Supplementary Material for Organic & Biomolecular Chemistry

Electronic Supplementary Information for B506178D (Organic and Biomolecular Chemistry)

Amino acid conjugates of 1,1′-diaminoferrocene. Synthesis and chiral organisation

Somenath Chowdhury,[a] Khaled A. Mahmoud,[a] Gabriele Schatte[b] and Heinz-Bernhard Kraatz[a*]

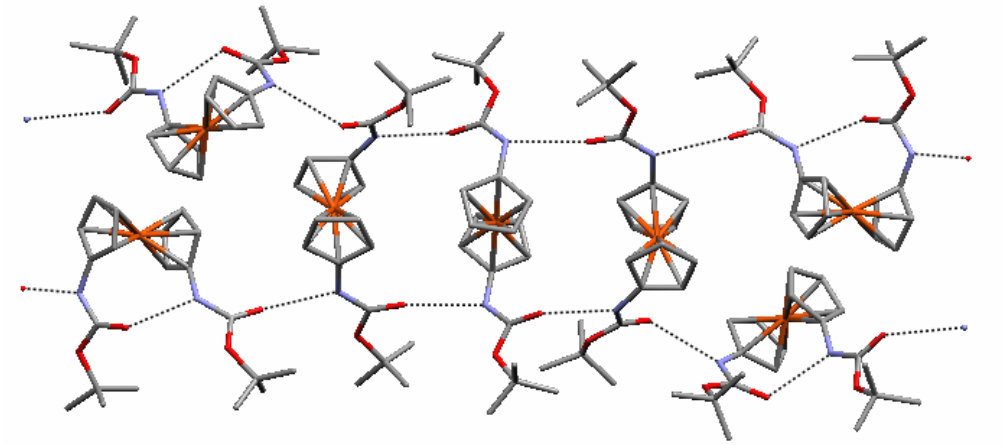

Fig. s1 Sheet like arrangement in the X-ray single crystal structure of compound **6** involving three different rotamers present in the asymmetric unit cell and their linkages though hydrogen bonding. Selected hydrogen bond distances O51…N41 2.709, N51A…O31 2.763, N51…O31A 2.763, O51A...N41A 2.709, O41…N11 2.781, N31…O21B 2.735, O11…N21 2.614, O21…N31B 2.735. [A =1-x,1-y,-z B=1.5-x,1/2+y,1/2-z].

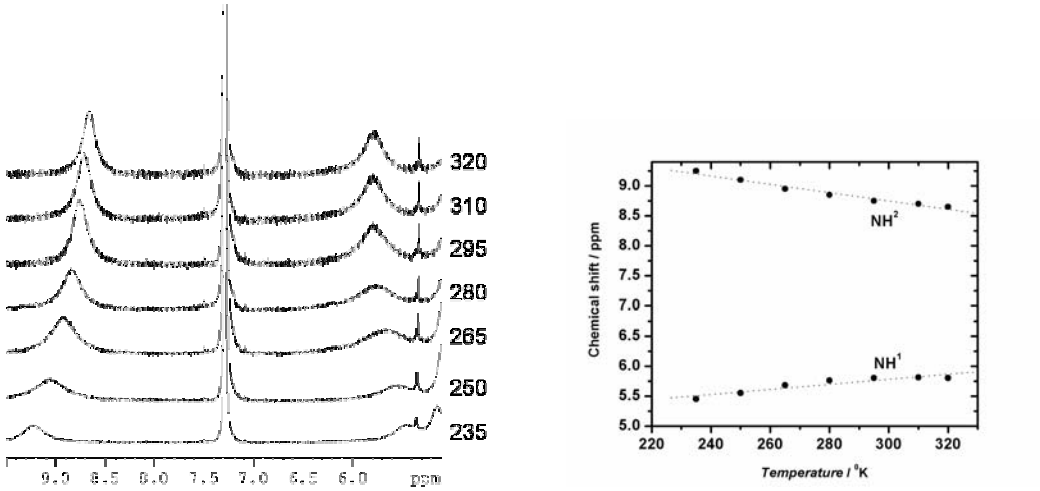

Fig. s2 Variable NMR study of 1,1'-bis(*tert*-butoxycarbonyl-L-alanine-amido) ferrocene (**7**), NH^1 is close to ferrocene and NH^2 is the one which is attached to Boc.

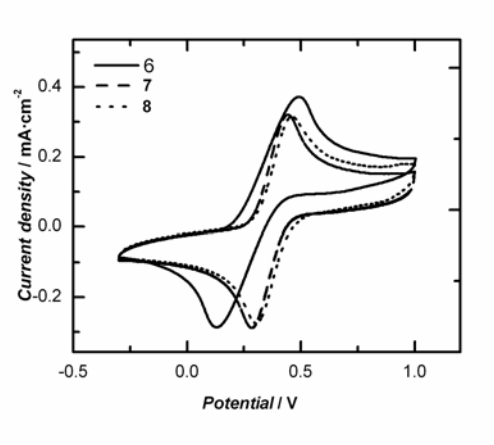

Fig. s3 Cyclic voltammogram SWV spectra of 0.1 M compounds **6**, **7**, **8** measured using GCE electrode *vs*. Ag/AgCl, scan rate 0.1 v/s, in CH_2Cl_2/0.1 M TBAP. The $E_{1/2}$ of the Fc/Fc^+ couple under the experimental conditions is 448(+/-5) mV (*vs*. Ag/AgCl)

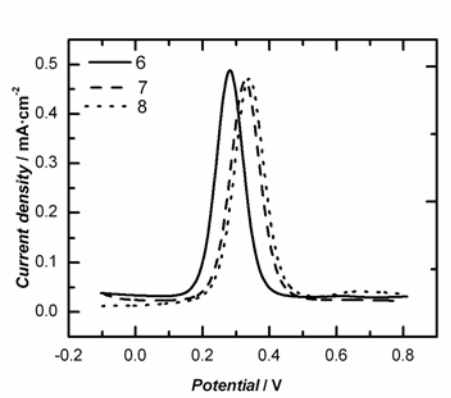

Fig. s4 SWV spectra of 0.1 M compounds **6**, **7**, **8** measured using GCE electrode *vs*. Ag/AgCl, scan rate 0.1 v/s, in CH_2Cl_2/0.1 M TBAP. The $E_{1/2}$ of the Fc/Fc^+ couple under the experimental conditions is 448(+/-5) mV (*vs*. Ag/AgCl).

Supplementary Material for Organic & Biomolecular Chemistry

Structural data for coumpounds **6**, **7** and **8**.

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# SUBMISSION DETAILS

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   in support of an upcoming communication to be published in
   Organic and Biomolecular Chemistry.
   Please forward any questions concerning
   this CIF to Dr. Gabriele Schatte
   (gabriele.schatte@usask.ca).
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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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based
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and R-
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C51 C 0.4620(2) 0.3697(2) -0.03482(7) 0.0222(6) Uani 1 1 d . . .
H51A H 0.4207 0.3839 -0.0551 0.027 Uiso 1 1 calc . . .
C52 C 0.5805(2) 0.3741(3) -0.02862(7) 0.0247(7) Uani 1 1 d . . .
H52 H 0.6427 0.3923 -0.0438 0.030 Uiso 1 1 calc . . .
C53 C 0.6004(2) 0.3468(3) 0.00500(7) 0.0258(7) Uani 1 1 d . . .
H53 H 0.6795 0.3439 0.0155 0.031 Uiso 1 1 calc . . .
C54 C 0.4936(2) 0.3258(3) 0.01997(7) 0.0242(7) Uani 1 1 d . . .
H54 H 0.4801 0.3064 0.0422 0.029 Uiso 1 1 calc . . .
C55 C 0.2299(2) 0.3428(3) 0.02462(7) 0.0236(7) Uani 1 1 d . . .
C56 C 0.0330(3) 0.3318(3) 0.04326(8) 0.0347(8) Uani 1 1 d . . .
C57 C 0.0200(3) 0.4669(3) 0.05105(9) 0.0470(10) Uani 1 1 d . . .
H57A H 0.0996 0.4964 0.0591 0.056 Uiso 1 1 calc R . .
H57B H -0.0428 0.4783 0.0677 0.056 Uiso 1 1 calc R . .
H57C H -0.0048 0.5071 0.0310 0.056 Uiso 1 1 calc R . .
C58 C 0.0617(3) 0.2572(3) 0.07352(9) 0.0491(10) Uani 1 1 d . . .
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H58B H -0.0112 0.2542 0.0874 0.059 Uiso 1 1 calc R . .
H58C H 0.1315 0.2897 0.0859 0.059 Uiso 1 1 calc R . .
C59 C -0.0714(3) 0.2797(4) 0.02605(10) 0.0658(13) Uani 1 1 d . . .
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H59B H -0.1446 0.2827 0.0398 0.079 Uiso 1 1 calc R . .
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H59C H -0.0518 0.2006 0.0211 0.079 Uiso 1 1 calc R . .

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0.0025(13)
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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# MOLECULAR GEOMETRY

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C15 O12 C16 C17 174.5(3) . . . . ?
C25 N21 C20 C21 90.7(4) . . . . ?
C25 N21 C20 C24 -93.2(4) . . . . ?
C25 N21 C20 Fe1 173.4(2) . . . . ?
C22 Fe1 C20 N21 -156.7(3) . . . . ?
C10 Fe1 C20 N21 32.7(3) . . . . ?
C21 Fe1 C20 N21 -114.4(4) . . . . ?
C14 Fe1 C20 N21 -15.0(3) . . . . ?
C11 Fe1 C20 N21 69.5(4) . . . . ?
C23 Fe1 C20 N21 155.7(3) . . . . ?
C12 Fe1 C20 N21 -75.5(7) . . . . ?
C13 Fe1 C20 N21 -52.3(3) . . . . ?
C24 Fe1 C20 N21 120.9(4) . . . . ?
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C22 Fe1 C20 C21 -42.3(2) . . . . ?
C10 Fe1 C20 C21 147.12(19) . . . . ?
C14 Fe1 C20 C21 99.4(2) . . . . ?
C11 Fe1 C20 C21 -176.1(2) . . . . ?
C23 Fe1 C20 C21 -89.9(2) . . . . ?
C12 Fe1 C20 C21 38.9(6) . . . . ?
C13 Fe1 C20 C21 62.1(2) . . . . ?
C24 Fe1 C20 C21 -124.7(3) . . . . ?
C22 Fe1 C20 C24 82.4(2) . . . . ?
C10 Fe1 C20 C24 -88.2(2) . . . . ?
C21 Fe1 C20 C24 124.7(3) . . . . ?
C14 Fe1 C20 C24 -135.91(18) . . . . ?
C11 Fe1 C20 C24 -51.4(3) . . . . ?
C23 Fe1 C20 C24 34.77(19) . . . . ?
C12 Fe1 C20 C24 163.6(5) . . . . ?
C13 Fe1 C20 C24 -173.18(17) . . . . ?
N21 C20 C21 C22 175.8(3) . . . . ?
C24 C20 C21 C22 -0.6(4) . . . . ?
Fe1 C20 C21 C22 60.7(2) . . . . ?
N21 C20 C21 Fe1 115.2(3) . . . . ?
C24 C20 C21 Fe1 -61.3(2) . . . . ?
C10 Fe1 C21 C22 -173.5(2) . . . . ?
C14 Fe1 C21 C22 151.4(2) . . . . ?
C20 Fe1 C21 C22 -110.8(3) . . . . ?
C23 Fe1 C21 C22 -38.3(2) . . . . ?
C12 Fe1 C21 C22 78.9(3) . . . . ?
C13 Fe1 C21 C22 113.0(2) . . . . ?
C24 Fe1 C21 C22 -76.4(2) . . . . ?
C22 Fe1 C21 C20 110.8(3) . . . . ?
C10 Fe1 C21 C20 -62.7(3) . . . . ?
C14 Fe1 C21 C20 -97.8(2) . . . . ?
C23 Fe1 C21 C20 72.54(19) . . . . ?
C12 Fe1 C21 C20 -170.31(18) . . . . ?
C13 Fe1 C21 C20 -136.18(18) . . . . ?
C24 Fe1 C21 C20 34.39(18) . . . . ?
C20 C21 C22 C23 0.3(4) . . . . ?
Fe1 C21 C22 C23 64.8(2) . . . . ?
C20 C21 C22 Fe1 -64.5(2) . . . . ?
C14 Fe1 C22 C21 -50.3(3) . . . . ?
C11 Fe1 C22 C21 -168.4(2) . . . . ?
C20 Fe1 C22 C21 41.8(2) . . . . ?
C23 Fe1 C22 C21 120.5(3) . . . . ?
C12 Fe1 C22 C21 -125.5(2) . . . . ?
C13 Fe1 C22 C21 -83.3(2) . . . . ?
C24 Fe1 C22 C21 86.1(2) . . . . ?
C21 Fe1 C22 C23 -120.5(3) . . . . ?
C14 Fe1 C22 C23 -170.74(19) . . . . ?
C11 Fe1 C22 C23 71.1(2) . . . . ?
C20 Fe1 C22 C23 -78.69(19) . . . . ?
C12 Fe1 C22 C23 114.02(19) . . . . ?
C13 Fe1 C22 C23 156.25(17) . . . . ?
C24 Fe1 C22 C23 -34.35(17) . . . . ?
C21 C22 C23 C24 0.2(4) . . . . ?
Fe1 C22 C23 C24 64.0(2) . . . . ?
C21 C22 C23 Fe1 -63.8(3) . . . . ?
C22 Fe1 C23 C24 -118.2(3) . . . . ?
C10 Fe1 C23 C24 68.9(3) . . . . ?
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C11 Fe1 C23 C24 108.7(2) . . . . ?
C20 Fe1 C23 C24 -38.9(2) . . . . ?
C12 Fe1 C23 C24 152.1(2) . . . . ?
C13 Fe1 C23 C24 -169.2(2) . . . . ?
C10 Fe1 C23 C22 -172.86(16) . . . . ?
C21 Fe1 C23 C22 36.38(17) . . . . ?
C11 Fe1 C23 C22 -133.11(17) . . . . ?
C20 Fe1 C23 C22 79.35(19) . . . . ?
C12 Fe1 C23 C22 -89.7(2) . . . . ?
C13 Fe1 C23 C22 -50.9(3) . . . . ?
C24 Fe1 C23 C22 118.2(3) . . . . ?
C22 C23 C24 C20 -0.5(4) . . . . ?
Fe1 C23 C24 C20 54.6(2) . . . . ?
C22 C23 C24 Fe1 -55.1(2) . . . . ?
N21 C20 C24 C23 -175.6(3) . . . . ?
C21 C20 C24 C23 0.8(4) . . . . ?
Fe1 C20 C24 C23 -56.7(2) . . . . ?
N21 C20 C24 Fe1 -118.9(3) . . . . ?
C21 C20 C24 Fe1 57.4(2) . . . . ?
C22 Fe1 C24 C23 40.8(2) . . . . ?
C10 Fe1 C24 C23 -130.0(2) . . . . ?
C21 Fe1 C24 C23 84.5(2) . . . . ?
C14 Fe1 C24 C23 -173.8(2) . . . . ?
C11 Fe1 C24 C23 -87.5(2) . . . . ?
C20 Fe1 C24 C23 118.8(3) . . . . ?
C12 Fe1 C24 C23 -54.4(4) . . . . ?
C22 Fe1 C24 C20 -78.0(2) . . . . ?
C10 Fe1 C24 C20 111.27(18) . . . . ?
C21 Fe1 C24 C20 -34.29(17) . . . . ?
C14 Fe1 C24 C20 67.4(2) . . . . ?
C11 Fe1 C24 C20 153.70(17) . . . . ?
C23 Fe1 C24 C20 -118.8(3) . . . . ?
C12 Fe1 C24 C20 -173.1(2) . . . . ?
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C26 O22 C25 N21 -165.0(3) . . . . ?
C20 N21 C25 O21 -12.1(6) . . . . ?
C20 N21 C25 O22 169.0(3) . . . . ?
C25 O22 C26 C29 167.9(3) . . . . ?
C25 O22 C26 C27 -78.0(3) . . . . ?
C25 O22 C26 C28 53.2(4) . . . . ?
C35 N31 C30 C31 -3.3(4) . . . . ?
C35 N31 C30 C34 175.4(3) . . . . ?
C35 N31 C30 Fe2 -99.0(3) . . . . ?
C34 Fe2 C30 C31 116.9(2) . . . . ?
C40 Fe2 C30 C31 -48.1(4) . . . . ?
C44 Fe2 C30 C31 -81.9(2) . . . . ?
C41 Fe2 C30 C31 163.4(3) . . . . ?
C42 Fe2 C30 C31 -162.16(19) . . . . ?
C33 Fe2 C30 C31 79.52(19) . . . . ?
C32 Fe2 C30 C31 37.99(18) . . . . ?
C43 Fe2 C30 C31 -121.99(19) . . . . ?
C40 Fe2 C30 C34 -165.0(3) . . . . ?
C44 Fe2 C30 C34 161.23(18) . . . . ?
C41 Fe2 C30 C34 46.6(4) . . . . ?
C31 Fe2 C30 C34 -116.9(2) . . . . ?
C42 Fe2 C30 C34 80.9(2) . . . . ?
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C32 Fe2 C30 C34 -78.90(19) . . . . ?
C43 Fe2 C30 C34 121.11(19) . . . . ?
C34 Fe2 C30 N31 -118.2(3) . . . . ?
C40 Fe2 C30 N31 76.9(4) . . . . ?
C44 Fe2 C30 N31 43.1(3) . . . . ?
C41 Fe2 C30 N31 -71.6(5) . . . . ?
C31 Fe2 C30 N31 124.9(3) . . . . ?
C42 Fe2 C30 N31 -37.2(3) . . . . ?
C33 Fe2 C30 N31 -155.6(3) . . . . ?
C32 Fe2 C30 N31 162.9(3) . . . . ?
C43 Fe2 C30 N31 2.9(3) . . . . ?
C34 C30 C31 C32 -1.2(3) . . . . ?
N31 C30 C31 C32 177.8(2) . . . . ?
Fe2 C30 C31 C32 -57.51(17) . . . . ?
C34 C30 C31 Fe2 56.34(17) . . . . ?
N31 C30 C31 Fe2 -124.7(3) . . . . ?
C34 Fe2 C31 C30 -41.86(18) . . . . ?
C40 Fe2 C31 C30 160.05(18) . . . . ?
C44 Fe2 C31 C30 112.65(18) . . . . ?
C41 Fe2 C31 C30 -164.5(3) . . . . ?
C42 Fe2 C31 C30 43.7(4) . . . . ?
C33 Fe2 C31 C30 -88.62(19) . . . . ?
C32 Fe2 C31 C30 -122.5(2) . . . . ?
C43 Fe2 C31 C30 72.2(2) . . . . ?
C34 Fe2 C31 C32 80.61(18) . . . . ?
C40 Fe2 C31 C32 -77.5(2) . . . . ?
C30 Fe2 C31 C32 122.5(2) . . . . ?
C44 Fe2 C31 C32 -124.88(18) . . . . ?
C41 Fe2 C31 C32 -42.1(4) . . . . ?
C42 Fe2 C31 C32 166.2(3) . . . . ?
C33 Fe2 C31 C32 33.85(17) . . . . ?
C43 Fe2 C31 C32 -165.34(17) . . . . ?
C30 C31 C32 C33 0.9(3) . . . . ?
Fe2 C31 C32 C33 -55.11(19) . . . . ?
C30 C31 C32 Fe2 56.04(18) . . . . ?
C34 Fe2 C32 C33 40.54(18) . . . . ?
C40 Fe2 C32 C33 -115.70(19) . . . . ?
C30 Fe2 C32 C33 88.26(19) . . . . ?
C44 Fe2 C32 C33 -162.43(18) . . . . ?
C41 Fe2 C32 C33 -72.5(2) . . . . ?
C31 Fe2 C32 C33 124.3(2) . . . . ?
C42 Fe2 C32 C33 -42.2(4) . . . . ?
C43 Fe2 C32 C33 164.0(3) . . . . ?
C34 Fe2 C32 C31 -83.77(18) . . . . ?
C40 Fe2 C32 C31 119.99(17) . . . . ?
C30 Fe2 C32 C31 -36.06(16) . . . . ?
C44 Fe2 C32 C31 73.3(2) . . . . ?
C41 Fe2 C32 C31 163.18(17) . . . . ?
C42 Fe2 C32 C31 -166.5(3) . . . . ?
C33 Fe2 C32 C31 -124.3(2) . . . . ?
C43 Fe2 C32 C31 39.7(4) . . . . ?
C31 C32 C33 C34 -0.2(3) . . . . ?
Fe2 C32 C33 C34 -52.95(18) . . . . ?
C31 C32 C33 Fe2 52.74(18) . . . . ?
C34 Fe2 C33 C32 -118.8(2) . . . . ?
C40 Fe2 C33 C32 78.70(19) . . . . ?
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C44 Fe2 C33 C32 44.9(4) . . . . ?
C41 Fe2 C33 C32 120.54(19) . . . . ?
C31 Fe2 C33 C32 -37.22(17) . . . . ?
C42 Fe2 C33 C32 162.11(18) . . . . ?
C43 Fe2 C33 C32 -164.7(3) . . . . ?
C40 Fe2 C33 C34 -162.47(17) . . . . ?
C30 Fe2 C33 C34 38.09(17) . . . . ?
C44 Fe2 C33 C34 163.8(3) . . . . ?
C41 Fe2 C33 C34 -120.62(18) . . . . ?
C31 Fe2 C33 C34 81.61(18) . . . . ?
C42 Fe2 C33 C34 -79.1(2) . . . . ?
C32 Fe2 C33 C34 118.8(2) . . . . ?
C43 Fe2 C33 C34 -45.8(4) . . . . ?
C31 C30 C34 C33 1.1(3) . . . . ?
N31 C30 C34 C33 -177.9(2) . . . . ?
Fe2 C30 C34 C33 61.0(2) . . . . ?
C31 C30 C34 Fe2 -59.88(17) . . . . ?
N31 C30 C34 Fe2 121.1(2) . . . . ?
C32 C33 C34 C30 -0.5(3) . . . . ?
Fe2 C33 C34 C30 -58.81(19) . . . . ?
C32 C33 C34 Fe2 58.28(19) . . . . ?
C40 Fe2 C34 C30 165.1(3) . . . . ?
C44 Fe2 C34 C30 -43.7(4) . . . . ?
C41 Fe2 C34 C30 -162.72(17) . . . . ?
C31 Fe2 C34 C30 38.87(17) . . . . ?
C42 Fe2 C34 C30 -117.81(19) . . . . ?
C33 Fe2 C34 C30 122.6(2) . . . . ?
C32 Fe2 C34 C30 85.89(18) . . . . ?
C43 Fe2 C34 C30 -74.7(2) . . . . ?
C40 Fe2 C34 C33 42.4(4) . . . . ?
C30 Fe2 C34 C33 -122.6(2) . . . . ?
C44 Fe2 C34 C33 -166.4(3) . . . . ?
C41 Fe2 C34 C33 74.7(2) . . . . ?
C31 Fe2 C34 C33 -83.76(18) . . . . ?
C42 Fe2 C34 C33 119.56(19) . . . . ?
C32 Fe2 C34 C33 -36.74(17) . . . . ?
C43 Fe2 C34 C33 162.66(18) . . . . ?
C36 O32 C35 O31 -4.2(4) . . . . ?
C36 O32 C35 N31 174.9(2) . . . . ?
C30 N31 C35 O31 -0.6(4) . . . . ?
C30 N31 C35 O32 -179.8(2) . . . . ?
C35 O32 C36 C38 64.0(4) . . . . ?
C35 O32 C36 C39 -57.5(3) . . . . ?
C35 O32 C36 C37 179.3(2) . . . . ?
C45 N41 C40 C41 -33.1(4) . . . . ?
C45 N41 C40 C44 150.8(2) . . . . ?
C45 N41 C40 Fe2 61.2(4) . . . . ?
C34 Fe2 C40 C41 43.7(4) . . . . ?
C30 Fe2 C40 C41 -163.9(3) . . . . ?
C44 Fe2 C40 C41 -120.1(2) . . . . ?
C31 Fe2 C40 C41 160.84(19) . . . . ?
C42 Fe2 C40 C41 -40.5(2) . . . . ?
C33 Fe2 C40 C41 75.6(2) . . . . ?
C32 Fe2 C40 C41 116.2(2) . . . . ?
C43 Fe2 C40 C41 -84.7(2) . . . . ?
C34 Fe2 C40 N41 -77.6(4) . . . . ?
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C30 Fe2 C40 N41 74.7(4) . . . . ?
C44 Fe2 C40 N41 118.5(3) . . . . ?
C41 Fe2 C40 N41 -121.3(4) . . . . ?
C31 Fe2 C40 N41 39.5(3) . . . . ?
C42 Fe2 C40 N41 -161.8(3) . . . . ?
C33 Fe2 C40 N41 -45.7(3) . . . . ?
C32 Fe2 C40 N41 -5.2(3) . . . . ?
C43 Fe2 C40 N41 154.0(3) . . . . ?
C34 Fe2 C40 C44 163.8(3) . . . . ?
C30 Fe2 C40 C44 -43.8(4) . . . . ?
C41 Fe2 C40 C44 120.1(2) . . . . ?
C31 Fe2 C40 C44 -79.04(18) . . . . ?
C42 Fe2 C40 C44 79.67(18) . . . . ?
C33 Fe2 C40 C44 -164.25(16) . . . . ?
C32 Fe2 C40 C44 -123.70(17) . . . . ?
C43 Fe2 C40 C44 35.45(16) . . . . ?
N41 C40 C41 C42 -176.3(2) . . . . ?
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Fe2 C40 C41 C42 59.05(18) . . . . ?
N41 C40 C41 Fe2 124.7(3) . . . . ?
C44 C40 C41 Fe2 -58.67(17) . . . . ?
C34 Fe2 C41 C40 -161.69(19) . . . . ?
C30 Fe2 C41 C40 162.2(3) . . . . ?
C44 Fe2 C41 C40 40.80(18) . . . . ?
C31 Fe2 C41 C40 -47.6(4) . . . . ?
C42 Fe2 C41 C40 117.1(3) . . . . ?
C33 Fe2 C41 C40 -118.3(2) . . . . ?
C32 Fe2 C41 C40 -79.5(2) . . . . ?
C43 Fe2 C41 C40 83.0(2) . . . . ?
C34 Fe2 C41 C42 81.2(2) . . . . ?
C40 Fe2 C41 C42 -117.1(3) . . . . ?
C30 Fe2 C41 C42 45.1(4) . . . . ?
C44 Fe2 C41 C42 -76.3(2) . . . . ?
C31 Fe2 C41 C42 -164.7(3) . . . . ?
C33 Fe2 C41 C42 124.6(2) . . . . ?
C32 Fe2 C41 C42 163.35(19) . . . . ?
C43 Fe2 C41 C42 -34.12(19) . . . . ?
C40 C41 C42 C43 -0.1(3) . . . . ?
Fe2 C41 C42 C43 56.6(2) . . . . ?
C40 C41 C42 Fe2 -56.76(17) . . . . ?
C34 Fe2 C42 C43 117.42(18) . . . . ?
C40 Fe2 C42 C43 -86.83(19) . . . . ?
C30 Fe2 C42 C43 70.7(2) . . . . ?
C44 Fe2 C42 C43 -36.94(17) . . . . ?
C41 Fe2 C42 C43 -126.3(3) . . . . ?
C31 Fe2 C42 C43 38.4(4) . . . . ?
C33 Fe2 C42 C43 162.80(17) . . . . ?
C32 Fe2 C42 C43 -166.8(3) . . . . ?
C34 Fe2 C42 C41 -116.2(2) . . . . ?
C40 Fe2 C42 C41 39.51(18) . . . . ?
C30 Fe2 C42 C41 -162.92(18) . . . . ?
C44 Fe2 C42 C41 89.4(2) . . . . ?
C31 Fe2 C42 C41 164.8(3) . . . . ?
C33 Fe2 C42 C41 -70.9(2) . . . . ?
C32 Fe2 C42 C41 -40.5(4) . . . . ?
C43 Fe2 C42 C41 126.3(3) . . . . ?
C41 C42 C43 C44 -0.2(3) . . . . ?
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Fe2 C42 C43 C44 53.80(18) . . . . ?
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C34 Fe2 C43 C44 160.51(18) . . . . ?
C40 Fe2 C43 C44 -40.50(18) . . . . ?
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C41 Fe2 C43 C44 -84.82(19) . . . . ?
C31 Fe2 C43 C44 75.8(2) . . . . ?
C42 Fe2 C43 C44 -120.0(2) . . . . ?
C33 Fe2 C43 C44 -164.3(3) . . . . ?
C32 Fe2 C43 C44 45.1(4) . . . . ?
C34 Fe2 C43 C42 -79.5(2) . . . . ?
C40 Fe2 C43 C42 79.52(19) . . . . ?
C30 Fe2 C43 C42 -123.78(18) . . . . ?
C44 Fe2 C43 C42 120.0(2) . . . . ?
C41 Fe2 C43 C42 35.20(18) . . . . ?
C31 Fe2 C43 C42 -164.21(17) . . . . ?
C33 Fe2 C43 C42 -44.3(4) . . . . ?
C32 Fe2 C43 C42 165.1(3) . . . . ?
C42 C43 C44 C40 0.4(3) . . . . ?
Fe2 C43 C44 C40 54.81(17) . . . . ?
C42 C43 C44 Fe2 -54.39(18) . . . . ?
C41 C40 C44 C43 -0.5(3) . . . . ?
N41 C40 C44 C43 176.1(2) . . . . ?
Fe2 C40 C44 C43 -60.93(19) . . . . ?
C41 C40 C44 Fe2 60.39(19) . . . . ?
N41 C40 C44 Fe2 -122.9(2) . . . . ?
C34 Fe2 C44 C43 -43.6(4) . . . . ?
C40 Fe2 C44 C43 121.2(2) . . . . ?
C30 Fe2 C44 C43 -76.4(2) . . . . ?
C41 Fe2 C44 C43 83.9(2) . . . . ?
C31 Fe2 C44 C43 -119.31(19) . . . . ?
C42 Fe2 C44 C43 38.28(18) . . . . ?
C33 Fe2 C44 C43 164.1(3) . . . . ?
C32 Fe2 C44 C43 -162.85(18) . . . . ?
C34 Fe2 C44 C40 -164.7(3) . . . . ?
C30 Fe2 C44 C40 162.43(15) . . . . ?
C41 Fe2 C44 C40 -37.30(16) . . . . ?
C31 Fe2 C44 C40 119.52(16) . . . . ?
C42 Fe2 C44 C40 -82.89(17) . . . . ?
C33 Fe2 C44 C40 42.9(4) . . . . ?
C32 Fe2 C44 C40 75.99(18) . . . . ?
C43 Fe2 C44 C40 -121.2(2) . . . . ?
C46 O42 C45 O41 -7.5(4) . . . . ?
C46 O42 C45 N41 171.8(2) . . . . ?
C40 N41 C45 O41 6.1(4) . . . . ?
C40 N41 C45 O42 -173.2(2) . . . . ?
C45 O42 C46 C48 -63.1(4) . . . . ?
C45 O42 C46 C49 -175.6(3) . . . . ?
C45 O42 C46 C47 61.7(3) . . . . ?
C55 N51 C50 C54 34.5(5) . . . . ?
C55 N51 C50 C51 -149.2(3) . . . . ?
C55 N51 C50 Fe3 -61.5(4) . . . . ?
C52 Fe3 C50 N51 -153.0(3) . . . . ?
C52 Fe3 C50 N51 27.0(3) 3_665 . . . ?
C53 Fe3 C50 N51 -19.0(3) 3_665 . . . ?
C53 Fe3 C50 N51 161.0(3) . . . . ?
C51 Fe3 C50 N51 -115.3(3) . . . . ?
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C54 Fe3 C50 N51 122.2(3) . . . . ?
C52 Fe3 C50 C54 84.78(18) . . . . ?
C52 Fe3 C50 C54 -95.22(18) 3_665 . . . ?
C53 Fe3 C50 C54 -141.14(16) 3_665 . . . ?
C53 Fe3 C50 C54 38.85(16) . . . . ?
C51 Fe3 C50 C54 122.5(2) . . . . ?
C51 Fe3 C50 C54 -57.5(2) 3_665 . . . ?
C54 Fe3 C50 C54 180.0 3_665 . . . ?
C52 Fe3 C50 C51 -37.72(17) . . . . ?
C52 Fe3 C50 C51 142.29(17) 3_665 . . . ?
C53 Fe3 C50 C51 96.36(18) 3_665 . . . ?
C53 Fe3 C50 C51 -83.65(18) . . . . ?
C51 Fe3 C50 C51 180.0 3_665 . . . ?
C54 Fe3 C50 C51 57.5(2) 3_665 . . . ?
C54 Fe3 C50 C51 -122.5(2) . . . . ?
N51 C50 C51 C52 -176.2(3) . . . . ?
C54 C50 C51 C52 0.5(4) . . . . ?
Fe3 C50 C51 C52 62.8(2) . . . . ?
N51 C50 C51 Fe3 121.0(3) . . . . ?
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C53 Fe3 C51 C50 74.19(18) . . . . ?
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C51 Fe3 C52 C51 180.0 3_665 . . . ?
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C54 Fe3 C52 C53 145.51(16) 3_665 . . . ?
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C51 C52 C53 C54 -0.3(4) . . . . ?
Fe3 C52 C53 C54 64.7(2) . . . . ?
C51 C52 C53 Fe3 -65.0(2) . . . . ?
C52 Fe3 C53 C54 -119.9(3) . . . . ?
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C51 Fe3 C53 C52 -143.64(15) 3_665 . . . ?
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C50 Fe3 C53 C52 80.29(17) . . . . ?
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C52 C53 C54 C50 0.6(3) . . . . ?
Fe3 C53 C54 C50 61.2(2) . . . . ?
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N51 C50 C54 Fe3 -123.5(3) . . . . ?
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C51 Fe3 C54 C50 -35.41(15) . . . . ?
C51 Fe3 C54 C50 144.59(15) 3_665 . . . ?
C50 Fe3 C54 C50 180.0 3_665 . . . ?
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C56 O52 C55 N51 -179.0(3) . . . . ?
C50 N51 C55 O51 0.6(5) . . . . ?
C50 N51 C55 O52 -179.9(3) . . . . ?
C55 O52 C56 C59 -174.5(3) . . . . ?
C55 O52 C56 C58 -63.4(4) . . . . ?
C55 O52 C56 C57 65.1(4) . . . . ?

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N11 H11 O41  0.88 2.05 2.887(3) 158.8 .
N21 H21 O11  0.88 1.99 2.753(3) 144.1 .
N31 H31 O21  0.88 1.94 2.818(3) 173.1 2_655
N41 H41 O51  0.88 2.00 2.831(3) 157.5 .
N51 H51 O31  0.88 2.16 2.845(3) 134.4 3_665
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_refine_diff_density_min   -0.378
_refine_diff_density_rms    0.068

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_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          'C26 H38 Fe N4 O6'
_chemical_formula_sum             'C26 H38 Fe N4 O6'
_chemical_formula_weight          558.45

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 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

# Crystal Data

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_symmetry_space_group_name_Hall   'C 2y'

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

_cell_length_a                    15.4790(3)
_cell_length_b                    9.3420(3)
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_cell_length_c                     11.0400(3)
_cell_angle_alpha                  90.00
_cell_angle_beta                   117.071(2)
_cell_angle_gamma                  90.00
_cell_volume                       1421.53(7)
_cell_formula_units_Z              2
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_cell_measurement_reflns_used      3809
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_cell_measurement_theta_max        30.03

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_exptl_crystal_colour              yellow
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_exptl_crystal_size_min            0.15
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_exptl_crystal_density_diffrn      1.305
_exptl_crystal_density_method      'not measured'
_exptl_crystal_F_000               592
_exptl_absorpt_coefficient_mu      0.575
_exptl_absorpt_correction_type     multi-scan
_exptl_absorpt_correction_T_min    0.8696
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_exptl_absorpt_process_details     'HKL Scalepack (Otwinowski & Minor
1997)'

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;

# EXPERIMENTAL DETAIL

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_diffrn_radiation_type             MoK\a
_diffrn_radiation_source           'Nonius FR590D, fine-focus sealed
tube'
_diffrn_radiation_monochromator    'horizonally mounted graphite
crystal'
_diffrn_measurement_device         '95mm CCD camera on \k-goniostat'
_diffrn_measurement_device_type    'KappaCCD (BruKer AXS-Nonius,
FR540C)'
_diffrn_measurement_method         'CCD rotation images, thick slices'
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_diffrn_standards_number           ?
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_diffrn_standards_decay_%          'no decay'
_diffrn_reflns_number              7467
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_diffrn_reflns_av_sigmaI/netI      0.0435
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_reflns_number_gt                 3656
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'HKL Scalepack (Otwinowski & Minor
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_computing_data_reduction
; HKL Denzo and Scalepack (Otwinowski & Minor 1997)
;
_computing_structure_solution
; 'SIR-97 (A. Altomare, G. Cascarano et al.)'
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
; Cameron (WinGX v1.70.01, 2005), Ortep (SHELXTL-NT v6.14, Bruker AXS)
;
_computing_publication_material   'WinGX v1.70.01 (L. J. Farrugia)'

# REFINEMENT DATA

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0279P)^2^+0.6901P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
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pairs'
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_refine_ls_abs_structure_Flack    -0.002(12)
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_refine_ls_wR_factor_ref          0.0753
_refine_ls_wR_factor_gt           0.0717
_refine_ls_goodness_of_fit_ref    1.069
_refine_ls_restrained_S_all       1.069
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_refine_ls_shift/su_mean          0.000

# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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O11 O 0.18569(9) 0.55835(14) -0.02474(14) 0.0288(3) Uani 1 1 d . . .
O12 O 0.13540(10) 0.74324(14) 0.17325(14) 0.0313(3) Uani 1 1 d . . .
O13 O 0.25441(10) 0.91279(14) 0.24656(13) 0.0280(3) Uani 1 1 d . . .
N11 N 0.02054(10) 0.56661(14) -0.14226(14) 0.0200(3) Uani 1 1 d . . .
H11 H -0.0284 0.6265 -0.1811 0.024 Uiso 1 1 calc . . .
N12 N 0.18035(11) 0.85584(16) 0.02912(15) 0.0232(3) Uani 1 1 d . . .
H12 H 0.2221 0.9153 0.0225 0.028 Uiso 1 1 calc . . .
C10 C -0.00352(15) 0.41951(19) -0.15196(19) 0.0200(4) Uani 1 1 d . . .
C11 C 0.05515(12) 0.2969(3) -0.13749(16) 0.0261(3) Uani 1 1 d . . .
H11A H 0.1218 0.2970 -0.1170 0.031 Uiso 1 1 calc . . .
C12 C -0.00472(18) 0.1745(2) -0.1595(2) 0.0305(5) Uani 1 1 d . . .
H12A H 0.0152 0.0778 -0.1564 0.037 Uiso 1 1 calc . . .
C13 C -0.09902(17) 0.2208(2) -0.1868(2) 0.0295(5) Uani 1 1 d . . .
H13 H -0.1531 0.1606 -0.2051 0.035 Uiso 1 1 calc . . .
C14 C -0.09864(15) 0.3734(2) -0.1819(2) 0.0234(4) Uani 1 1 d . . .
H14 H -0.1521 0.4331 -0.1960 0.028 Uiso 1 1 calc . . .
C15 C 0.10941(12) 0.62563(18) -0.08062(16) 0.0195(3) Uani 1 1 d . . .
C16 C 0.10767(10) 0.7894(2) -0.09278(14) 0.0208(3) Uani 1 1 d . . .
H16 H 0.0421 0.8254 -0.1105 0.025 Uiso 1 1 calc R . .
C17 C 0.12695(16) 0.8297(2) -0.2125(2) 0.0356(5) Uani 1 1 d . . .
H17A H 0.1271 0.9341 -0.2205 0.043 Uiso 1 1 calc R . .
H17B H 0.0760 0.7891 -0.2965 0.043 Uiso 1 1 calc R . .
H17C H 0.1901 0.7916 -0.1971 0.043 Uiso 1 1 calc R . .
C18 C 0.18621(12) 0.82982(17) 0.15184(18) 0.0218(3) Uani 1 1 d . . .
C19 C 0.29240(16) 0.8806(2) 0.3927(2) 0.0336(4) Uani 1 1 d . . .
C110 C 0.34269(19) 0.7374(3) 0.4214(3) 0.0506(6) Uani 1 1 d . . .
H11B H 0.2947 0.6618 0.3768 0.061 Uiso 1 1 calc R . .
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H11C H 0.3755 0.7206 0.5198 0.061 Uiso 1 1 calc R . .
H11D H 0.3905 0.7368 0.3863 0.061 Uiso 1 1 calc R . .
C111 C 0.2133(2) 0.8875(3) 0.4364(2) 0.0476(6) Uani 1 1 d . . .
H11E H 0.1749 0.9746 0.3999 0.057 Uiso 1 1 calc R . .
H11F H 0.2424 0.8889 0.5360 0.057 Uiso 1 1 calc R . .
H11G H 0.1712 0.8035 0.4018 0.057 Uiso 1 1 calc R . .
C112 C 0.3637(2) 1.0022(3) 0.4560(2) 0.0619(8) Uani 1 1 d . . .
H11H H 0.4121 1.0004 0.4219 0.074 Uiso 1 1 calc R . .
H11I H 0.3962 0.9913 0.5552 0.074 Uiso 1 1 calc R . .
H11J H 0.3289 1.0937 0.4320 0.074 Uiso 1 1 calc R . .

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O12 0.0310(7) 0.0319(7) 0.0351(7) -0.0037(5) 0.0186(6) -0.0128(5)
O13 0.0308(7) 0.0237(6) 0.0249(6) -0.0017(5) 0.0085(6) -0.0101(5)
N11 0.0187(7) 0.0153(6) 0.0240(7) -0.0009(5) 0.0080(6) 0.0007(5)
N12 0.0230(7) 0.0202(7) 0.0280(7) -0.0031(6) 0.0131(6) -0.0067(6)
C10 0.0246(9) 0.0131(8) 0.0214(8) -0.0023(7) 0.0098(7) -0.0002(7)
C11 0.0320(8) 0.0182(7) 0.0307(7) -0.0051(9) 0.0167(7) -0.0008(9)
C12 0.0418(13) 0.0172(10) 0.0328(11) -0.0080(8) 0.0174(10) -0.0019(9)
C13 0.0321(11) 0.0225(10) 0.0282(11) -0.0055(8) 0.0088(9) -0.0083(8)
C14 0.0231(10) 0.0199(9) 0.0235(9) -0.0013(7) 0.0075(8) -0.0008(7)
C15 0.0212(8) 0.0185(7) 0.0213(7) -0.0004(6) 0.0117(7) 0.0025(6)
C16 0.0207(7) 0.0159(6) 0.0255(7) -0.0014(9) 0.0103(6) -0.0022(9)
C17 0.0484(12) 0.0310(11) 0.0303(9) 0.0012(7) 0.0204(9) -0.0073(8)
C18 0.0188(8) 0.0182(8) 0.0284(8) -0.0036(6) 0.0108(7) -0.0038(6)
C19 0.0369(11) 0.0330(10) 0.0232(9) 0.0023(7) 0.0068(8) -0.0045(8)
C110 0.0494(14) 0.0495(13) 0.0447(13) 0.0149(11) 0.0144(12) 0.0119(12)
C111 0.0561(15) 0.0582(15) 0.0322(11) -0.0033(10) 0.0232(11) -
0.0016(12)
C112 0.0680(18) 0.0653(17) 0.0278(11) -0.0047(11) 0.0003(11) -
0.0323(15)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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# MOLECULAR GEOMETRY

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Fe1 C14 2.038(2) . ?
Fe1 C10 2.0383(18) 2 ?
Fe1 C10 2.0384(18) . ?
Fe1 C13 2.041(2) 2 ?
Fe1 C13 2.041(2) . ?
Fe1 C12 2.048(2) 2 ?
Fe1 C12 2.048(2) . ?
Fe1 C11 2.0528(15) 2 ?
Fe1 C11 2.0528(15) . ?
O11 C15 1.227(2) . ?
O12 C18 1.224(2) . ?
O13 C18 1.343(2) . ?
O13 C19 1.475(2) . ?
N11 C15 1.344(2) . ?
N11 C10 1.415(2) . ?
N11 H11 0.8800 . ?
N12 C18 1.338(2) . ?
N12 C16 1.444(2) . ?
N12 H12 0.8800 . ?
C10 C14 1.421(3) . ?
C10 C11 1.425(3) . ?
C11 C12 1.421(3) . ?
C11 H11A 0.9500 . ?
C12 C13 1.417(3) . ?
C12 H12A 0.9500 . ?
C13 C14 1.426(2) . ?
C13 H13 0.9500 . ?
C14 H14 0.9500 . ?
C15 C16 1.535(3) . ?
C16 C17 1.528(2) . ?
C16 H16 1.0000 . ?
C17 H17A 0.9800 . ?
C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
C19 C110 1.507(3) . ?
C19 C111 1.508(3) . ?
C19 C112 1.515(3) . ?
C110 H11B 0.9800 . ?
C110 H11C 0.9800 . ?
C110 H11D 0.9800 . ?
C111 H11E 0.9800 . ?
C111 H11F 0.9800 . ?
C111 H11G 0.9800 . ?
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C112 H11I 0.9800 . ?
C112 H11J 0.9800 . ?

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C14 Fe1 C10 40.82(8) 2 2 ?
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C14 Fe1 C10 108.67(7) 2 . ?
C14 Fe1 C10 40.82(8) . . ?
C10 Fe1 C10 108.43(10) 2 . ?
C14 Fe1 C13 40.94(6) 2 2 ?
C14 Fe1 C13 176.94(10) . 2 ?
C10 Fe1 C13 68.44(9) 2 2 ?
C10 Fe1 C13 138.44(9) . 2 ?
C14 Fe1 C13 176.94(10) 2 . ?
C14 Fe1 C13 40.94(6) . . ?
C10 Fe1 C13 138.45(9) 2 . ?
C10 Fe1 C13 68.44(9) . . ?
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 '-x, y, -z'
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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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O13 O 0.25443(15) 0.5876(2) 0.24617(18) 0.0309(5) Uani 1 1 d . . .
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H11D H 0.3751 0.7812 0.5195 0.064 Uiso 1 1 calc R . .
C111 C 0.2131(3) 0.6128(4) 0.4360(3) 0.0521(9) Uani 1 1 d . . .
H11E H 0.1763 0.5239 0.4022 0.063 Uiso 1 1 calc R . .
H11F H 0.1697 0.6950 0.3982 0.063 Uiso 1 1 calc R . .
H11G H 0.2419 0.6150 0.5355 0.063 Uiso 1 1 calc R . .
C112 C 0.3639(3) 0.4981(4) 0.4563(3) 0.0637(12) Uani 1 1 d . . .
H11H H 0.4125 0.5006 0.4226 0.076 Uiso 1 1 calc R . .
H11I H 0.3293 0.4065 0.4316 0.076 Uiso 1 1 calc R . .
H11J H 0.3961 0.5085 0.5555 0.076 Uiso 1 1 calc R . .

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O12 0.0330(12) 0.0350(12) 0.0372(11) 0.0022(8) 0.0191(10) 0.0126(9)
O13 0.0344(13) 0.0275(10) 0.0257(10) 0.0003(8) 0.0092(10) 0.0093(9)
N11 0.0223(13) 0.0157(11) 0.0258(12) -0.0012(9) 0.0092(10) -0.0007(10)
N12 0.0248(13) 0.0217(11) 0.0283(12) 0.0025(9) 0.0128(11) 0.0074(10)
C10 0.0248(17) 0.0157(15) 0.0205(14) 0.0021(12) 0.0067(13) -0.0019(13)
C11 0.0341(15) 0.0207(12) 0.0318(12) 0.0045(16) 0.0171(12) 0.0000(17)
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C12 0.048(2) 0.0171(17) 0.0385(18) 0.0051(14) 0.0215(18) 0.0014(15)
C13 0.036(2) 0.0233(17) 0.0295(18) 0.0062(13) 0.0110(16) 0.0080(14)
C14 0.0250(18) 0.0218(17) 0.0280(17) 0.0014(13) 0.0090(15) 0.0004(13)
C15 0.0253(16) 0.0207(13) 0.0214(13) -0.0017(11) 0.0121(12) -0.0045(12)
C16 0.0216(13) 0.0186(11) 0.0285(12) 0.0008(16) 0.0102(10) 0.0009(16)
C17 0.050(2) 0.035(2) 0.0325(15) -0.0012(12) 0.0214(15) 0.0061(14)
C18 0.0206(15) 0.0200(16) 0.0323(15) 0.0034(10) 0.0116(13) 0.0029(11)
C19 0.040(2) 0.0366(19) 0.0265(16) -0.0023(13) 0.0084(15) 0.0065(15)
C110 0.054(2) 0.055(2) 0.045(2) -0.0164(16) 0.0161(19) -0.0123(19)
C111 0.061(3) 0.062(2) 0.0362(18) 0.0018(16) 0.0249(18) -0.0001(19)
C112 0.070(3) 0.068(3) 0.0278(17) 0.0050(17) 0.0006(18) 0.030(2)

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;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

# MOLECULAR GEOMETRY

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Fe1 C11 2.048(2) 2 ?
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O12 C18 1.228(3) . ?
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N11 C15 1.349(3) . ?
N11 C10 1.419(4) . ?
N11 H11 0.8800 . ?
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N12 H12 0.8800 . ?
C10 C14 1.419(5) . ?
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C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
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C19 C112 1.517(5) . ?
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C110 H11C 0.9800 . ?
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Fe1 C11 H11A 126.4 . . ?
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H17A C17 H17B 109.5 . . ?
C16 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
O12 C18 N12 124.0(3) . . ?
O12 C18 O13 125.4(3) . . ?
N12 C18 O13 110.6(2) . . ?
O13 C19 C111 111.2(3) . . ?
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C10 C11 C12 Fe1 59.27(16) . . . . ?
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C14 Fe1 C12 C13 37.7(2) . . . . ?
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C11 Fe1 C12 C11 -177.90(18) 2 . . . ?
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Fe1 C12 C13 C14 -59.4(3) . . . . ?
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Fe1 C13 C14 C10 -59.8(2) . . . . ?
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