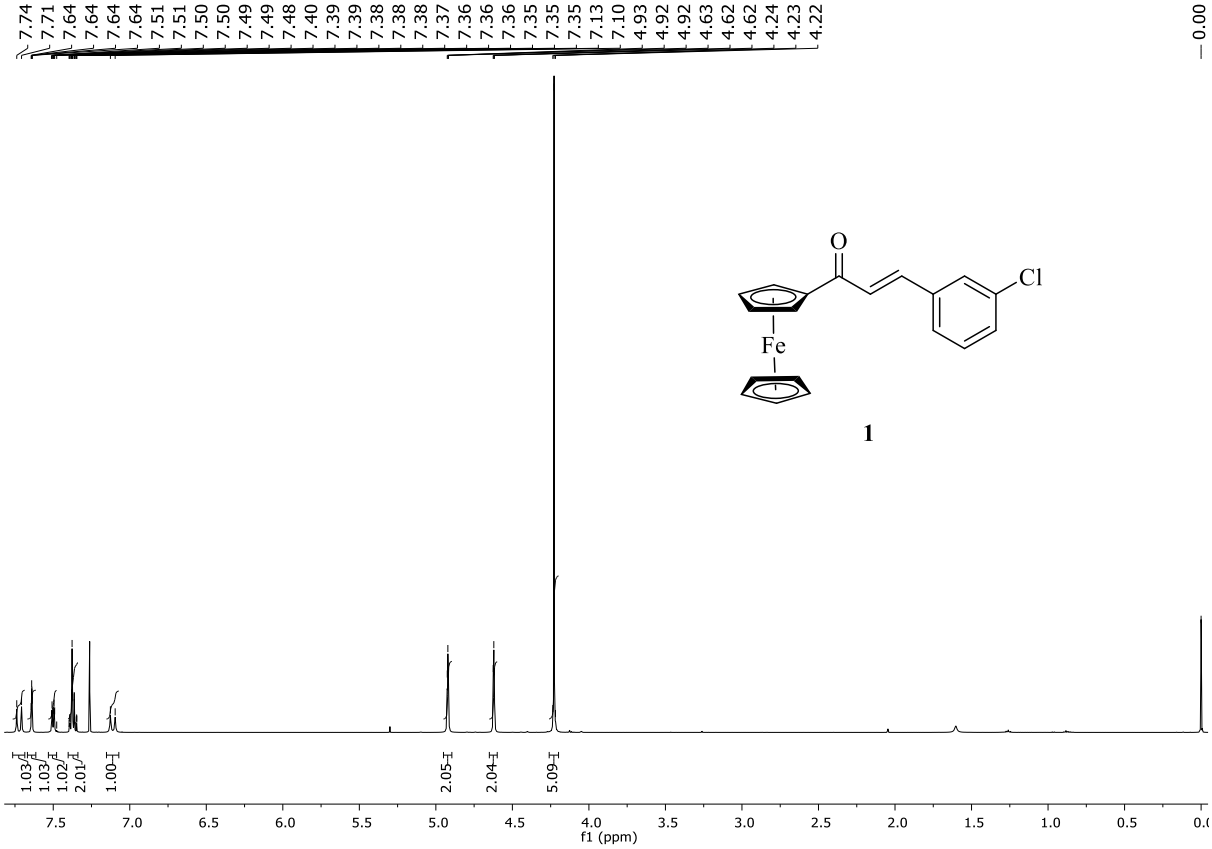
(2*E*)-1-ferrocenyl-3-(3-chlorophenyl)prop-2-en-1-one, FcC **1**.

Red solid (97 % yield). M.p. 131–133 °C. FT–IR $\nu_{max}/cm^{-1}$: 1657 (C=O), 1598 (C=C). $^{1}H$ NMR (500 MHz, $CDCl_3$) δ (ppm): 7.74 (d, 1H, *J* = 15.0 Hz), 7.64–7.35 (m, 4H), 7.13 (d, 1H, *J* = 15 Hz), 4.93 (m, 2H), 4.63 (m, 2H), 4.22 (s, 5H). $^{13}C$ NMR (125 MHz, $CDCl_3$) δ (ppm): 192.6, 139.1, 137.0, 134.9, 130.2, 129.9, 127.5, 126.8, 124.1, 80.4, 73.0, 70.2, 69.7. Anal. Calcd. for $C_{19}H_{15}ClFeO$ (%): C 65.09; H 4.31. Found (%): C 65.14; H 4.25.

(2*E*)-1-ferrocenyl-3-(3-methylphenyl)prop-2-en-1-one, FcC **2**.

Red solid (95 % yield). M.p. 139–141 °C. FT–IR $\nu_{max}/cm^{-1}$: 1652 (C=O), 1598 (C=C). $^{1}H$ NMR (500 MHz, $CDCl_3$) δ (ppm): 7.79 (d, 1H, *J* = 15 Hz), 7.47–7.22 (m, 4H), 7.14 (d, 1H, *J* = 15 Hz), 4.93 (m, 2H), 4.60 (m, 2H), 4.22 (s, 5H), 2.42 (s, 3H). $^{13}C$ NMR (125 MHz, $CDCl_3$) δ (ppm): 193.0, 141.0, 138.6, 135.1, 130.9, 128.8, 128.8, 125.4, 122.7, 80.6, 72.7, 70.1, 69.7, 21.4. Anal. Calcd. for $C_{20}H_{18}FeO$ (%): C 72.75; H 5.49. Found (%): C 72.64; H 5.31.

**Fig. S1. $^{1}$H (top) and $^{13}$C NMR (bottom) for (2*E*)-1-ferrocenyl-3-(3-chlorophenyl)prop-2-en-1-one, FcC 1.**



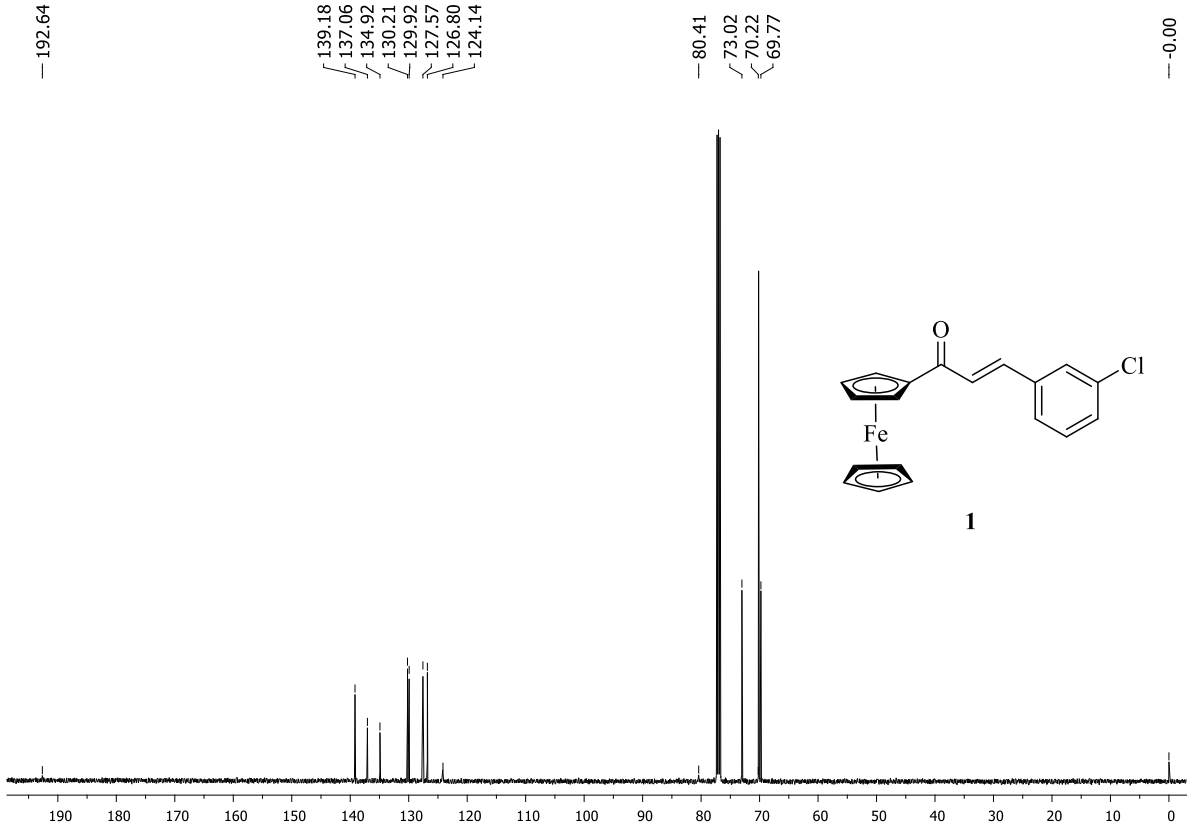
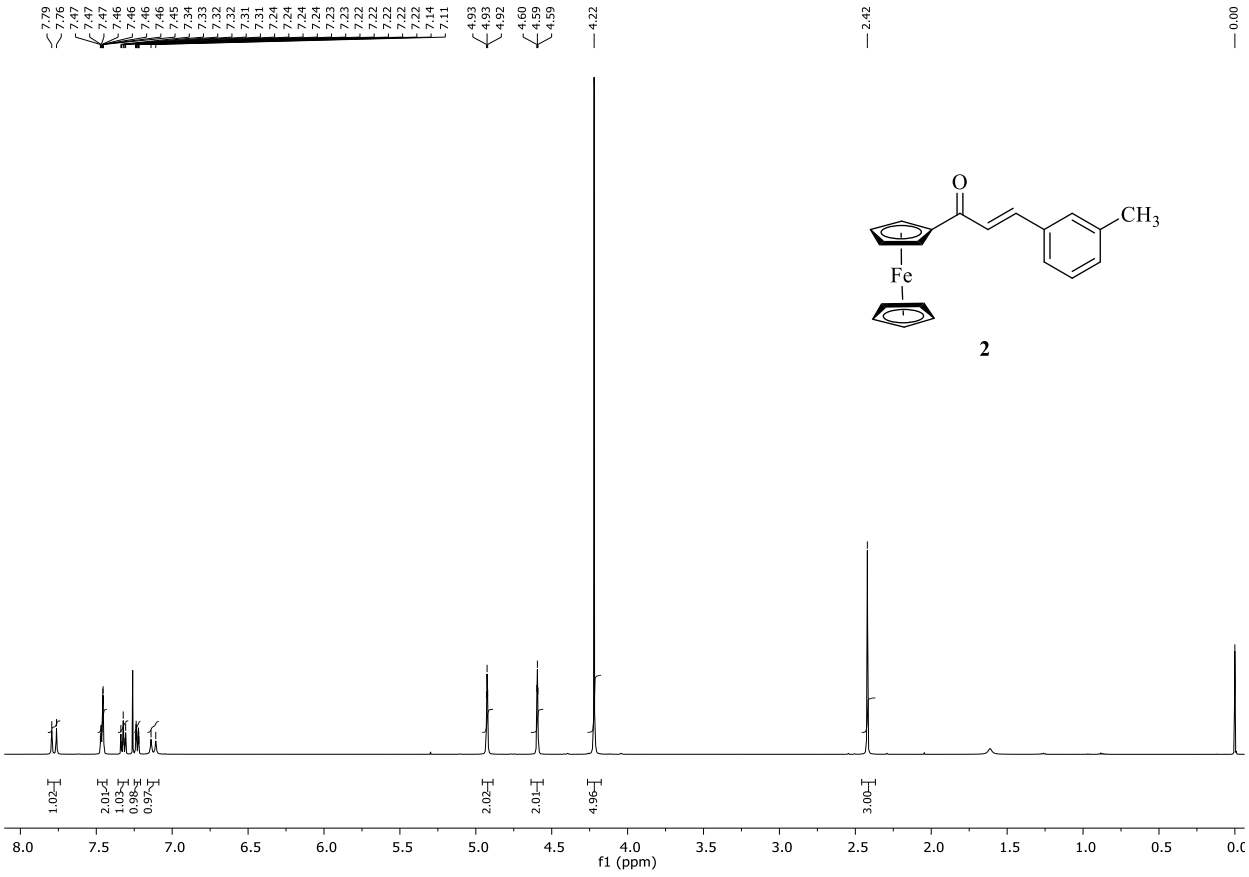



**Fig. S2. $^{1}$H (top) and $^{13}$C NMR (bottom) $^{1}$H and $^{13}$C NMR for (2E)-1-ferrocenyl-3-(3-methylphenyl)prop-2-en-1-one, FcC 2.**



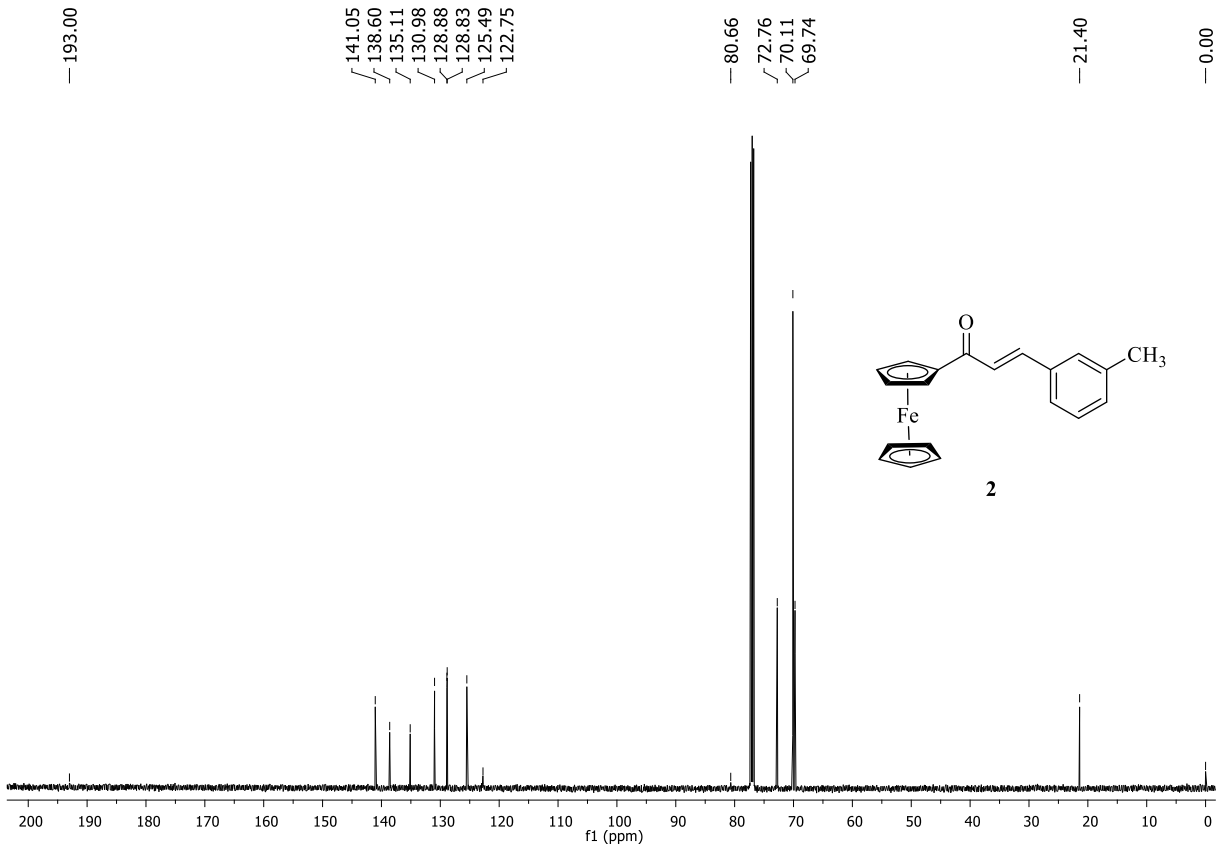



**Table S1. Crystal data and structure refinement for FcC-1.**

| | | |
|---|---|---|
| Identification code | JVB-9-Fe | |
| Empirical formula | C19 H15 Cl Fe O | |
| Formula weight | 350.61 | |
| Temperature | 293(2) K | |
| Wavelength | 0.56083 Å | |
| Crystal system | Orthorhombic | |
| Space group | $P2_12_12_1$ | |
| Unit cell dimensions | a = 5.8022(3) Å | α= 90°. |
| | b = 10.5286(5) Å | β= 90°. |
| | c = 25.5874(12) Å | γ = 90°. |
| Volume | 1563.11(13) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.490 $Mg/m^3$ | |
| Absorption coefficient | 0.591 $mm^{-1}$ | |
| F(000) | 720 | |
| Theta range for data collection | 1.977 to 20.517°. | |
| Index ranges | -7<=h<=7, -13<=k<=13, -31<=l<=31 | |
| Reflections collected | 42477 | |

| | |
|---|---|
| Independent reflections | 3196 [R(int) = 0.0951] |
| Completeness to theta = 19.664° | 99.9 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3196 / 0 / 199 |
| Goodness-of-fit on $F^2$ | 1.019 |
| Final R indices [I>2sigma(I)] | R1 = 0.0500, wR2 = 0.1175 |
| R indices (all data) | R1 = 0.0595, wR2 = 0.1257 |
| Absolute structure parameter | 0.08(3) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.971 and -0.246 e.$Å^{-3}$ |

**Table S2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for FcC-1. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1) | 5177(1) | 4980(1) | 4128(1) | 48(1) |
| Cl(1) | 5508(4) | 7735(2) | 7786(1) | 95(1) |
| O(1) | 1012(6) | 4912(4) | 5261(2) | 73(1) |
| C(1) | 3764(8) | 3957(5) | 4719(2) | 51(1) |
| C(2) | 2993(9) | 4573(5) | 5202(2) | 57(1) |
| C(3) | 4730(9) | 4752(5) | 5618(2) | 59(1) |
| C(4) | 4236(9) | 5362(5) | 6055(2) | 56(1) |
| C(5) | 5765(9) | 5580(5) | 6500(2) | 52(1) |
| C(6) | 5043(10) | 6402(4) | 6889(2) | 56(1) |
| C(7) | 6440(10) | 6630(5) | 7317(2) | 63(1) |
| C(8) | 8529(10) | 6048(6) | 7377(2) | 70(2) |
| C(9) | 9232(10) | 5209(5) | 6992(2) | 69(1) |
| C(10) | 7900(8) | 4991(6) | 6555(2) | 59(1) |
| C(11) | 2381(9) | 3849(5) | 4261(2) | 56(1) |
| C(12) | 3752(12) | 3309(5) | 3862(2) | 63(2) |
| C(13) | 5995(11) | 3089(5) | 4063(2) | 63(1) |
| C(14) | 6001(10) | 3486(4) | 4590(2) | 55(1) |
| C(15) | 5574(12) | 6805(5) | 4382(3) | 76(2) |
| C(16) | 4117(13) | 6772(6) | 3941(3) | 79(2) |
| C(17) | 5370(14) | 6242(6) | 3527(3) | 84(2) |
| C(18) | 7589(12) | 5955(6) | 3713(3) | 78(2) |
| C(19) | 7705(10) | 6307(5) | 4239(3) | 70(2) |

**Table S3. Bond lengths [Å] and angles [°] for FcC-1.**

| | |
|---|---|
| Fe(1)-C(14) | 2.025(5) |
| Fe(1)-C(1) | 2.028(5) |
| Fe(1)-C(18) | 2.035(6) |
| Fe(1)-C(17) | 2.036(5) |
| Fe(1)-C(15) | 2.041(5) |
| Fe(1)-C(11) | 2.041(5) |
| Fe(1)-C(16) | 2.041(6) |
| Fe(1)-C(19) | 2.045(5) |
| Fe(1)-C(13) | 2.053(5) |
| Fe(1)-C(12) | 2.061(6) |
| Cl(1)-C(7) | 1.758(6) |
| O(1)-C(2) | 1.213(7) |
| C(1)-C(11) | 1.424(7) |
| C(1)-C(14) | 1.427(7) |
| C(1)-C(2) | 1.466(8) |
| C(2)-C(3) | 1.479(7) |
| C(3)-C(4) | 1.320(8) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.463(7) |
| C(4)-H(4) | 0.9300 |
| C(5)-C(6) | 1.383(7) |
| C(5)-C(10) | 1.393(7) |
| C(6)-C(7) | 1.383(8) |
| C(6)-H(6) | 0.9300 |
| C(7)-C(8) | 1.367(8) |
| C(8)-C(9) | 1.384(8) |
| C(8)-H(8) | 0.9300 |
| C(9)-C(10) | 1.378(8) |
| C(9)-H(9) | 0.9300 |
| C(10)-H(10) | 0.9300 |
| C(11)-C(12) | 1.414(8) |
| C(11)-H(11) | 0.9300 |
| C(12)-C(13) | 1.419(9) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.412(8) |
| C(13)-H(13) | 0.9300 |

| | |
|---|---|
| C(14)-H(14) | 0.9300 |
| C(15)-C(19) | 1.392(9) |
| C(15)-C(16) | 1.411(10) |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.400(10) |
| C(16)-H(16) | 0.9300 |
| C(17)-C(18) | 1.406(10) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(19) | 1.396(10) |
| C(18)-H(18) | 0.9300 |
| C(19)-H(19) | 0.9300 |

| | |
|---|---|
| C(14)-Fe(1)-C(1) | 41.2(2) |
| C(14)-Fe(1)-C(18) | 122.3(2) |
| C(1)-Fe(1)-C(18) | 159.2(2) |
| C(14)-Fe(1)-C(17) | 159.3(3) |
| C(1)-Fe(1)-C(17) | 158.7(3) |
| C(18)-Fe(1)-C(17) | 40.4(3) |
| C(14)-Fe(1)-C(15) | 121.3(3) |
| C(1)-Fe(1)-C(15) | 108.0(2) |
| C(18)-Fe(1)-C(15) | 67.3(3) |
| C(17)-Fe(1)-C(15) | 67.7(3) |
| C(14)-Fe(1)-C(11) | 68.7(2) |
| C(1)-Fe(1)-C(11) | 41.0(2) |
| C(18)-Fe(1)-C(11) | 158.1(3) |
| C(17)-Fe(1)-C(11) | 123.4(3) |
| C(15)-Fe(1)-C(11) | 125.9(3) |
| C(14)-Fe(1)-C(16) | 157.9(3) |
| C(1)-Fe(1)-C(16) | 123.0(3) |
| C(18)-Fe(1)-C(16) | 67.6(3) |
| C(17)-Fe(1)-C(16) | 40.2(3) |
| C(15)-Fe(1)-C(16) | 40.5(3) |
| C(11)-Fe(1)-C(16) | 109.8(3) |
| C(14)-Fe(1)-C(19) | 106.3(2) |
| C(1)-Fe(1)-C(19) | 123.4(2) |
| C(18)-Fe(1)-C(19) | 40.0(3) |
| C(17)-Fe(1)-C(19) | 67.6(3) |
| C(15)-Fe(1)-C(19) | 39.8(3) |

| | |
|---|---|
| C(11)-Fe(1)-C(19) | 161.0(3) |
| C(16)-Fe(1)-C(19) | 67.5(3) |
| C(14)-Fe(1)-C(13) | 40.5(2) |
| C(1)-Fe(1)-C(13) | 68.8(2) |
| C(18)-Fe(1)-C(13) | 106.7(3) |
| C(17)-Fe(1)-C(13) | 124.0(3) |
| C(15)-Fe(1)-C(13) | 155.8(3) |
| C(11)-Fe(1)-C(13) | 68.4(2) |
| C(16)-Fe(1)-C(13) | 161.2(3) |
| C(19)-Fe(1)-C(13) | 120.5(2) |
| C(14)-Fe(1)-C(12) | 67.9(2) |
| C(1)-Fe(1)-C(12) | 68.3(2) |
| C(18)-Fe(1)-C(12) | 122.3(3) |
| C(17)-Fe(1)-C(12) | 109.2(3) |
| C(15)-Fe(1)-C(12) | 162.7(3) |
| C(11)-Fe(1)-C(12) | 40.3(2) |
| C(16)-Fe(1)-C(12) | 126.2(3) |
| C(19)-Fe(1)-C(12) | 156.5(3) |
| C(13)-Fe(1)-C(12) | 40.4(2) |
| C(11)-C(1)-C(14) | 107.2(4) |
| C(11)-C(1)-C(2) | 123.8(5) |
| C(14)-C(1)-C(2) | 128.7(5) |
| C(11)-C(1)-Fe(1) | 70.0(3) |
| C(14)-C(1)-Fe(1) | 69.3(3) |
| C(2)-C(1)-Fe(1) | 121.1(3) |
| O(1)-C(2)-C(1) | 121.6(5) |
| O(1)-C(2)-C(3) | 121.3(5) |
| C(1)-C(2)-C(3) | 117.1(4) |
| C(4)-C(3)-C(2) | 121.6(5) |
| C(4)-C(3)-H(3) | 119.2 |
| C(2)-C(3)-H(3) | 119.2 |
| C(3)-C(4)-C(5) | 127.2(5) |
| C(3)-C(4)-H(4) | 116.4 |
| C(5)-C(4)-H(4) | 116.4 |
| C(6)-C(5)-C(10) | 118.4(5) |
| C(6)-C(5)-C(4) | 118.3(5) |
| C(10)-C(5)-C(4) | 123.2(5) |
| C(5)-C(6)-C(7) | 120.0(5) |

| | |
|---|---|
| C(5)-C(6)-H(6) | 120.0 |
| C(7)-C(6)-H(6) | 120.0 |
| C(8)-C(7)-C(6) | 122.1(5) |
| C(8)-C(7)-Cl(1) | 119.5(5) |
| C(6)-C(7)-Cl(1) | 118.4(5) |
| C(7)-C(8)-C(9) | 117.8(5) |
| C(7)-C(8)-H(8) | 121.1 |
| C(9)-C(8)-H(8) | 121.1 |
| C(10)-C(9)-C(8) | 121.2(5) |
| C(10)-C(9)-H(9) | 119.4 |
| C(8)-C(9)-H(9) | 119.4 |
| C(9)-C(10)-C(5) | 120.4(5) |
| C(9)-C(10)-H(10) | 119.8 |
| C(5)-C(10)-H(10) | 119.8 |
| C(12)-C(11)-C(1) | 108.0(5) |
| C(12)-C(11)-Fe(1) | 70.6(3) |
| C(1)-C(11)-Fe(1) | 69.0(3) |
| C(12)-C(11)-H(11) | 126.0 |
| C(1)-C(11)-H(11) | 126.0 |
| Fe(1)-C(11)-H(11) | 126.0 |
| C(11)-C(12)-C(13) | 108.6(5) |
| C(11)-C(12)-Fe(1) | 69.1(3) |
| C(13)-C(12)-Fe(1) | 69.6(3) |
| C(11)-C(12)-H(12) | 125.7 |
| C(13)-C(12)-H(12) | 125.7 |
| Fe(1)-C(12)-H(12) | 127.2 |
| C(14)-C(13)-C(12) | 107.5(5) |
| C(14)-C(13)-Fe(1) | 68.7(3) |
| C(12)-C(13)-Fe(1) | 70.1(3) |
| C(14)-C(13)-H(13) | 126.2 |
| C(12)-C(13)-H(13) | 126.2 |
| Fe(1)-C(13)-H(13) | 126.5 |
| C(13)-C(14)-C(1) | 108.7(5) |
| C(13)-C(14)-Fe(1) | 70.8(3) |
| C(1)-C(14)-Fe(1) | 69.5(3) |
| C(13)-C(14)-H(14) | 125.7 |
| C(1)-C(14)-H(14) | 125.7 |
| Fe(1)-C(14)-H(14) | 125.6 |

| | |
|---|---|
| C(19)-C(15)-C(16) | 108.2(6) |
| C(19)-C(15)-Fe(1) | 70.3(3) |
| C(16)-C(15)-Fe(1) | 69.8(3) |
| C(19)-C(15)-H(15) | 125.9 |
| C(16)-C(15)-H(15) | 125.9 |
| Fe(1)-C(15)-H(15) | 125.6 |
| C(17)-C(16)-C(15) | 107.7(6) |
| C(17)-C(16)-Fe(1) | 69.7(3) |
| C(15)-C(16)-Fe(1) | 69.8(3) |
| C(17)-C(16)-H(16) | 126.2 |
| C(15)-C(16)-H(16) | 126.2 |
| Fe(1)-C(16)-H(16) | 125.9 |
| C(16)-C(17)-C(18) | 107.7(6) |
| C(16)-C(17)-Fe(1) | 70.1(3) |
| C(18)-C(17)-Fe(1) | 69.7(3) |
| C(16)-C(17)-H(17) | 126.1 |
| C(18)-C(17)-H(17) | 126.1 |
| Fe(1)-C(17)-H(17) | 125.6 |
| C(19)-C(18)-C(17) | 108.3(6) |
| C(19)-C(18)-Fe(1) | 70.4(3) |
| C(17)-C(18)-Fe(1) | 69.9(3) |
| C(19)-C(18)-H(18) | 125.9 |
| C(17)-C(18)-H(18) | 125.9 |
| Fe(1)-C(18)-H(18) | 125.4 |
| C(15)-C(19)-C(18) | 108.1(6) |
| C(15)-C(19)-Fe(1) | 69.9(3) |
| C(18)-C(19)-Fe(1) | 69.6(3) |
| C(15)-C(19)-H(19) | 125.9 |
| C(18)-C(19)-H(19) | 125.9 |
| Fe(1)-C(19)-H(19) | 126.2 |

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Symmetry transformations used to generate equivalent atoms:

**Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for FcC-1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$**

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 45(1) | 44(1) | 55(1) | 6(1) | -3(1) | -2(1) |
| Cl(1) | 100(1) | 107(1) | 77(1) | -31(1) | 8(1) | -1(1) |
| O(1) | 51(2) | 96(3) | 72(2) | -7(2) | -1(2) | 6(2) |
| C(1) | 51(3) | 47(2) | 56(2) | 8(2) | 2(2) | -6(2) |
| C(2) | 53(3) | 59(3) | 58(3) | 6(2) | 0(2) | -2(2) |
| C(3) | 53(3) | 68(3) | 56(2) | 1(2) | -3(2) | 8(2) |
| C(4) | 47(3) | 58(3) | 63(3) | 8(2) | 2(2) | 2(2) |
| C(5) | 52(3) | 49(2) | 55(2) | 9(2) | 4(2) | -4(2) |
| C(6) | 52(3) | 56(3) | 61(2) | 3(2) | 5(2) | 2(2) |
| C(7) | 64(3) | 68(3) | 57(3) | -4(3) | 11(2) | -9(3) |
| C(8) | 67(4) | 80(4) | 64(3) | 4(3) | -9(3) | -9(3) |
| C(9) | 57(3) | 74(4) | 77(3) | 10(3) | -6(2) | 6(3) |
| C(10) | 54(3) | 58(3) | 65(3) | 1(3) | 3(2) | 1(3) |
| C(11) | 48(3) | 55(3) | 64(3) | 7(2) | -2(2) | -14(2) |
| C(12) | 72(4) | 55(3) | 61(3) | -5(2) | -5(3) | -11(3) |
| C(13) | 70(3) | 47(3) | 73(3) | -2(2) | 8(3) | 3(2) |
| C(14) | 61(3) | 44(2) | 60(3) | 10(2) | -6(2) | 1(2) |
| C(15) | 80(5) | 41(2) | 105(5) | -6(3) | 7(4) | -7(3) |
| C(16) | 62(4) | 53(3) | 123(6) | 30(3) | -6(4) | 4(3) |
| C(17) | 99(5) | 72(3) | 80(4) | 37(3) | -12(4) | -20(4) |
| C(18) | 68(4) | 69(4) | 96(4) | 20(3) | 17(3) | -9(3) |
| C(19) | 54(3) | 58(3) | 98(4) | 4(3) | -14(3) | -17(3) |

**Table S5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for FcC-1.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 6206 | 4428 | 5571 | 71 |
| H(4) | 2752 | 5689 | 6082 | 67 |
| H(6) | 3618 | 6801 | 6862 | 67 |
| H(8) | 9448 | 6210 | 7667 | 85 |
| H(9) | 10629 | 4786 | 7029 | 83 |
| H(10) | 8431 | 4447 | 6295 | 71 |
| H(11) | 845 | 4090 | 4230 | 67 |
| H(12) | 3264 | 3128 | 3524 | 75 |
| H(13) | 7236 | 2747 | 3881 | 76 |
| H(14) | 7253 | 3446 | 4817 | 66 |
| H(15) | 5179 | 7106 | 4712 | 91 |
| H(16) | 2597 | 7051 | 3927 | 95 |
| H(17) | 4831 | 6105 | 3189 | 100 |
| H(18) | 8776 | 5592 | 3520 | 93 |
| H(19) | 8984 | 6224 | 4455 | 84 |

**Table S6. Torsion angles [°] for FcC-1.**

| | |
|---|---|
| C(11)-C(1)-C(2)-O(1) | 8.2(8) |
| C(14)-C(1)-C(2)-O(1) | -178.8(5) |
| Fe(1)-C(1)-C(2)-O(1) | 93.8(6) |
| C(11)-C(1)-C(2)-C(3) | -172.4(4) |
| C(14)-C(1)-C(2)-C(3) | 0.5(7) |
| Fe(1)-C(1)-C(2)-C(3) | -86.8(5) |
| O(1)-C(2)-C(3)-C(4) | -4.6(8) |
| C(1)-C(2)-C(3)-C(4) | 176.0(5) |
| C(2)-C(3)-C(4)-C(5) | 178.5(4) |
| C(3)-C(4)-C(5)-C(6) | 170.5(5) |
| C(3)-C(4)-C(5)-C(10) | -10.2(8) |
| C(10)-C(5)-C(6)-C(7) | 0.6(7) |
| C(4)-C(5)-C(6)-C(7) | 179.9(5) |
| C(5)-C(6)-C(7)-C(8) | -1.2(8) |
| C(5)-C(6)-C(7)-Cl(1) | 177.2(4) |
| C(6)-C(7)-C(8)-C(9) | 0.1(9) |
| Cl(1)-C(7)-C(8)-C(9) | -178.3(4) |
| C(7)-C(8)-C(9)-C(10) | 1.6(9) |
| C(8)-C(9)-C(10)-C(5) | -2.3(8) |
| C(6)-C(5)-C(10)-C(9) | 1.1(7) |
| C(4)-C(5)-C(10)-C(9) | -178.1(5) |
| C(14)-C(1)-C(11)-C(12) | 0.5(5) |
| C(2)-C(1)-C(11)-C(12) | 174.7(5) |
| Fe(1)-C(1)-C(11)-C(12) | 60.0(4) |
| C(14)-C(1)-C(11)-Fe(1) | -59.6(3) |
| C(2)-C(1)-C(11)-Fe(1) | 114.7(5) |
| C(1)-C(11)-C(12)-C(13) | -0.6(6) |
| Fe(1)-C(11)-C(12)-C(13) | 58.5(4) |
| C(1)-C(11)-C(12)-Fe(1) | -59.1(3) |
| C(11)-C(12)-C(13)-C(14) | 0.5(6) |
| Fe(1)-C(12)-C(13)-C(14) | 58.7(4) |
| C(11)-C(12)-C(13)-Fe(1) | -58.2(4) |
| C(12)-C(13)-C(14)-C(1) | -0.2(6) |
| Fe(1)-C(13)-C(14)-C(1) | 59.4(3) |
| C(12)-C(13)-C(14)-Fe(1) | -59.6(4) |
| C(11)-C(1)-C(14)-C(13) | -0.2(5) |

| | |
|---|---|
| C(2)-C(1)-C(14)-C(13) | -174.1(5) |
| Fe(1)-C(1)-C(14)-C(13) | -60.2(3) |
| C(11)-C(1)-C(14)-Fe(1) | 60.0(3) |
| C(2)-C(1)-C(14)-Fe(1) | -113.9(5) |
| C(19)-C(15)-C(16)-C(17) | 0.4(7) |
| Fe(1)-C(15)-C(16)-C(17) | -59.6(4) |
| C(19)-C(15)-C(16)-Fe(1) | 60.0(4) |
| C(15)-C(16)-C(17)-C(18) | -0.2(7) |
| Fe(1)-C(16)-C(17)-C(18) | -59.8(4) |
| C(15)-C(16)-C(17)-Fe(1) | 59.7(4) |
| C(16)-C(17)-C(18)-C(19) | -0.1(7) |
| Fe(1)-C(17)-C(18)-C(19) | -60.2(4) |
| C(16)-C(17)-C(18)-Fe(1) | 60.1(4) |
| C(16)-C(15)-C(19)-C(18) | -0.5(7) |
| Fe(1)-C(15)-C(19)-C(18) | 59.3(4) |
| C(16)-C(15)-C(19)-Fe(1) | -59.7(4) |
| C(17)-C(18)-C(19)-C(15) | 0.4(7) |
| Fe(1)-C(18)-C(19)-C(15) | -59.5(4) |
| C(17)-C(18)-C(19)-Fe(1) | 59.8(4) |

Symmetry transformations used to generate equivalent atoms:

**Table S7. Crystal data and structure refinement for FcC-2.**

| | | |
|---|---|---|
| Identification code | JVB-10-Fe | |
| Empirical formula | C20 H18 Fe O | |
| Formula weight | 330.19 | |
| Temperature | 295(1) K | |
| Wavelength | 0.56083 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1/c$ | |
| Unit cell dimensions | a = 28.5538(16) Å | α= 90°. |
| | b = 5.9183(2) Å | β= 110.119(4)°. |
| | c = 19.7317(11) Å | γ = 90°. |
| Volume | 3131.0(3) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.401 $Mg/m^3$ | |
| Absorption coefficient | 0.505 $mm^{-1}$ | |
| F(000) | 1376 | |
| Theta range for data collection | 2.398 to 20.518°. | |
| Index ranges | -35<=h<=35, -7<=k<=7, -24<=l<=24 | |
| Reflections collected | 54422 | |
| Independent reflections | 6415 [R(int) = 0.0889] | |
| Completeness to theta = 19.664° | 99.9 % | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6415 / 0 / 400 | |
| Goodness-of-fit on $F^2$ | 0.969 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0470, wR2 = 0.1043 | |
| R indices (all data) | R1 = 0.0627, wR2 = 0.1087 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 1.509 and -0.269 $e.Å^{-3}$ | |

**Table S8. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for FcC-2. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1) | 6879(1) | 11368(1) | 10934(1) | 42(1) |
| O(1) | 6507(1) | 15500(5) | 9362(2) | 60(1) |
| C(1) | 7012(2) | 12664(7) | 10065(2) | 40(1) |
| C(2) | 6608(2) | 13465(7) | 9429(3) | 47(1) |
| C(3) | 6344(2) | 11803(7) | 8878(2) | 47(1) |
| C(4) | 5979(2) | 12411(7) | 8269(2) | 44(1) |
| C(5) | 5720(2) | 11021(6) | 7647(2) | 43(1) |
| C(6) | 5328(2) | 11955(8) | 7099(3) | 49(1) |
| C(7) | 5091(2) | 10819(8) | 6458(3) | 56(1) |
| C(8) | 5259(2) | 8646(8) | 6383(3) | 63(1) |
| C(9) | 5642(2) | 7695(8) | 6935(3) | 56(1) |
| C(10) | 5880(2) | 8847(7) | 7548(3) | 51(1) |
| C(11) | 7257(2) | 14013(7) | 10701(3) | 51(1) |
| C(12) | 7588(2) | 12647(9) | 11192(3) | 55(1) |
| C(13) | 7566(2) | 10415(8) | 10930(3) | 54(1) |
| C(14) | 7213(2) | 10426(8) | 10228(2) | 48(1) |
| C(15) | 6128(2) | 11110(9) | 10698(3) | 62(1) |
| C(16) | 6335(2) | 12477(9) | 11307(4) | 69(2) |
| C(17) | 6684(2) | 11169(10) | 11839(3) | 70(2) |
| C(18) | 6690(2) | 9035(8) | 11549(3) | 60(1) |
| C(19) | 6349(2) | 8970(7) | 10844(3) | 60(1) |
| C(20) | 4679(2) | 11927(11) | 5852(3) | 82(2) |
| Fe(2) | 8150(1) | 8245(1) | 9033(1) | 40(1) |
| O(51) | 8466(1) | 4115(5) | 7764(2) | 58(1) |
| C(51) | 7966(2) | 6881(7) | 8033(2) | 44(1) |
| C(52) | 8360(2) | 6112(6) | 7758(2) | 42(1) |
| C(53) | 8615(2) | 7848(7) | 7470(2) | 43(1) |
| C(54) | 8994(2) | 7349(6) | 7254(2) | 43(1) |
| C(55) | 9262(2) | 8790(6) | 6911(2) | 42(1) |
| C(56) | 9675(2) | 7918(7) | 6769(2) | 45(1) |
| C(57) | 9912(2) | 9131(8) | 6381(3) | 52(1) |
| C(58) | 9744(2) | 11281(8) | 6152(3) | 56(1) |
| C(59) | 9341(2) | 12226(8) | 6290(3) | 53(1) |

| | | | | |
|---|---|---|---|---|
| C(60) | 9095(2) | 10981(7) | 6670(2) | 46(1) |
| C(61) | 7769(2) | 5514(7) | 8468(3) | 47(1) |
| C(62) | 7442(2) | 6899(7) | 8703(3) | 57(1) |
| C(63) | 7437(2) | 9084(7) | 8409(3) | 51(1) |
| C(64) | 7765(2) | 9082(7) | 8003(2) | 45(1) |
| C(65) | 8912(2) | 8615(7) | 9442(3) | 59(1) |
| C(66) | 8749(2) | 7129(8) | 9880(3) | 59(1) |
| C(67) | 8415(2) | 8264(9) | 10132(3) | 66(1) |
| C(68) | 8365(2) | 10538(8) | 9857(3) | 58(1) |
| C(69) | 8674(2) | 10702(7) | 9428(3) | 61(1) |
| C(70) | 10331(2) | 8099(10) | 6190(4) | 79(2) |

**Table S9. Bond lengths [Å] and angles [°] for FcC-2.**

| | |
|---|---|
| Fe(1)-C(14) | 2.018(4) |
| Fe(1)-C(18) | 2.029(5) |
| Fe(1)-C(1) | 2.030(4) |
| Fe(1)-C(15) | 2.036(5) |
| Fe(1)-C(19) | 2.037(5) |
| Fe(1)-C(11) | 2.042(4) |
| Fe(1)-C(16) | 2.042(5) |
| Fe(1)-C(13) | 2.045(5) |
| Fe(1)-C(17) | 2.048(5) |
| Fe(1)-C(12) | 2.054(4) |
| O(1)-C(2) | 1.235(5) |
| C(1)-C(14) | 1.435(6) |
| C(1)-C(11) | 1.447(6) |
| C(1)-C(2) | 1.461(7) |
| C(2)-C(3) | 1.467(6) |
| C(3)-C(4) | 1.342(6) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.451(6) |
| C(4)-H(4) | 0.9300 |
| C(5)-C(6) | 1.377(6) |
| C(5)-C(10) | 1.402(5) |
| C(6)-C(7) | 1.387(7) |
| C(6)-H(6) | 0.9300 |
| C(7)-C(8) | 1.398(7) |
| C(7)-C(20) | 1.509(7) |
| C(8)-C(9) | 1.372(8) |
| C(8)-H(8) | 0.9300 |
| C(9)-C(10) | 1.351(7) |
| C(9)-H(9) | 0.9300 |
| C(10)-H(10) | 0.9300 |
| C(11)-C(12) | 1.363(7) |
| C(11)-H(11) | 0.9300 |
| C(12)-C(13) | 1.412(7) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.404(6) |
| C(13)-H(13) | 0.9300 |

| | |
|---|---|
| C(14)-H(14) | 0.9300 |
| C(15)-C(19) | 1.400(6) |
| C(15)-C(16) | 1.400(8) |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.405(8) |
| C(16)-H(16) | 0.9300 |
| C(17)-C(18) | 1.389(7) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(19) | 1.397(7) |
| C(18)-H(18) | 0.9300 |
| C(19)-H(19) | 0.9300 |
| C(20)-H(20A) | 0.9600 |
| C(20)-H(20B) | 0.9600 |
| C(20)-H(20C) | 0.9600 |
| Fe(2)-C(64) | 2.012(4) |
| Fe(2)-C(51) | 2.026(4) |
| Fe(2)-C(67) | 2.037(5) |
| Fe(2)-C(69) | 2.039(4) |
| Fe(2)-C(68) | 2.043(5) |
| Fe(2)-C(63) | 2.046(5) |
| Fe(2)-C(66) | 2.046(5) |
| Fe(2)-C(61) | 2.051(4) |
| Fe(2)-C(65) | 2.055(5) |
| Fe(2)-C(62) | 2.061(4) |
| O(51)-C(52) | 1.219(5) |
| C(51)-C(64) | 1.416(6) |
| C(51)-C(61) | 1.428(6) |
| C(51)-C(52) | 1.479(6) |
| C(52)-C(53) | 1.480(6) |
| C(53)-C(54) | 1.327(6) |
| C(53)-H(53) | 0.9300 |
| C(54)-C(55) | 1.458(6) |
| C(54)-H(54) | 0.9300 |
| C(55)-C(56) | 1.401(6) |
| C(55)-C(60) | 1.407(5) |
| C(56)-C(57) | 1.383(7) |
| C(56)-H(56) | 0.9300 |
| C(57)-C(58) | 1.380(7) |

| | |
|---|---|
| C(57)-C(70) | 1.504(7) |
| C(58)-C(59) | 1.388(7) |
| C(58)-H(58) | 0.9300 |
| C(59)-C(60) | 1.400(7) |
| C(59)-H(59) | 0.9300 |
| C(60)-H(60) | 0.9300 |
| C(61)-C(62) | 1.435(7) |
| C(61)-H(61) | 0.9300 |
| C(62)-C(63) | 1.416(6) |
| C(62)-H(62) | 0.9300 |
| C(63)-C(64) | 1.428(6) |
| C(63)-H(63) | 0.9300 |
| C(64)-H(64) | 0.9300 |
| C(65)-C(69) | 1.405(6) |
| C(65)-C(66) | 1.418(7) |
| C(65)-H(65) | 0.9300 |
| C(66)-C(67) | 1.392(7) |
| C(66)-H(66) | 0.9300 |
| C(67)-C(68) | 1.440(7) |
| C(67)-H(67) | 0.9300 |
| C(68)-C(69) | 1.422(7) |
| C(68)-H(68) | 0.9300 |
| C(69)-H(69) | 0.9300 |
| C(70)-H(70A) | 0.9600 |
| C(70)-H(70B) | 0.9600 |
| C(70)-H(70C) | 0.9600 |
| C(14)-Fe(1)-C(18) | 120.7(2) |
| C(14)-Fe(1)-C(1) | 41.53(17) |
| C(18)-Fe(1)-C(1) | 158.03(19) |
| C(14)-Fe(1)-C(15) | 122.1(2) |
| C(18)-Fe(1)-C(15) | 67.1(2) |
| C(1)-Fe(1)-C(15) | 108.9(2) |
| C(14)-Fe(1)-C(19) | 105.1(2) |
| C(18)-Fe(1)-C(19) | 40.2(2) |
| C(1)-Fe(1)-C(19) | 122.61(19) |
| C(15)-Fe(1)-C(19) | 40.21(19) |
| C(14)-Fe(1)-C(11) | 69.17(18) |
| C(18)-Fe(1)-C(11) | 157.9(2) |

| | |
|---|---|
| C(1)-Fe(1)-C(11) | 41.64(18) |
| C(15)-Fe(1)-C(11) | 127.0(2) |
| C(19)-Fe(1)-C(11) | 161.6(2) |
| C(14)-Fe(1)-C(16) | 159.4(2) |
| C(18)-Fe(1)-C(16) | 67.2(2) |
| C(1)-Fe(1)-C(16) | 124.7(2) |
| C(15)-Fe(1)-C(16) | 40.2(2) |
| C(19)-Fe(1)-C(16) | 67.8(2) |
| C(11)-Fe(1)-C(16) | 111.15(19) |
| C(14)-Fe(1)-C(13) | 40.43(18) |
| C(18)-Fe(1)-C(13) | 105.5(2) |
| C(1)-Fe(1)-C(13) | 69.01(18) |
| C(15)-Fe(1)-C(13) | 156.1(2) |
| C(19)-Fe(1)-C(13) | 119.49(19) |
| C(11)-Fe(1)-C(13) | 68.19(18) |
| C(16)-Fe(1)-C(13) | 160.1(3) |
| C(14)-Fe(1)-C(17) | 156.9(2) |
| C(18)-Fe(1)-C(17) | 39.8(2) |
| C(1)-Fe(1)-C(17) | 160.7(2) |
| C(15)-Fe(1)-C(17) | 67.4(2) |
| C(19)-Fe(1)-C(17) | 67.7(2) |
| C(11)-Fe(1)-C(17) | 124.3(2) |
| C(16)-Fe(1)-C(17) | 40.2(2) |
| C(13)-Fe(1)-C(17) | 122.5(2) |
| C(14)-Fe(1)-C(12) | 67.2(2) |
| C(18)-Fe(1)-C(12) | 123.0(2) |
| C(1)-Fe(1)-C(12) | 67.4(2) |
| C(15)-Fe(1)-C(12) | 162.6(2) |
| C(19)-Fe(1)-C(12) | 156.5(2) |
| C(11)-Fe(1)-C(12) | 38.9(2) |
| C(16)-Fe(1)-C(12) | 126.8(2) |
| C(13)-Fe(1)-C(12) | 40.3(2) |
| C(17)-Fe(1)-C(12) | 110.2(2) |
| C(14)-C(1)-C(11) | 106.2(4) |
| C(14)-C(1)-C(2) | 129.0(4) |
| C(11)-C(1)-C(2) | 124.6(4) |
| C(14)-C(1)-Fe(1) | 68.8(2) |
| C(11)-C(1)-Fe(1) | 69.6(3) |

| | |
|---|---|
| C(2)-C(1)-Fe(1) | 121.8(3) |
| O(1)-C(2)-C(1) | 119.7(4) |
| O(1)-C(2)-C(3) | 122.2(4) |
| C(1)-C(2)-C(3) | 118.1(4) |
| C(4)-C(3)-C(2) | 121.8(4) |
| C(4)-C(3)-H(3) | 119.1 |
| C(2)-C(3)-H(3) | 119.1 |
| C(3)-C(4)-C(5) | 128.3(4) |
| C(3)-C(4)-H(4) | 115.9 |
| C(5)-C(4)-H(4) | 115.9 |
| C(6)-C(5)-C(10) | 118.4(4) |
| C(6)-C(5)-C(4) | 118.5(4) |
| C(10)-C(5)-C(4) | 122.8(4) |
| C(5)-C(6)-C(7) | 122.1(4) |
| C(5)-C(6)-H(6) | 118.9 |
| C(7)-C(6)-H(6) | 118.9 |
| C(6)-C(7)-C(8) | 117.8(5) |
| C(6)-C(7)-C(20) | 121.0(5) |
| C(8)-C(7)-C(20) | 121.2(5) |
| C(9)-C(8)-C(7) | 120.1(5) |
| C(9)-C(8)-H(8) | 119.9 |
| C(7)-C(8)-H(8) | 119.9 |
| C(10)-C(9)-C(8) | 121.5(5) |
| C(10)-C(9)-H(9) | 119.2 |
| C(8)-C(9)-H(9) | 119.2 |
| C(9)-C(10)-C(5) | 120.0(5) |
| C(9)-C(10)-H(10) | 120.0 |
| C(5)-C(10)-H(10) | 120.0 |
| C(12)-C(11)-C(1) | 107.4(4) |
| C(12)-C(11)-Fe(1) | 71.1(3) |
| C(1)-C(11)-Fe(1) | 68.7(2) |
| C(12)-C(11)-H(11) | 126.3 |
| C(1)-C(11)-H(11) | 126.3 |
| Fe(1)-C(11)-H(11) | 125.4 |
| C(11)-C(12)-C(13) | 111.2(4) |
| C(11)-C(12)-Fe(1) | 70.1(3) |
| C(13)-C(12)-Fe(1) | 69.5(3) |
| C(11)-C(12)-H(12) | 124.4 |

| | |
|---|---|
| C(13)-C(12)-H(12) | 124.4 |
| Fe(1)-C(12)-H(12) | 127.8 |
| C(14)-C(13)-C(12) | 106.4(4) |
| C(14)-C(13)-Fe(1) | 68.8(3) |
| C(12)-C(13)-Fe(1) | 70.2(3) |
| C(14)-C(13)-H(13) | 126.8 |
| C(12)-C(13)-H(13) | 126.8 |
| Fe(1)-C(13)-H(13) | 125.8 |
| C(13)-C(14)-C(1) | 108.8(4) |
| C(13)-C(14)-Fe(1) | 70.8(3) |
| C(1)-C(14)-Fe(1) | 69.7(2) |
| C(13)-C(14)-H(14) | 125.6 |
| C(1)-C(14)-H(14) | 125.6 |
| Fe(1)-C(14)-H(14) | 125.5 |
| C(19)-C(15)-C(16) | 108.6(5) |
| C(19)-C(15)-Fe(1) | 69.9(3) |
| C(16)-C(15)-Fe(1) | 70.1(3) |
| C(19)-C(15)-H(15) | 125.7 |
| C(16)-C(15)-H(15) | 125.7 |
| Fe(1)-C(15)-H(15) | 125.8 |
| C(15)-C(16)-C(17) | 107.7(5) |
| C(15)-C(16)-Fe(1) | 69.7(3) |
| C(17)-C(16)-Fe(1) | 70.1(3) |
| C(15)-C(16)-H(16) | 126.2 |
| C(17)-C(16)-H(16) | 126.2 |
| Fe(1)-C(16)-H(16) | 125.6 |
| C(18)-C(17)-C(16) | 107.4(5) |
| C(18)-C(17)-Fe(1) | 69.4(3) |
| C(16)-C(17)-Fe(1) | 69.7(3) |
| C(18)-C(17)-H(17) | 126.3 |
| C(16)-C(17)-H(17) | 126.3 |
| Fe(1)-C(17)-H(17) | 126.2 |
| C(17)-C(18)-C(19) | 109.4(5) |
| C(17)-C(18)-Fe(1) | 70.8(3) |
| C(19)-C(18)-Fe(1) | 70.2(3) |
| C(17)-C(18)-H(18) | 125.3 |
| C(19)-C(18)-H(18) | 125.3 |
| Fe(1)-C(18)-H(18) | 125.3 |

| | |
|---|---|
| C(18)-C(19)-C(15) | 106.9(4) |
| C(18)-C(19)-Fe(1) | 69.6(3) |
| C(15)-C(19)-Fe(1) | 69.9(3) |
| C(18)-C(19)-H(19) | 126.6 |
| C(15)-C(19)-H(19) | 126.6 |
| Fe(1)-C(19)-H(19) | 125.5 |
| C(7)-C(20)-H(20A) | 109.5 |
| C(7)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(7)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(64)-Fe(2)-C(51) | 41.05(17) |
| C(64)-Fe(2)-C(67) | 161.5(2) |
| C(51)-Fe(2)-C(67) | 156.3(2) |
| C(64)-Fe(2)-C(69) | 106.5(2) |
| C(51)-Fe(2)-C(69) | 124.5(2) |
| C(67)-Fe(2)-C(69) | 68.6(2) |
| C(64)-Fe(2)-C(68) | 123.40(19) |
| C(51)-Fe(2)-C(68) | 161.0(2) |
| C(67)-Fe(2)-C(68) | 41.3(2) |
| C(69)-Fe(2)-C(68) | 40.8(2) |
| C(64)-Fe(2)-C(63) | 41.18(18) |
| C(51)-Fe(2)-C(63) | 68.86(18) |
| C(67)-Fe(2)-C(63) | 124.6(2) |
| C(69)-Fe(2)-C(63) | 120.31(19) |
| C(68)-Fe(2)-C(63) | 106.35(19) |
| C(64)-Fe(2)-C(66) | 156.5(2) |
| C(51)-Fe(2)-C(66) | 122.1(2) |
| C(67)-Fe(2)-C(66) | 39.9(2) |
| C(69)-Fe(2)-C(66) | 67.7(2) |
| C(68)-Fe(2)-C(66) | 68.1(2) |
| C(63)-Fe(2)-C(66) | 161.6(2) |
| C(64)-Fe(2)-C(61) | 68.99(18) |
| C(51)-Fe(2)-C(61) | 41.00(18) |
| C(67)-Fe(2)-C(61) | 121.1(2) |
| C(69)-Fe(2)-C(61) | 162.3(2) |
| C(68)-Fe(2)-C(61) | 156.01(19) |

| | |
|---|---|
| C(63)-Fe(2)-C(61) | 68.37(18) |
| C(66)-Fe(2)-C(61) | 109.14(19) |
| C(64)-Fe(2)-C(65) | 120.50(19) |
| C(51)-Fe(2)-C(65) | 108.09(19) |
| C(67)-Fe(2)-C(65) | 68.0(2) |
| C(69)-Fe(2)-C(65) | 40.15(17) |
| C(68)-Fe(2)-C(65) | 68.26(19) |
| C(63)-Fe(2)-C(65) | 155.62(19) |
| C(66)-Fe(2)-C(65) | 40.46(19) |
| C(61)-Fe(2)-C(65) | 126.16(18) |
| C(64)-Fe(2)-C(62) | 68.9(2) |
| C(51)-Fe(2)-C(62) | 69.0(2) |
| C(67)-Fe(2)-C(62) | 107.6(2) |
| C(69)-Fe(2)-C(62) | 155.2(2) |
| C(68)-Fe(2)-C(62) | 120.0(2) |
| C(63)-Fe(2)-C(62) | 40.34(18) |
| C(66)-Fe(2)-C(62) | 125.9(2) |
| C(61)-Fe(2)-C(62) | 40.85(19) |
| C(65)-Fe(2)-C(62) | 163.11(19) |
| C(64)-C(51)-C(61) | 108.0(4) |
| C(64)-C(51)-C(52) | 128.0(4) |
| C(61)-C(51)-C(52) | 123.6(4) |
| C(64)-C(51)-Fe(2) | 69.0(2) |
| C(61)-C(51)-Fe(2) | 70.4(3) |
| C(52)-C(51)-Fe(2) | 120.3(3) |
| O(51)-C(52)-C(51) | 120.8(4) |
| O(51)-C(52)-C(53) | 121.6(4) |
| C(51)-C(52)-C(53) | 117.6(4) |
| C(54)-C(53)-C(52) | 122.1(4) |
| C(54)-C(53)-H(53) | 118.9 |
| C(52)-C(53)-H(53) | 118.9 |
| C(53)-C(54)-C(55) | 129.5(4) |
| C(53)-C(54)-H(54) | 115.3 |
| C(55)-C(54)-H(54) | 115.3 |
| C(56)-C(55)-C(60) | 118.9(4) |
| C(56)-C(55)-C(54) | 119.3(4) |
| C(60)-C(55)-C(54) | 121.7(4) |
| C(57)-C(56)-C(55) | 121.7(4) |

| | |
|---|---|
| C(57)-C(56)-H(56) | 119.2 |
| C(55)-C(56)-H(56) | 119.2 |
| C(58)-C(57)-C(56) | 118.6(4) |
| C(58)-C(57)-C(70) | 120.6(5) |
| C(56)-C(57)-C(70) | 120.8(4) |
| C(57)-C(58)-C(59) | 121.7(4) |
| C(57)-C(58)-H(58) | 119.2 |
| C(59)-C(58)-H(58) | 119.2 |
| C(58)-C(59)-C(60) | 119.7(4) |
| C(58)-C(59)-H(59) | 120.1 |
| C(60)-C(59)-H(59) | 120.1 |
| C(59)-C(60)-C(55) | 119.5(4) |
| C(59)-C(60)-H(60) | 120.3 |
| C(55)-C(60)-H(60) | 120.3 |
| C(51)-C(61)-C(62) | 107.8(4) |
| C(51)-C(61)-Fe(2) | 68.6(2) |
| C(62)-C(61)-Fe(2) | 69.9(2) |
| C(51)-C(61)-H(61) | 126.1 |
| C(62)-C(61)-H(61) | 126.1 |
| Fe(2)-C(61)-H(61) | 127.0 |
| C(63)-C(62)-C(61) | 107.7(4) |
| C(63)-C(62)-Fe(2) | 69.3(3) |
| C(61)-C(62)-Fe(2) | 69.2(2) |
| C(63)-C(62)-H(62) | 126.2 |
| C(61)-C(62)-H(62) | 126.2 |
| Fe(2)-C(62)-H(62) | 126.9 |
| C(62)-C(63)-C(64) | 108.4(4) |
| C(62)-C(63)-Fe(2) | 70.4(3) |
| C(64)-C(63)-Fe(2) | 68.2(3) |
| C(62)-C(63)-H(63) | 125.8 |
| C(64)-C(63)-H(63) | 125.8 |
| Fe(2)-C(63)-H(63) | 127.2 |
| C(51)-C(64)-C(63) | 108.1(4) |
| C(51)-C(64)-Fe(2) | 70.0(2) |
| C(63)-C(64)-Fe(2) | 70.7(3) |
| C(51)-C(64)-H(64) | 126.0 |
| C(63)-C(64)-H(64) | 126.0 |
| Fe(2)-C(64)-H(64) | 125.0 |

| | |
|---|---|
| C(69)-C(65)-C(66) | 107.4(5) |
| C(69)-C(65)-Fe(2) | 69.3(3) |
| C(66)-C(65)-Fe(2) | 69.4(3) |
| C(69)-C(65)-H(65) | 126.3 |
| C(66)-C(65)-H(65) | 126.3 |
| Fe(2)-C(65)-H(65) | 126.5 |
| C(67)-C(66)-C(65) | 109.1(4) |
| C(67)-C(66)-Fe(2) | 69.7(3) |
| C(65)-C(66)-Fe(2) | 70.1(3) |
| C(67)-C(66)-H(66) | 125.4 |
| C(65)-C(66)-H(66) | 125.4 |
| Fe(2)-C(66)-H(66) | 126.3 |
| C(66)-C(67)-C(68) | 107.9(5) |
| C(66)-C(67)-Fe(2) | 70.4(3) |
| C(68)-C(67)-Fe(2) | 69.6(3) |
| C(66)-C(67)-H(67) | 126.1 |
| C(68)-C(67)-H(67) | 126.1 |
| Fe(2)-C(67)-H(67) | 125.6 |
| C(69)-C(68)-C(67) | 106.7(4) |
| C(69)-C(68)-Fe(2) | 69.5(3) |
| C(67)-C(68)-Fe(2) | 69.1(3) |
| C(69)-C(68)-H(68) | 126.7 |
| C(67)-C(68)-H(68) | 126.7 |
| Fe(2)-C(68)-H(68) | 126.3 |
| C(65)-C(69)-C(68) | 108.8(4) |
| C(65)-C(69)-Fe(2) | 70.5(3) |
| C(68)-C(69)-Fe(2) | 69.8(3) |
| C(65)-C(69)-H(69) | 125.6 |
| C(68)-C(69)-H(69) | 125.6 |
| Fe(2)-C(69)-H(69) | 125.7 |
| C(57)-C(70)-H(70A) | 109.5 |
| C(57)-C(70)-H(70B) | 109.5 |
| H(70A)-C(70)-H(70B) | 109.5 |
| C(57)-C(70)-H(70C) | 109.5 |
| H(70A)-C(70)-H(70C) | 109.5 |
| H(70B)-C(70)-H(70C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

**Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for FcC-2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$**

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 42(1) | 45(1) | 42(1) | -6(1) | 16(1) | -3(1) |
| O(1) | 71(2) | 41(2) | 62(2) | 0(1) | 17(2) | 1(2) |
| C(1) | 36(3) | 42(2) | 41(3) | 0(2) | 14(2) | -4(2) |
| C(2) | 48(3) | 50(3) | 51(3) | -8(2) | 28(2) | -8(2) |
| C(3) | 50(3) | 43(2) | 49(3) | 2(2) | 20(2) | 1(2) |
| C(4) | 46(3) | 42(2) | 44(3) | 2(2) | 15(2) | 2(2) |
| C(5) | 41(2) | 42(2) | 47(3) | 3(2) | 17(2) | 1(2) |
| C(6) | 45(3) | 52(2) | 51(3) | 5(2) | 16(2) | 1(2) |
| C(7) | 46(3) | 70(3) | 52(3) | 10(2) | 15(2) | -8(2) |
| C(8) | 67(4) | 68(3) | 55(3) | -13(2) | 24(3) | -22(3) |
| C(9) | 63(4) | 46(2) | 65(4) | -14(2) | 31(3) | -11(2) |
| C(10) | 51(3) | 48(2) | 57(3) | 7(2) | 22(2) | 0(2) |
| C(11) | 48(3) | 45(2) | 59(3) | -8(2) | 18(2) | -9(2) |
| C(12) | 42(3) | 78(3) | 41(3) | -12(2) | 9(2) | -16(3) |
| C(13) | 50(3) | 65(3) | 48(3) | -4(2) | 16(2) | 9(2) |
| C(14) | 42(3) | 61(3) | 44(3) | -7(2) | 19(2) | 5(2) |
| C(15) | 37(3) | 82(3) | 67(4) | 10(3) | 18(3) | 0(2) |
| C(16) | 73(4) | 55(3) | 106(5) | -4(3) | 64(4) | 0(3) |
| C(17) | 76(4) | 90(4) | 54(3) | -16(3) | 36(3) | -19(3) |
| C(18) | 61(3) | 57(3) | 65(3) | 12(2) | 25(3) | -3(2) |
| C(19) | 60(3) | 54(2) | 68(3) | -7(2) | 25(3) | -11(2) |
| C(20) | 62(4) | 110(5) | 56(4) | 14(3) | -3(3) | -4(4) |
| Fe(2) | 40(1) | 42(1) | 39(1) | 1(1) | 16(1) | -3(1) |
| O(51) | 65(2) | 47(2) | 70(2) | -4(2) | 33(2) | 2(2) |
| C(51) | 37(2) | 56(2) | 35(2) | -3(2) | 9(2) | 0(2) |
| C(52) | 46(3) | 41(2) | 39(2) | -5(2) | 13(2) | 0(2) |
| C(53) | 45(3) | 43(2) | 44(3) | 1(2) | 17(2) | 4(2) |
| C(54) | 46(3) | 35(2) | 45(3) | -1(2) | 13(2) | -2(2) |
| C(55) | 43(2) | 44(2) | 37(2) | -3(2) | 10(2) | 1(2) |
| C(56) | 42(3) | 44(2) | 48(3) | -5(2) | 14(2) | 2(2) |
| C(57) | 47(3) | 59(3) | 50(3) | -10(2) | 16(2) | -7(2) |
| C(58) | 57(3) | 64(3) | 50(3) | -4(2) | 21(3) | -19(3) |
| C(59) | 59(3) | 43(2) | 50(3) | -1(2) | 9(3) | -4(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(60) | 45(3) | 43(2) | 50(3) | -4(2) | 15(2) | -2(2) |
| C(61) | 50(3) | 39(2) | 55(3) | -5(2) | 21(2) | -12(2) |
| C(62) | 47(3) | 71(3) | 56(3) | 11(3) | 21(3) | -17(2) |
| C(63) | 41(3) | 56(2) | 53(3) | -5(2) | 14(2) | 7(2) |
| C(64) | 43(3) | 47(2) | 44(3) | 4(2) | 14(2) | 1(2) |
| C(65) | 43(3) | 74(3) | 56(3) | -11(3) | 13(2) | 1(2) |
| C(66) | 57(3) | 56(3) | 53(3) | 9(2) | 5(3) | 5(2) |
| C(67) | 63(4) | 94(4) | 37(3) | -4(2) | 15(3) | -5(3) |
| C(68) | 59(3) | 51(2) | 62(3) | -15(2) | 17(3) | -1(2) |
| C(69) | 57(3) | 47(2) | 81(4) | -7(2) | 26(3) | -13(2) |
| C(70) | 65(4) | 92(4) | 94(5) | -14(3) | 46(4) | -10(3) |

**Table S11. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for FcC-2.**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 6433 | 10287 | 8954 | 56 |
| H(4) | 5880 | 13915 | 8241 | 53 |
| H(6) | 5218 | 13394 | 7161 | 59 |
| H(8) | 5110 | 7843 | 5957 | 75 |
| H(9) | 5740 | 6223 | 6887 | 67 |
| H(10) | 6151 | 8198 | 7905 | 61 |
| H(11) | 7198 | 15533 | 10762 | 61 |
| H(12) | 7801 | 13123 | 11641 | 66 |
| H(13) | 7749 | 9181 | 11173 | 65 |
| H(14) | 7124 | 9188 | 9920 | 57 |
| H(15) | 5885 | 11550 | 10268 | 74 |
| H(16) | 6256 | 13981 | 11352 | 83 |
| H(17) | 6876 | 11644 | 12300 | 84 |
| H(18) | 6890 | 7836 | 11787 | 72 |
| H(19) | 6282 | 7740 | 10532 | 72 |
| H(20A) | 4377 | 11922 | 5964 | 123 |
| H(20B) | 4626 | 11108 | 5412 | 123 |
| H(20C) | 4771 | 13457 | 5794 | 123 |
| H(53) | 8505 | 9337 | 7440 | 52 |
| H(54) | 9105 | 5862 | 7331 | 51 |
| H(56) | 9793 | 6488 | 6939 | 54 |
| H(58) | 9904 | 12118 | 5898 | 67 |
| H(59) | 9235 | 13680 | 6132 | 64 |
| H(60) | 8823 | 11597 | 6762 | 56 |
| H(61) | 7840 | 3997 | 8579 | 57 |
| H(62) | 7265 | 6444 | 8997 | 69 |
| H(63) | 7252 | 10310 | 8470 | 61 |
| H(64) | 7835 | 10313 | 7760 | 54 |
| H(65) | 9136 | 8271 | 9208 | 70 |
| H(66) | 8849 | 5634 | 9981 | 71 |
| H(67) | 8253 | 7661 | 10427 | 79 |
| H(68) | 8168 | 11677 | 9943 | 69 |

| | | | | |
|---|---|---|---|---|
| H(69) | 8713 | 11982 | 9179 | 73 |
| H(70A) | 10494 | 6965 | 6540 | 119 |
| H(70B) | 10567 | 9253 | 6188 | 119 |
| H(70C) | 10201 | 7421 | 5720 | 119 |

**Table S12. Torsion angles [°] for FcC-2.**

| | |
|---|---|
| C(14)-C(1)-C(2)-O(1) | -175.4(4) |
| C(11)-C(1)-C(2)-O(1) | 11.3(7) |
| Fe(1)-C(1)-C(2)-O(1) | 97.3(4) |
| C(14)-C(1)-C(2)-C(3) | 3.0(7) |
| C(11)-C(1)-C(2)-C(3) | -170.3(4) |
| Fe(1)-C(1)-C(2)-C(3) | -84.4(4) |
| O(1)-C(2)-C(3)-C(4) | 0.3(7) |
| C(1)-C(2)-C(3)-C(4) | -178.0(4) |
| C(2)-C(3)-C(4)-C(5) | 173.3(4) |
| C(3)-C(4)-C(5)-C(6) | 175.0(5) |
| C(3)-C(4)-C(5)-C(10) | -11.4(7) |
| C(10)-C(5)-C(6)-C(7) | -0.2(7) |
| C(4)-C(5)-C(6)-C(7) | 173.7(4) |
| C(5)-C(6)-C(7)-C(8) | 0.9(7) |
| C(5)-C(6)-C(7)-C(20) | -177.0(5) |
| C(6)-C(7)-C(8)-C(9) | 0.6(7) |
| C(20)-C(7)-C(8)-C(9) | 178.4(5) |
| C(7)-C(8)-C(9)-C(10) | -2.8(8) |
| C(8)-C(9)-C(10)-C(5) | 3.5(7) |
| C(6)-C(5)-C(10)-C(9) | -1.9(6) |
| C(4)-C(5)-C(10)-C(9) | -175.6(4) |
| C(14)-C(1)-C(11)-C(12) | 1.5(5) |
| C(2)-C(1)-C(11)-C(12) | 176.1(4) |
| Fe(1)-C(1)-C(11)-C(12) | 60.9(3) |
| C(14)-C(1)-C(11)-Fe(1) | -59.4(3) |
| C(2)-C(1)-C(11)-Fe(1) | 115.2(4) |
| C(1)-C(11)-C(12)-C(13) | -2.2(6) |
| Fe(1)-C(11)-C(12)-C(13) | 57.2(4) |
| C(1)-C(11)-C(12)-Fe(1) | -59.4(3) |
| C(11)-C(12)-C(13)-C(14) | 2.0(6) |
| Fe(1)-C(12)-C(13)-C(14) | 59.5(3) |
| C(11)-C(12)-C(13)-Fe(1) | -57.6(4) |
| C(12)-C(13)-C(14)-C(1) | -0.9(5) |
| Fe(1)-C(13)-C(14)-C(1) | 59.5(3) |
| C(12)-C(13)-C(14)-Fe(1) | -60.5(3) |
| C(11)-C(1)-C(14)-C(13) | -0.3(5) |

| | |
|---|---|
| C(2)-C(1)-C(14)-C(13) | -174.6(4) |
| Fe(1)-C(1)-C(14)-C(13) | -60.2(3) |
| C(11)-C(1)-C(14)-Fe(1) | 59.9(3) |
| C(2)-C(1)-C(14)-Fe(1) | -114.4(5) |
| C(19)-C(15)-C(16)-C(17) | -0.6(6) |
| Fe(1)-C(15)-C(16)-C(17) | -60.1(4) |
| C(19)-C(15)-C(16)-Fe(1) | 59.5(4) |
| C(15)-C(16)-C(17)-C(18) | 0.5(6) |
| Fe(1)-C(16)-C(17)-C(18) | -59.3(4) |
| C(15)-C(16)-C(17)-Fe(1) | 59.8(4) |
| C(16)-C(17)-C(18)-C(19) | -0.3(6) |
| Fe(1)-C(17)-C(18)-C(19) | -59.8(4) |
| C(16)-C(17)-C(18)-Fe(1) | 59.5(4) |
| C(17)-C(18)-C(19)-C(15) | -0.1(6) |
| Fe(1)-C(18)-C(19)-C(15) | -60.2(3) |
| C(17)-C(18)-C(19)-Fe(1) | 60.2(4) |
| C(16)-C(15)-C(19)-C(18) | 0.4(6) |
| Fe(1)-C(15)-C(19)-C(18) | 60.1(3) |
| C(16)-C(15)-C(19)-Fe(1) | -59.7(4) |
| C(64)-C(51)-C(52)-O(51) | -173.4(4) |
| C(61)-C(51)-C(52)-O(51) | 15.2(7) |
| Fe(2)-C(51)-C(52)-O(51) | 100.7(5) |
| C(64)-C(51)-C(52)-C(53) | 5.9(7) |
| C(61)-C(51)-C(52)-C(53) | -165.5(4) |
| Fe(2)-C(51)-C(52)-C(53) | -80.0(5) |
| O(51)-C(52)-C(53)-C(54) | -5.0(7) |
| C(51)-C(52)-C(53)-C(54) | 175.7(4) |
| C(52)-C(53)-C(54)-C(55) | 175.1(4) |
| C(53)-C(54)-C(55)-C(56) | 176.0(5) |
| C(53)-C(54)-C(55)-C(60) | -8.9(7) |
| C(60)-C(55)-C(56)-C(57) | -1.8(6) |
| C(54)-C(55)-C(56)-C(57) | 173.4(4) |
| C(55)-C(56)-C(57)-C(58) | 2.1(7) |
| C(55)-C(56)-C(57)-C(70) | -175.7(5) |
| C(56)-C(57)-C(58)-C(59) | -1.1(7) |
| C(70)-C(57)-C(58)-C(59) | 176.7(5) |
| C(57)-C(58)-C(59)-C(60) | -0.2(7) |
| C(58)-C(59)-C(60)-C(55) | 0.5(7) |

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| C(56)-C(55)-C(60)-C(59) | 0.5(6) |
| C(54)-C(55)-C(60)-C(59) | -174.6(4) |
| C(64)-C(51)-C(61)-C(62) | 0.2(5) |
| C(52)-C(51)-C(61)-C(62) | 173.1(4) |
| Fe(2)-C(51)-C(61)-C(62) | 59.1(3) |
| C(64)-C(51)-C(61)-Fe(2) | -58.9(3) |
| C(52)-C(51)-C(61)-Fe(2) | 114.0(4) |
| C(51)-C(61)-C(62)-C(63) | 0.5(6) |
| Fe(2)-C(61)-C(62)-C(63) | 58.8(3) |
| C(51)-C(61)-C(62)-Fe(2) | -58.3(3) |
| C(61)-C(62)-C(63)-C(64) | -1.0(6) |
| Fe(2)-C(62)-C(63)-C(64) | 57.7(3) |
| C(61)-C(62)-C(63)-Fe(2) | -58.7(3) |
| C(61)-C(51)-C(64)-C(63) | -0.8(5) |
| C(52)-C(51)-C(64)-C(63) | -173.3(4) |
| Fe(2)-C(51)-C(64)-C(63) | -60.7(3) |
| C(61)-C(51)-C(64)-Fe(2) | 59.8(3) |
| C(52)-C(51)-C(64)-Fe(2) | -112.6(5) |
| C(62)-C(63)-C(64)-C(51) | 1.2(5) |
| Fe(2)-C(63)-C(64)-C(51) | 60.2(3) |
| C(62)-C(63)-C(64)-Fe(2) | -59.1(4) |
| C(69)-C(65)-C(66)-C(67) | 0.1(6) |
| Fe(2)-C(65)-C(66)-C(67) | -59.0(4) |
| C(69)-C(65)-C(66)-Fe(2) | 59.1(4) |
| C(65)-C(66)-C(67)-C(68) | -0.5(6) |
| Fe(2)-C(66)-C(67)-C(68) | -59.7(4) |
| C(65)-C(66)-C(67)-Fe(2) | 59.2(4) |
| C(66)-C(67)-C(68)-C(69) | 0.6(6) |
| Fe(2)-C(67)-C(68)-C(69) | -59.6(3) |
| C(66)-C(67)-C(68)-Fe(2) | 60.2(4) |
| C(66)-C(65)-C(69)-C(68) | 0.3(6) |
| Fe(2)-C(65)-C(69)-C(68) | 59.5(3) |
| C(66)-C(65)-C(69)-Fe(2) | -59.2(4) |
| C(67)-C(68)-C(69)-C(65) | -0.6(6) |
| Fe(2)-C(68)-C(69)-C(65) | -59.9(3) |
| C(67)-C(68)-C(69)-Fe(2) | 59.4(3) |

Symmetry transformations used to generate equivalent atoms: