Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1997, 36(11), 2400-2405, DOI:10.1021/ic961454t

Space Group and Cell Dimensions Monoclinic, P 21
a 11.8142(5) b 9.7560(5) c 22.9456(10)
beta 90.246(5)
Volume 2644.67(21)A**3

Empirical formula : Fe2 O10 N2 C60 H58

Cell dimensions were obtained from8100 reflections with 2Theta angle
in the range 3.00 - 50.00 degrees.

Crystal dimensions : 0.30 X 0.30 X 0.12 mm

FW = 1078.81 Z = 2 F(000) = 1129.67

Dcalc 1.355Mg.m-3, mu 0.61mm-1, lambda 0.70930A, 2Theta(max) 49.3

The intensity data were collected on a Siemens diffractometer,
using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -13 13; Kmin,max -11 11; Lmin,max -26 26
No. of reflections measured 11939
No. of unique reflections 7933
No. of reflections with Inet > 2.5sigma(Inet) 7532
Merging R-value on intensities 0.019
No correction was made for absorption

The last least squares cycle was calculated with
132 atoms, 666 parameters and 4473 out of 4738 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000300

The residuals are as follows :--
For significant reflections, RF 0.046, Rw 0.061 GoF 2.41
For all reflections, RF 0.046, Rw 0.061.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.007.

In the last D-map, the deepest hole was -0.420e/A**3,
and the highest peak 0.770e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S.
(1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)
Kynoch Press, Birmingham, England.

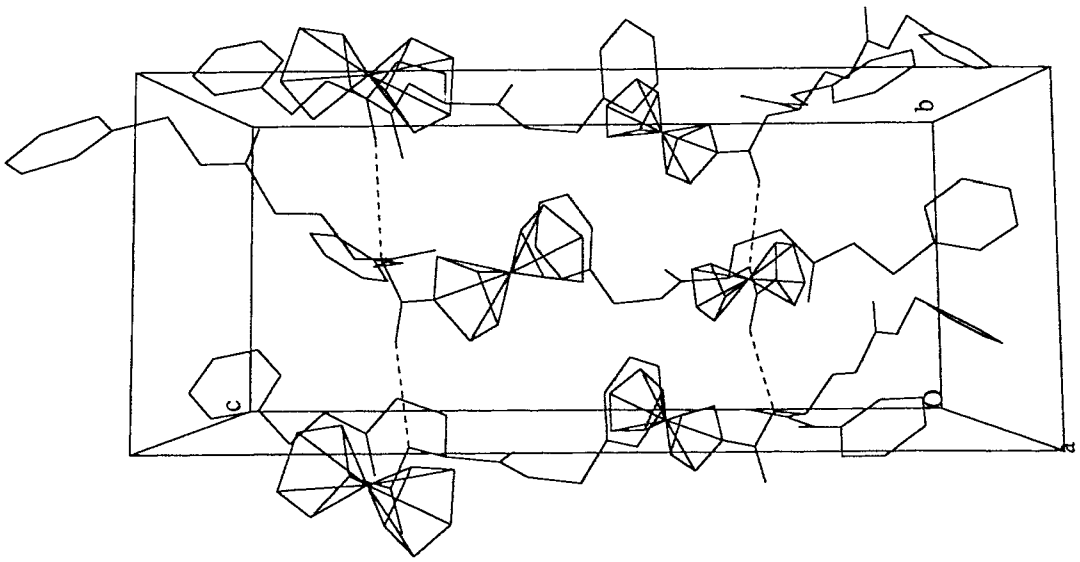
The following references may also be relevant.

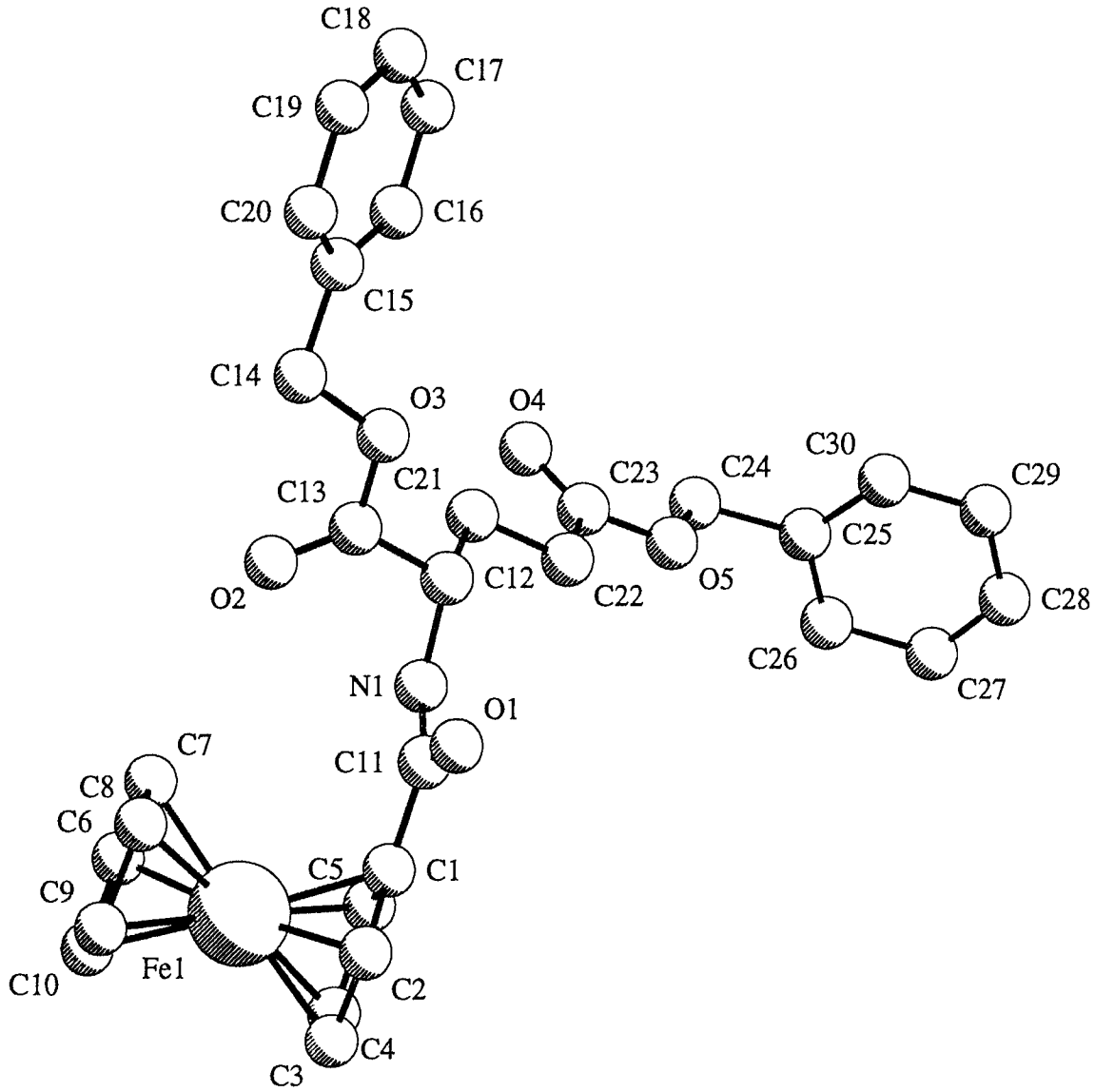
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot
Program, Technical Report ORNL-5138, Oak Ridge

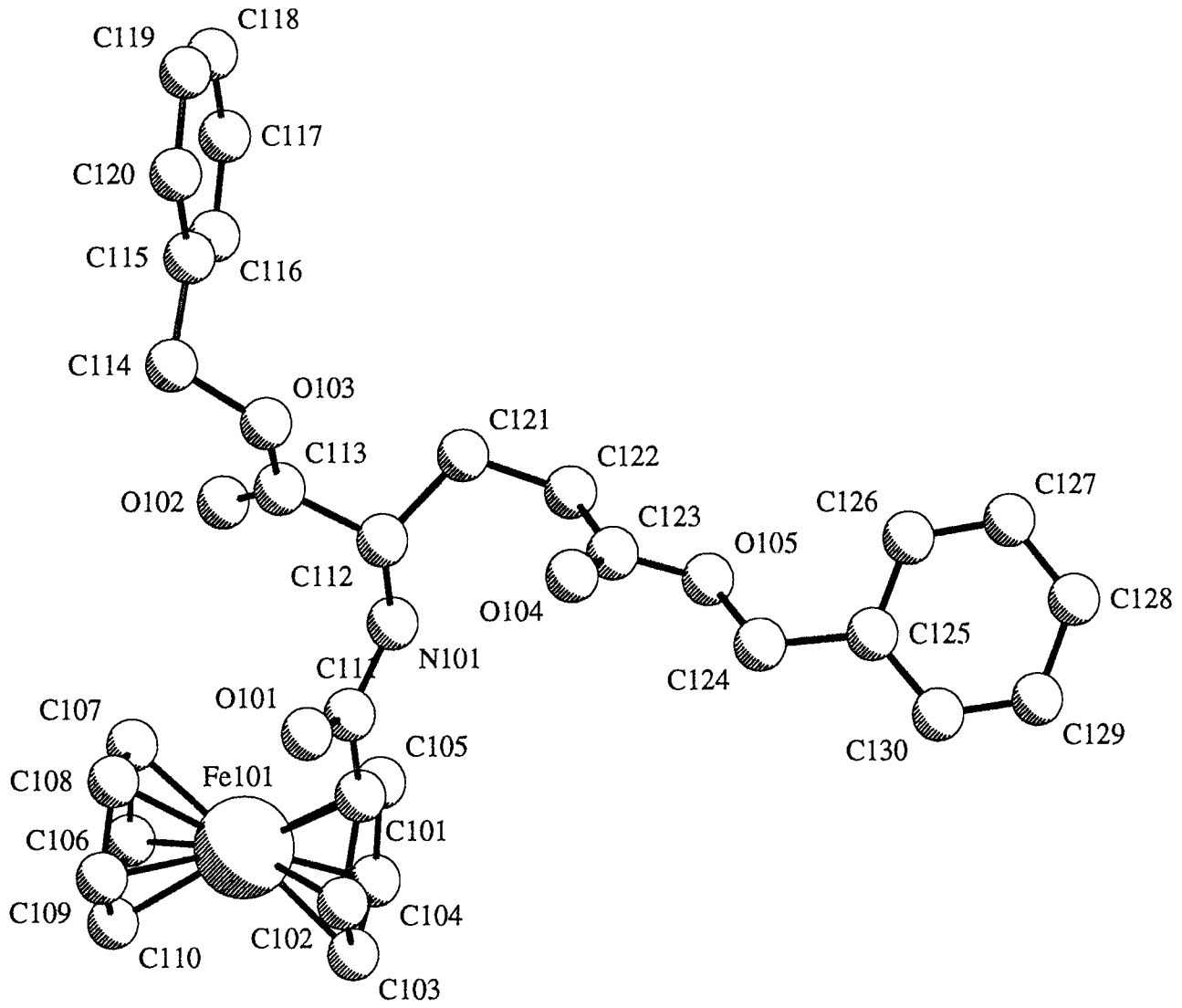
4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.


b
c
a


C18
C17
C19
C20
C16
C15
C14
O3
O4
C30
C23
C24
C29
C13
C21
C25
O2
C12
C22
O5
C28
C26
C27
N1
O1
C7
C11
C8
C6
C5
C1
C9
Fe1
C10
C2
C4
C3


C119
C118
C117
C120
C115
C116
C114
O103
C113
O102
C121
C122
C112
C123
O105
C126
C127
C128
O104
C125
C124
C111
N101
O101
C107
C105
C108
Fe101
C101
C106
C109
C104
C102
C110
C103
C130
C129

25-Apr-1996

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Fe1	-0.96887(5)	-0.03368	-0.59604(3)	2.43(3)
O1	-0.8369 (3)	-0.2209 (4)	-0.73110(16)	3.28(15)
O2	-0.6434 (3)	0.0380 (7)	-0.69660(16)	6.3 (3)
O3	-0.5549 (3)	-0.0074 (4)	-0.77955(14)	3.34(16)
O4	-0.8250 (3)	0.3713 (4)	-0.88683(19)	4.16(18)
O5	-0.9628 (3)	0.2572 (4)	-0.93360(17)	3.80(16)
N1	-0.8533 (3)	0.0069 (4)	-0.74594(16)	2.13(15)
C1	-0.9809 (4)	-0.1044 (6)	-0.67865(20)	2.47(18)
C2	-1.0069 (4)	-0.2123 (6)	-0.63862(21)	2.89(20)
C3	-1.1015 (5)	-0.1670 (6)	-0.60549(21)	3.11(21)
C4	-1.1332 (4)	-0.0330 (7)	-0.62488(20)	3.05(21)
C5	-1.0573 (4)	0.0071 (5)	-0.67065(20)	2.55(18)
C6	-0.9180 (5)	0.1480 (6)	-0.56023(25)	3.56(23)
C7	-0.8267 (4)	0.0835 (6)	-0.58845(22)	3.19(21)
C8	-0.8085 (4)	-0.0458 (7)	-0.56219(24)	3.91(23)
C9	-0.8900 (5)	-0.0590 (8)	-0.51676(24)	4.7 (3)
C10	-0.9567 (5)	0.0597 (8)	-0.51608(23)	4.2 (3)
C11	-0.8837 (4)	-0.1117 (5)	-0.72032(20)	2.23(18)
C12	-0.7545 (4)	0.0107 (5)	-0.78386(19)	2.35(18)
C13	0.3526 (4)	1.0147 (6)	0.25326(20)	2.83(20)
C14	0.5517 (4)	1.0065 (7)	0.25014(23)	4.0 (3)
C15	0.6440 (4)	1.0167 (6)	0.20520(22)	3.29(23)
C16	0.6300 (5)	1.0947 (7)	0.1555 (3)	4.1 (3)
C17	0.7169 (5)	1.1074 (7)	0.11470(25)	4.0 (3)
C18	0.8183 (5)	1.0402 (7)	0.1243 (3)	4.2 (3)
C19	0.8335 (4)	0.9624 (8)	0.17329(23)	3.65(24)
C20	0.7463 (4)	0.9494 (7)	0.21393(23)	3.66(23)
C21	0.2405 (4)	1.1376 (6)	0.17733(20)	2.58(19)
C22	0.1378 (4)	1.1338 (6)	0.13676(21)	2.68(18)
C23	0.1218 (4)	1.2685 (6)	0.10519(23)	3.07(21)
C24	0.0097 (6)	1.3822 (7)	0.0340 (3)	4.6 (3)
C25	-0.0697 (5)	1.3352 (6)	-0.01387(24)	3.44(22)
C26	-0.1862 (5)	1.3548 (8)	-0.0075 (3)	4.6 (3)
C27	-0.2587 (6)	1.2998 (9)	-0.0517 (4)	5.8 (4)
C28	-0.2158 (8)	1.2359 (9)	-0.0971 (3)	6.2 (4)
C29	-0.1022 (9)	1.2195 (8)	-0.1049 (3)	6.4 (5)
C30	-0.0299 (6)	1.2689 (8)	-0.0618 (3)	4.9 (3)
Fe101	-0.18313(6)	0.45321(12)	0.26767(4)	4.24(4)
O101	0.0877 (3)	0.2768 (4)	0.28249(18)	3.57(17)
O102	0.1287 (3)	0.4850 (4)	0.40417(14)	3.12(14)
O103	0.3008 (3)	0.3880 (4)	0.41486(14)	2.82(13)
O104	0.4252 (4)	0.3758 (5)	0.22431(20)	4.45(21)
O105	0.4382 (4)	0.5575 (6)	0.16349(17)	5.80(24)
N101	0.1529 (3)	0.4937 (4)	0.28518(16)	2.57(16)
C101	-0.0242 (4)	0.4476 (6)	0.23567(20)	3.11(21)
C102	-0.0968 (5)	0.3568 (7)	0.2036 (3)	3.87(25)
C103	-0.1859 (7)	0.4394 (9)	0.1796 (3)	5.8 (4)
C104	-0.1701 (8)	0.5768 (8)	0.1975 (4)	6.5 (4)
C105	-0.0687 (6)	0.5816 (7)	0.2315 (3)	4.6 (3)
C106	-0.3121 (8)	0.5153 (11)	0.3202 (6)	10.4 (7)
C107	-0.2004 (6)	0.4916 (8)	0.3545 (3)	5.3 (3)
C108	-0.1750 (7)	0.3538 (9)	0.3496 (4)	5.8 (4)
C109	-0.2522 (5)	0.2983 (10)	0.3187 (3)	5.4 (4)
C110	-0.3373 (5)	0.3861 (8)	0.2969 (4)	6.3 (4)
C111	0.0762 (4)	0.3981 (5)	0.27045(21)	2.67(19)
C112	0.2498 (4)	0.4541 (6)	0.32025(18)	2.59(18)
C113	0.2152 (4)	0.4442 (5)	0.38443(19)	2.56(19)
C114	0.2845 (5)	0.3730 (6)	0.47774(21)	3.35(23)
C115	0.3468 (4)	0.4845 (8)	0.50986(21)	3.7 (3)
C116	0.3131 (5)	0.6210 (8)	0.5067 (3)	4.3 (3)
C117	0.3656 (7)	0.7220 (9)	0.5388 (3)	5.8 (3)
C118	0.4557 (6)	0.6894 (13)	0.5748 (3)	6.5 (5)
C119	0.4904 (6)	0.5537 (16)	0.5799 (3)	7.6 (6)
C120	0.4368 (5)	0.4526 (12)	0.54668(24)	5.8 (4)
C121	0.3472 (5)	0.5584 (7)	0.31574(23)	3.44(22)
C122	0.3783 (5)	0.6048 (8)	0.2551 (3)	4.7 (3)
C123	0.4144 (5)	0.4982 (6)	0.2148 (3)	3.74(25)

C124	0.4724 (8)	0.4613 (11)	0.1170 (3)	7.7 (5)
C125	0.5291 (6)	0.5554 (9)	0.0712 (3)	5.2 (3)
C126	0.6003 (6)	0.6577 (8)	0.0905 (3)	5.4 (3)
C127	0.6639 (6)	0.7339 (9)	0.0525 (4)	5.8 (4)
C128	0.6566 (9)	0.7068 (13)	-0.0050 (5)	9.0 (6)
C129	0.5814 (10)	0.6044 (16)	-0.0253 (3)	9.2 (7)
C130	0.5191 (7)	0.5323 (12)	0.0127 (4)	7.4 (5)
H1	0.100	1.100	0.262	2.9
H2	0.037	0.691	0.367	3.7
H3	-0.142	0.776	0.429	3.9
H4	-0.204	1.026	0.391	3.8
H5	-0.058	1.102	0.305	3.3
H6	0.054	1.247	0.425	4.4
H7	0.227	1.118	0.376	4.0
H8	0.253	0.875	0.430	4.7
H9	0.093	0.858	0.513	5.5
H10	-0.027	1.092	0.511	5.0
H12	0.246	0.918	0.190	3.1
H14a	0.565	0.920	0.279	4.8
H14b	0.552	1.099	0.276	4.8
H16	0.550	1.142	0.146	4.8
H17	0.705	1.164	0.075	4.8
H18	0.887	1.051	0.093	5.0
H19	0.914	0.916	0.183	4.4
H20	0.759	0.893	0.254	4.4
H21a	0.315	1.140	0.150	3.4
H21b	0.238	1.228	0.204	3.4
H22a	0.144	1.047	0.108	3.5
H22b	0.064	1.122	0.164	3.5
H24a	-0.035	1.456	0.060	5.3
H24b	0.087	1.428	0.018	5.3
H26	-0.216	1.400	0.033	5.3
H27	-0.348	1.308	-0.043	6.6
H28	-0.279	1.198	-0.127	7.0
H29	-0.081	1.170	-0.146	7.2
H30	0.058	1.255	-0.073	5.7
H101	0.139	0.599	0.273	3.4
H102	-0.086	0.247	0.199	4.7
H103	-0.252	0.397	0.152	6.6
H104	-0.227	0.659	0.187	7.3
H105	-0.032	0.673	0.250	5.4
H106	-0.355	0.612	0.315	11.2
H107	-0.151	0.564	0.379	6.1
H108	-0.106	0.298	0.370	6.7
H109	-0.255	0.190	0.309	6.2
H110	-0.405	0.359	0.267	7.1
H112	0.278	0.353	0.308	3.4
H114a	0.307	0.270	0.490	4.1
H114b	0.196	0.391	0.487	4.1
H116	0.246	0.655	0.478	5.1
H117	0.346	0.830	0.536	6.6
H118	0.504	0.762	0.600	7.2
H119	0.558	0.519	0.608	8.4
H120	0.457	0.345	0.549	6.6
H121a	0.422	0.513	0.335	4.2
H121b	0.325	0.649	0.340	4.2
H122a	0.302	0.643	0.234	5.4
H122b	0.440	0.686	0.257	5.4
H124a	0.403	0.397	0.103	8.5
H124b	0.539	0.397	0.135	8.5
H126	0.598	0.677	0.137	6.2
H127	0.717	0.811	0.072	6.6
H128	0.713	0.766	-0.032	9.8
H129	0.583	0.586	-0.072	10.0
H130	0.465	0.455	-0.007	8.2

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Fe1-C1	2.022(5)	Fe101-C101	2.019(5)
Fe1-C2	2.047(5)	Fe101-C102	2.025(6)
Fe1-C3	2.048(5)	Fe101-C103	2.025(7)
Fe1-C4	2.049(5)	Fe101-C104	2.019(8)
Fe1-C5	2.041(5)	Fe101-C105	2.024(7)
Fe1-C6	2.043(5)	Fe101-C106	2.038(9)
Fe1-C7	2.039(5)	Fe101-C107	2.037(7)
Fe1-C8	2.047(5)	Fe101-C108	2.117(9)
Fe1-C9	2.055(5)	Fe101-C109	2.081(9)
Fe1-C10	2.053(5)	Fe101-C110	2.051(8)
O1-C11	1.226(6)	O101-C111	1.222(6)
O2-C13	1.173(6)	O102-C113	1.188(6)
O3-C13	1.348(6)	O103-C113	1.343(6)
O3-C14	1.435(6)	O103-C114	1.464(6)
O4-C23	1.198(7)	O104-C123	1.220(8)
O5-C23	1.340(6)	O105-C123	1.344(7)
O5-C24	1.464(7)	O105-C124	1.479(9)
N1-C11	1.347(6)	N101-C111	1.342(7)
N1-C12	1.459(6)	N101-C112	1.449(6)
N1-H1	1.079(4)	N101-H101	1.079(4)
C1-C2	1.432(7)	C101-C102	1.434(8)
C1-C5	1.426(7)	C101-C105	1.412(9)
C1-C11	1.499(7)	C101-C111	1.507(7)
C2-C3	1.425(7)	C102-C103	1.433(10)
C2-H2	1.082(6)	C102-H102	1.081(6)
C3-C4	1.430(9)	C103-C104	1.414(12)
C3-H3	1.081(5)	C103-H103	1.081(6)
C4-C5	1.438(7)	C104-C105	1.428(9)
C4-H4	1.079(5)	C104-H104	1.080(7)
C5-H5	1.079(5)	C105-H105	1.079(7)
C6-C7	1.409(8)	C106-C107	1.551(15)
C6-C10	1.407(9)	C106-C110	1.401(14)
C6-H6	1.078(6)	C106-H106	1.080(10)
C7-C8	1.413(9)	C107-C108	1.382(12)
C7-H7	1.080(5)	C107-H107	1.079(7)
C8-C9	1.428(8)	C108-C109	1.273(11)
C8-H8	1.081(6)	C108-H108	1.080(9)
C9-C10	1.400(12)	C109-C110	1.411(10)
C9-H9	1.081(7)	C109-H109	1.081(10)
C10-H10	1.079(6)	C110-H110	1.080(8)
C12-C13	1.522(6)	C112-C113	1.533(6)
C12-C21	1.526(7)	C112-C121	1.540(8)
C12-H12	1.082(5)	C112-H112	1.081(5)
C14-C15	1.507(7)	C114-C115	1.505(9)
C14-H14a	1.083(7)	C114-H114a	1.082(6)
C14-H14b	1.078(7)	C114-H114b	1.080(6)
C15-C16	1.381(8)	C115-C116	1.392(11)
C15-C20	1.390(7)	C115-C120	1.391(8)
C16-C17	1.398(8)	C116-C117	1.376(10)
C16-H16	1.079(6)	C116-H116	1.079(6)
C17-C18	1.382(9)	C117-C118	1.382(12)
C17-H17	1.079(6)	C117-H117	1.079(10)
C18-C19	1.369(10)	C118-C119	1.391(20)
C18-H18	1.081(5)	C118-H118	1.079(8)
C19-C20	1.398(7)	C119-C120	1.396(14)
C19-H19	1.081(5)	C119-H119	1.081(8)
C20-H20	1.081(6)	C120-H120	1.081(11)
C21-C22	1.527(7)	C121-C122	1.510(8)
C21-H21a	1.080(4)	C121-H121a	1.081(6)
C21-H21b	1.079(5)	C121-H121b	1.079(6)
C22-C23	1.512(8)	C122-C123	1.457(10)
C22-H22a	1.081(5)	C122-H122a	1.080(7)
C22-H22b	1.080(5)	C122-H122b	1.078(7)
C24-C25	1.512(8)	C124-C125	1.549(11)
C24-H24a	1.078(8)	C124-H124a	1.082(9)
C24-H24b	1.080(7)	C124-H124b	1.081(12)
C25-C26	1.398(9)	C125-C126	1.378(10)
C25-C30	1.361(10)	C125-C130	1.365(10)
C26-C27	1.428(10)	C126-C127	1.371(10)
C26-H26	1.080(7)	C126-H126	1.080(7)
C27-C28	1.318(14)	C127-C128	1.349(16)

C27-H27	1.081(8)	C127-H127	1.078(8)
C28-C29	1.364(15)	C128-C129	1.415(21)
C28-H28	1.081(7)	C128-H128	1.079(9)
C29-C30	1.392(12)	C129-C130	1.343(16)
C29-H29	1.079(8)	C129-H129	1.081(8)
C30-H30	1.079(7)	C130-H130	1.081(9)

C1-Fe1-C2	41.20(20)	C101-Fe101-C102	41.55(23)
C1-Fe1-C3	68.50(19)	C101-Fe101-C103	69.3(3)
C1-Fe1-C4	68.63(19)	C101-Fe101-C104	69.6(3)
C1-Fe1-C5	41.10(20)	C101-Fe101-C105	40.9(3)
C1-Fe1-C6	133.82(22)	C101-Fe101-C106	157.1(4)
C1-Fe1-C7	109.01(20)	C101-Fe101-C107	117.2(3)
C1-Fe1-C8	113.39(22)	C101-Fe101-C108	105.8(3)
C1-Fe1-C9	145.0(3)	C101-Fe101-C109	123.5(3)
C1-Fe1-C10	173.6(3)	C101-Fe101-C110	159.8(3)
C2-Fe1-C3	40.73(20)	C102-Fe101-C103	41.5(3)
C2-Fe1-C4	69.06(23)	C102-Fe101-C104	70.0(3)
C2-Fe1-C5	69.82(21)	C102-Fe101-C105	69.5(3)
C2-Fe1-C6	173.85(21)	C102-Fe101-C106	161.3(4)
C2-Fe1-C7	134.21(22)	C102-Fe101-C107	148.0(3)
C2-Fe1-C8	109.45(25)	C102-Fe101-C108	114.3(3)
C2-Fe1-C9	114.7(3)	C102-Fe101-C109	105.7(3)
C2-Fe1-C10	144.98(25)	C102-Fe101-C110	122.7(3)
C3-Fe1-C4	40.9(3)	C103-Fe101-C104	40.9(3)
C3-Fe1-C5	69.27(21)	C103-Fe101-C105	68.9(3)
C3-Fe1-C6	144.84(22)	C103-Fe101-C106	126.9(5)
C3-Fe1-C7	174.43(24)	C103-Fe101-C107	170.5(3)
C3-Fe1-C8	135.2(3)	C103-Fe101-C108	148.8(3)
C3-Fe1-C9	111.18(24)	C103-Fe101-C109	120.5(3)
C3-Fe1-C10	115.31(21)	C103-Fe101-C110	107.1(3)
C4-Fe1-C5	41.17(19)	C104-Fe101-C105	41.4(3)
C4-Fe1-C6	113.83(24)	C104-Fe101-C106	110.7(5)
C4-Fe1-C7	143.6(3)	C104-Fe101-C107	132.7(3)
C4-Fe1-C8	175.33(24)	C104-Fe101-C108	168.2(3)
C4-Fe1-C9	135.37(22)	C104-Fe101-C109	156.1(3)
C4-Fe1-C10	110.49(22)	C104-Fe101-C110	121.5(3)
C5-Fe1-C6	108.48(22)	C105-Fe101-C106	124.1(4)
C5-Fe1-C7	112.40(20)	C105-Fe101-C107	110.9(3)
C5-Fe1-C8	143.02(21)	C105-Fe101-C108	128.3(3)
C5-Fe1-C9	173.9(3)	C105-Fe101-C109	160.87(24)
C5-Fe1-C10	134.2(3)	C105-Fe101-C110	158.0(3)
C6-Fe1-C7	40.39(23)	C106-Fe101-C107	44.7(5)
C6-Fe1-C8	68.1(3)	C106-Fe101-C108	69.1(5)
C6-Fe1-C9	67.5(3)	C106-Fe101-C109	65.6(4)
C6-Fe1-C10	40.2(3)	C106-Fe101-C110	40.1(4)
C7-Fe1-C8	40.5(3)	C107-Fe101-C108	38.8(3)
C7-Fe1-C9	67.76(23)	C107-Fe101-C109	62.7(3)
C7-Fe1-C10	67.67(21)	C107-Fe101-C110	69.3(3)
C8-Fe1-C9	40.74(24)	C108-Fe101-C109	35.3(3)
C8-Fe1-C10	67.99(25)	C108-Fe101-C110	66.4(3)
C9-Fe1-C10	39.9(3)	C109-Fe101-C110	39.9(3)
C13-O3-C14	115.6(4)	C113-O103-C114	116.8(4)
C23-O5-C24	115.6(4)	C123-O105-C124	114.7(6)
C11-N1-C12	119.8(4)	C111-N101-C112	119.0(4)
C11-N1-H1	120.9(4)	C111-N101-H101	119.6(4)
C12-N1-H1	119.2(4)	C112-N101-H101	121.3(4)
Fe1-C1-C2	70.3(3)	Fe101-C101-C102	69.4(3)
Fe1-C1-C5	70.2(3)	Fe101-C101-C105	69.7(4)
Fe1-C1-C11	124.3(3)	Fe101-C101-C111	123.2(3)
C2-C1-C5	109.9(4)	C102-C101-C105	108.4(5)
C2-C1-C11	122.8(5)	C102-C101-C111	122.8(5)
C5-C1-C11	127.3(4)	C105-C101-C111	128.6(5)
Fe1-C2-C1	68.4(3)	Fe101-C102-C101	69.0(3)
Fe1-C2-C3	69.7(3)	Fe101-C102-C103	69.3(4)
Fe1-C2-H2	125.3(4)	Fe101-C102-H102	126.3(5)
C1-C2-C3	106.6(5)	C101-C102-C103	106.6(5)
C1-C2-H2	127.6(5)	C101-C102-H102	126.2(6)
C3-C2-H2	125.8(5)	C103-C102-H102	127.2(6)
Fe1-C3-C2	69.6(3)	Fe101-C103-C102	69.3(3)
Fe1-C3-C4	69.6(3)	Fe101-C103-C104	69.3(4)

Fe1-C3-H3	126.4(4)	Fe101-C103-H103	128.1(6)
C2-C3-C4	108.8(4)	C102-C103-C104	109.0(5)
C2-C3-H3	125.7(5)	C102-C103-H103	122.0(7)
C4-C3-H3	125.5(5)	C104-C103-H103	129.0(7)
Fe1-C4-C3	69.5(3)	Fe101-C104-C103	69.7(4)
Fe1-C4-C5	69.1(3)	Fe101-C104-C105	69.5(4)
Fe1-C4-H4	129.0(4)	Fe101-C104-H104	125.2(8)
C3-C4-C5	108.2(4)	C103-C104-C105	107.4(6)
C3-C4-H4	125.9(5)	C103-C104-H104	123.9(6)
C5-C4-H4	125.8(6)	C105-C104-H104	128.7(7)
Fe1-C5-C1	68.7(3)	Fe101-C105-C101	69.4(4)
Fe1-C5-C4	69.7(3)	Fe101-C105-C104	69.2(5)
Fe1-C5-H5	126.7(3)	Fe101-C105-H105	127.9(5)
C1-C5-C4	106.5(5)	C101-C105-C104	108.5(6)
C1-C5-H5	126.4(4)	C101-C105-H105	126.2(5)
C4-C5-H5	127.2(5)	C104-C105-H105	125.2(6)
Fe1-C6-C7	69.7(3)	Fe101-C106-C107	67.6(4)
Fe1-C6-C10	70.3(3)	Fe101-C106-C110	70.4(5)
Fe1-C6-H6	124.4(4)	Fe101-C106-H106	123.0(9)
C7-C6-C10	108.0(6)	C107-C106-C110	103.8(7)
C7-C6-H6	119.3(5)	C107-C106-H106	126.0(10)
C10-C6-H6	132.7(6)	C110-C106-H106	130.2(12)
Fe1-C7-C6	70.0(3)	Fe101-C107-C106	67.7(5)
Fe1-C7-C8	70.1(3)	Fe101-C107-C108	73.7(5)
Fe1-C7-H7	126.6(4)	Fe101-C107-H107	125.5(5)
C6-C7-C8	108.5(5)	C106-C107-C108	106.8(7)
C6-C7-H7	130.7(6)	C106-C107-H107	129.2(7)
C8-C7-H7	120.8(5)	C108-C107-H107	124.0(8)
Fe1-C8-C7	69.4(3)	Fe101-C108-C107	67.5(5)
Fe1-C8-C9	69.9(3)	Fe101-C108-C109	70.8(5)
Fe1-C8-H8	127.1(4)	Fe101-C108-H108	130.0(5)
C7-C8-C9	106.9(6)	C107-C108-C109	107.7(8)
C7-C8-H8	131.7(5)	C107-C108-H108	128.1(8)
C9-C8-H8	121.4(6)	C109-C108-H108	124.1(8)
Fe1-C9-C8	69.3(3)	Fe101-C109-C108	73.9(6)
Fe1-C9-C10	70.0(3)	Fe101-C109-C110	68.9(5)
Fe1-C9-H9	124.5(4)	Fe101-C109-H109	127.1(5)
C8-C9-C10	108.3(6)	C108-C109-C110	116.5(9)
C8-C9-H9	131.3(8)	C108-C109-H109	123.8(7)
C10-C9-H9	120.3(6)	C110-C109-H109	119.7(6)
Fe1-C10-C6	69.5(3)	Fe101-C110-C106	69.5(5)
Fe1-C10-C9	70.1(3)	Fe101-C110-C109	71.2(4)
Fe1-C10-H10	125.7(4)	Fe101-C110-H110	122.2(7)
C6-C10-C9	108.3(5)	C106-C110-C109	105.1(8)
C6-C10-H10	119.0(7)	C106-C110-H110	127.9(8)
C9-C10-H10	132.7(6)	C109-C110-H110	126.9(8)
O1-C11-N1	122.5(4)	O101-C111-N101	122.8(5)
O1-C11-C1	121.2(5)	O101-C111-C101	121.1(5)
N1-C11-C1	116.3(4)	N101-C111-C101	116.1(5)
N1-C12-C13	109.4(4)	N101-C112-C113	109.7(4)
N1-C12-C21	109.9(4)	N101-C112-C121	112.0(4)
N1-C12-H12	108.2(4)	N101-C112-H112	110.0(4)
C13-C12-C21	109.6(4)	C113-C112-C121	108.0(4)
C13-C12-H12	109.1(4)	C113-C112-H112	106.2(4)
C21-C12-H12	110.7(4)	C121-C112-H112	110.6(4)
O2-C13-O3	123.3(4)	O102-C113-O103	125.8(4)
O2-C13-C12	125.7(4)	O102-C113-C112	125.3(4)
O3-C13-C12	111.0(4)	O103-C113-C112	108.8(4)
O3-C14-C15	108.5(4)	O103-C114-C115	110.1(4)
O3-C14-H14a	110.0(5)	O103-C114-H114a	108.9(5)
O3-C14-H14b	109.7(5)	O103-C114-H114b	108.1(4)
C15-C14-H14a	110.9(5)	C115-C114-H114a	115.1(5)
C15-C14-H14b	108.6(5)	C115-C114-H114b	104.9(5)
H14a-C14-H14b	109.2(5)	H114a-C114-H114b	109.4(5)
C14-C15-C16	121.1(5)	C114-C115-C116	121.8(5)
C14-C15-C20	120.1(5)	C114-C115-C120	120.5(7)
C16-C15-C20	118.7(5)	C116-C115-C120	117.7(7)
C15-C16-C17	121.1(5)	C115-C116-C117	121.9(6)
C15-C16-H16	120.4(5)	C115-C116-H116	122.6(6)
C17-C16-H16	118.4(6)	C117-C116-H116	115.5(7)
C16-C17-C18	119.4(6)	C116-C117-C118	120.0(9)
C16-C17-H17	121.0(6)	C116-C117-H117	124.7(7)
C18-C17-H17	119.5(5)	C118-C117-H117	115.2(7)

C17-C18-C19	120.3(5)	C117-C118-C119	119.7(8)
C17-C18-H18	120.0(6)	C117-C118-H118	125.0(12)
C19-C18-H18	119.7(6)	C119-C118-H118	115.3(8)
C18-C19-C20	120.3(5)	C118-C119-C120	119.6(7)
C18-C19-H19	120.9(5)	C118-C119-H119	124.7(10)
C20-C19-H19	118.6(5)	C120-C119-H119	115.6(13)
C15-C20-C19	120.3(5)	C115-C120-C119	121.1(10)
C15-C20-H20	118.6(5)	C115-C120-H120	114.5(8)
C19-C20-H20	121.0(5)	C119-C120-H120	124.3(7)
C12-C21-C22	111.4(4)	C112-C121-C122	116.4(5)
C12-C21-H21a	108.8(4)	C112-C121-H121a	108.1(5)
C12-C21-H21b	109.5(4)	C112-C121-H121b	108.8(4)
C22-C21-H21a	107.2(4)	C122-C121-H121a	107.3(4)
C22-C21-H21b	110.3(4)	C122-C121-H121b	106.9(5)
H21a-C21-H21b	109.6(4)	H121a-C121-H121b	109.1(5)
C21-C22-C23	111.6(4)	C121-C122-C123	116.3(6)
C21-C22-H22a	110.2(4)	C121-C122-H122a	107.9(5)
C21-C22-H22b	106.9(4)	C121-C122-H122b	110.0(6)
C23-C22-H22a	113.0(4)	C123-C122-H122a	102.3(6)
C23-C22-H22b	105.5(4)	C123-C122-H122b	110.7(5)
H22a-C22-H22b	109.3(4)	H122a-C122-H122b	109.2(6)
O4-C23-O5	124.1(5)	O104-C123-O105	123.8(6)
O4-C23-C22	126.2(5)	O104-C123-C122	128.1(6)
O5-C23-C22	109.8(5)	O105-C123-C122	108.1(5)
O5-C24-C25	104.6(5)	O105-C124-C125	103.5(7)
O5-C24-H24a	112.8(5)	O105-C124-H124a	111.8(6)
O5-C24-H24b	109.5(5)	O105-C124-H124b	107.4(7)
C25-C24-H24a	107.3(5)	C125-C124-H124a	118.2(7)
C25-C24-H24b	113.6(6)	C125-C124-H124b	106.4(6)
H24a-C24-H24b	109.1(6)	H124a-C124-H124b	109.0(9)
C24-C25-C26	119.4(6)	C124-C125-C126	118.5(6)
C24-C25-C30	121.0(6)	C124-C125-C130	122.2(7)
C26-C25-C30	119.5(6)	C126-C125-C130	119.1(7)
C25-C26-C27	117.5(7)	C125-C126-C127	121.6(7)
C25-C26-H26	117.7(6)	C125-C126-H126	115.1(6)
C27-C26-H26	124.4(6)	C127-C126-H126	123.2(7)
C26-C27-C28	120.5(7)	C126-C127-C128	118.9(8)
C26-C27-H27	115.0(8)	C126-C127-H127	116.0(8)
C28-C27-H27	124.3(7)	C128-C127-H127	125.0(8)
C27-C28-C29	122.8(7)	C127-C128-C129	119.8(8)
C27-C28-H28	113.2(9)	C127-C128-H128	115.1(12)
C29-C28-H28	124.0(9)	C129-C128-H128	125.1(11)
C28-C29-C30	117.9(7)	C128-C129-C130	120.1(8)
C28-C29-H29	113.3(8)	C128-C129-H129	115.2(11)
C30-C29-H29	128.9(10)	C130-C129-H129	124.6(14)
C25-C30-C29	121.8(7)	C125-C130-C129	120.5(9)
C25-C30-H30	125.7(7)	C125-C130-H130	124.6(9)
C29-C30-H30	112.3(7)	C129-C130-H130	114.9(8)

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Fe1	3.82(4)	2.81(3)	2.60(3)	-0.53(3)	0.186(24)	-0.04(3)
O1	5.12(21)	2.68(19)	4.67(21)	0.80(17)	1.80 (17)	0.50(16)
O2	3.73(21)	17.2 (6)	2.87(21)	0.9 (3)	-0.42 (16)	-1.4 (3)
O3	2.82(16)	5.9 (3)	3.92(18)	0.29(16)	0.15 (14)	-1.04(19)
O4	5.46(24)	4.04(24)	6.3 (3)	-1.21(20)	-1.81 (19)	1.22(20)
O5	5.31(23)	3.93(22)	5.17(23)	-1.02(18)	-2.34 (18)	1.36(19)
N1	3.06(19)	2.77(21)	2.26(18)	0.10(15)	0.23 (15)	0.08(16)
C1	3.3 (3)	3.3 (3)	2.79(24)	-0.30(21)	0.09 (20)	0.12(22)
C2	5.0 (3)	2.9 (3)	3.1 (3)	-0.79(23)	0.42 (23)	-0.61(22)
C3	5.0 (3)	3.5 (3)	3.2 (3)	-1.91(24)	0.92 (23)	-0.77(23)
C4	3.80(24)	4.3 (3)	3.54(24)	-0.4 (3)	0.51 (19)	-1.1 (3)
C5	2.99(23)	3.5 (3)	3.23(24)	-0.26(19)	-0.22 (19)	-0.40(20)
C6	4.5 (3)	3.6 (3)	5.4 (3)	-0.95(24)	-0.4 (3)	-1.1 (3)
C7	4.5 (3)	4.6 (3)	3.1 (3)	-1.4 (3)	-0.13 (22)	-0.39(25)
C8	4.7 (3)	4.7 (3)	5.5 (3)	-0.1 (3)	-1.28 (24)	0.1 (3)
C9	7.0 (4)	7.4 (5)	3.5 (3)	-2.9 (4)	-1.8 (3)	1.6 (3)
C10	5.0 (3)	8.0 (5)	2.9 (3)	-2.4 (3)	0.81 (24)	-1.7 (3)
C11	3.08(25)	2.9 (3)	2.50(23)	0.15(20)	-0.25 (19)	0.22(21)
C12	2.93(22)	3.4 (3)	2.56(21)	-0.19(19)	0.09 (18)	-0.04(19)
C13	3.00(24)	5.1 (3)	2.69(25)	0.42(22)	-0.18 (19)	0.15(22)
C14	3.1 (3)	8.0 (5)	4.1 (3)	-0.4 (3)	-0.46 (22)	-0.3 (3)
C15	2.75(24)	5.7 (4)	4.0 (3)	0.09(23)	0.17 (21)	-0.4 (3)
C16	3.8 (3)	5.2 (4)	6.4 (4)	0.5 (3)	0.1 (3)	0.0 (3)
C17	5.4 (3)	5.8 (4)	4.1 (3)	-0.8 (3)	0.4 (3)	0.2 (3)
C18	4.2 (3)	6.8 (4)	5.2 (3)	-2.2 (3)	1.0 (3)	-2.6 (3)
C19	3.14(24)	5.4 (3)	5.3 (3)	-0.3 (3)	-0.02 (21)	-0.5 (3)
C20	3.5 (3)	5.6 (4)	4.8 (3)	-0.2 (3)	-0.79 (21)	0.1 (3)
C21	2.93(24)	3.7 (3)	3.19(25)	-0.72(21)	0.06 (19)	0.32(22)
C22	3.6 (3)	3.3 (3)	3.21(25)	-0.39(21)	-0.46 (20)	0.50(22)
C23	3.7 (3)	4.2 (3)	3.8 (3)	-0.28(25)	-0.64 (22)	0.72(25)
C24	7.0 (4)	4.0 (3)	6.4 (4)	-1.2 (3)	-3.0 (3)	2.0 (3)
C25	5.1 (3)	3.9 (3)	4.1 (3)	-0.3 (3)	-1.33 (25)	1.5 (3)
C26	5.8 (4)	6.8 (4)	4.7 (3)	-0.9 (3)	-0.4 (3)	1.6 (3)
C27	5.9 (4)	8.2 (6)	8.0 (5)	-1.7 (4)	-2.4 (4)	2.5 (5)
C28	11.4 (7)	6.4 (5)	5.7 (5)	-2.4 (5)	-3.8 (5)	2.0 (4)
C29	14.3 (9)	4.7 (4)	5.2 (4)	0.6 (5)	-0.7 (5)	0.4 (4)
C30	7.4 (5)	5.3 (4)	6.0 (4)	0.8 (3)	-0.1 (3)	1.1 (4)
Fe101	3.86(4)	4.95(5)	7.29(6)	1.09(4)	-1.74 (4)	-2.31(5)
O101	4.89(22)	2.33(19)	6.36(25)	0.48(16)	0.62 (19)	0.34(18)
O102	3.83(18)	4.83(24)	3.21(16)	0.96(17)	0.43 (14)	0.53(18)
O103	4.01(19)	3.98(20)	2.73(17)	0.53(16)	-0.28 (14)	0.39(16)
O104	5.3 (3)	5.7 (3)	5.9 (3)	-0.05(22)	0.27 (21)	0.06(23)
O105	10.1 (4)	8.2 (4)	3.77(23)	1.4 (3)	2.50 (23)	0.41(25)
N101	4.41(22)	2.65(23)	2.68(19)	1.01(17)	-0.47 (16)	-0.03(17)
C101	5.2 (3)	3.6 (3)	3.01(24)	0.6 (3)	-0.52 (20)	-0.81(24)
C102	6.3 (4)	4.5 (3)	4.0 (3)	0.1 (3)	-0.6 (3)	-1.4 (3)
C103	8.2 (5)	7.0 (5)	6.9 (4)	-0.9 (4)	-4.7 (4)	-0.4 (4)
C104	10.6 (6)	4.9 (4)	9.2 (5)	0.2 (4)	-6.8 (5)	1.7 (4)
C105	7.0 (4)	4.3 (3)	6.1 (4)	0.2 (3)	-3.7 (3)	0.4 (3)
C106	8.2 (6)	7.0 (6)	24.6 (15)	1.0 (5)	7.7 (8)	-3.6 (8)
C107	7.7 (5)	5.3 (5)	7.2 (4)	-1.1 (4)	0.9 (4)	-0.9 (4)
C108	7.4 (5)	6.9 (5)	7.9 (5)	-1.0 (4)	1.9 (4)	-0.9 (4)
C109	3.7 (3)	11.4 (7)	5.4 (4)	1.2 (4)	-0.7 (3)	0.0 (4)
C110	3.7 (3)	5.4 (4)	14.7 (8)	0.6 (3)	-2.3 (4)	-0.3 (5)
C111	4.4 (3)	2.8 (3)	2.90(24)	0.80(22)	0.83 (21)	-0.10(21)
C112	4.51(25)	2.87(25)	2.46(21)	0.71(24)	0.03 (18)	-0.11(23)
C113	4.1 (3)	2.6 (3)	3.04(23)	0.29(22)	-0.10 (19)	0.46(21)
C114	5.5 (3)	4.7 (3)	2.54(25)	-0.1 (3)	-0.82 (22)	0.48(24)
C115	3.24(24)	8.0 (5)	2.68(23)	-0.4 (3)	0.26 (19)	-0.1 (3)
C116	5.8 (4)	6.2 (4)	4.5 (3)	-2.0 (3)	-0.6 (3)	0.7 (3)
C117	8.1 (5)	9.5 (6)	4.5 (4)	-4.1 (5)	0.0 (3)	-1.1 (4)
C118	4.9 (4)	14.6 (9)	5.0 (4)	-3.3 (5)	0.7 (3)	-2.6 (5)
C119	3.4 (3)	21.5 (13)	4.0 (4)	0.5 (5)	-1.2 (3)	-3.3 (6)
C120	4.5 (3)	13.9 (8)	3.5 (3)	2.4 (5)	-1.11 (24)	-0.8 (5)
C121	4.2 (3)	5.0 (3)	3.9 (3)	0.5 (3)	0.92 (23)	0.7 (3)
C122	5.9 (4)	7.0 (5)	4.8 (3)	0.3 (3)	1.8 (3)	1.2 (3)
C123	4.3 (3)	4.4 (4)	5.6 (3)	-0.12(24)	-0.3 (3)	0.9 (3)
C124	13.5 (7)	8.3 (6)	7.3 (5)	-4.0 (6)	5.3 (5)	-3.0 (6)

C125	6.5 (4)	8.4 (5)	5.0 (4)	-1.8 (4)	1.6 (3)	-2.0 (4)
C126	7.3 (5)	7.2 (5)	6.0 (4)	-2.0 (4)	-0.1 (3)	-0.8 (4)
C127	4.9 (4)	6.5 (5)	10.6 (6)	-0.7 (3)	2.3 (4)	-0.2 (5)
C128	12.1 (9)	9.6 (8)	12.5 (9)	0.3 (7)	6.9 (7)	3.8 (7)
C129	15.1 (10)	16.2 (12)	3.7 (4)	4.2 (10)	1.4 (5)	1.5 (6)
C130	7.9 (5)	13.3 (9)	6.7 (5)	-2.6 (6)	-1.2 (4)	-2.9 (5)
H1	3.7					
H2	4.7					
H3	5.0					
H4	4.9					
H5	4.2					
H6	5.5					
H7	5.0					
H8	6.0					
H9	7.0					
H10	6.3					
H12	4.0					
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H21a	4.3					
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H22a	4.4					
H22b	4.4					
H24a	6.8					
H24b	6.8					
H26	6.8					
H27	8.4					
H28	8.8					
H29	9.1					
H30	7.2					
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H107	7.7					
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H119	10.6					
H120	8.3					
H121a	5.4					
H121b	5.4					
H122a	6.9					
H122b	6.9					
H124a	10.7					
H124b	10.7					
H126	7.8					
H127	8.4					
H128	12.4					
H129	12.7					
H130	10.3					

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

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 are based on F, with F set to zero for negative F^2^. The observed criterion
 of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_obs etc. and is
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O2 O 0.6956(18) -0.4129(14) 0.8396(4) 0.105(6) Uani 1 d . .
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C13 C 0.6367(29) -0.5156(23) 0.8398(7) 0.059(8) Uiso 1 d . .
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H14A H 0.7042(29) -0.2619(22) 0.8157(6) 0.195 Uiso 1 calc R .
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C17 C 0.7505(2) -0.8871(2) 0.82256(6) 0.058(6) Uiso 1 d R .
C18 C 0.6805(2) -0.9899(2) 0.82077(6) 0.120(10) Uiso 1 d R .
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S101 S -0.0795(2) 0.9022(2) 0.66953(6) 0.075(2) Uani 1 d R .
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O101 O -0.4368(2) 1.0164(2) 0.58834(6) 0.071(5) Uani 1 d R .
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C8 C9 Fe1 69.0(12) . . ?
C9 C10 C6 106.4(25) . . ?
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O1 C11 N1 118.5(21) . . ?
O1 C11 C1 123.6(26) . . ?
N1 C11 C1 117.8(24) . . ?
N1 C12 C13 115.4(16) . . ?
N1 C12 C15 112.9(15) . . ?
C13 C12 C15 108.3(17) . . ?
O3 C13 O2 122.1(25) . . ?
O3 C13 C12 130.5(27) . . ?
O2 C13 C12 107.3(22) . . ?
C12 C15 S1 116.2(14) . . ?
C17 C16 S1 111.0(2) . . ?
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C105 Fe2 C109 125.5 . . ?
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C103 Fe2 C102 39.3 . . ?
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C104 Fe2 C107 104.2 . . ?
C110 Fe2 C107 71.2 . . ?
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C101 Fe2 C108 124.4 . . ?
C104 Fe2 C108 123.2 . . ?
C110 Fe2 C108 67.8 . . ?
C103 Fe2 C108 158.5 . . ?
C105 Fe2 C108 109.8 . . ?
C109 Fe2 C108 41.6 . . ?
C102 Fe2 C108 161.5 . . ?
C107 Fe2 C108 40.1 . . ?
C106 Fe2 C108 67.8 . . ?
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C113 O103 C114 100.9 . . ?
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C117 C118 C119 120.0 . . ?
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O102 O -0.3122(2) 1.2468(2) 0.66224(6) 0.162(8) Uani 1 d R .
O103 O -0.2313(2) 1.2432(2) 0.60585(6) 0.091(5) Uani 1 d R .
C101 C -0.2892(2) 0.9212(2) 0.54572(6) 0.027(5) Uiso 1 d R .
C102 C -0.1574(2) 0.8981(2) 0.52831(6) 0.040(6) Uiso 1 d R .
H10C H -0.0685(2) 0.9248(2) 0.53597(6) 0.048 Uiso 1 calc R .
C103 C -0.1902(2) 0.8315(2) 0.49861(6) 0.044(6) Uiso 1 d R .
H10D H -0.1223(2) 0.7973(2) 0.48256(6) 0.052 Uiso 1 calc R .
C104 C -0.3251(2) 0.8077(2) 0.49523(6) 0.060(7) Uiso 1 d R .
H10E H -0.3686(2) 0.7617(2) 0.47613(6) 0.071 Uiso 1 calc R .
C105 C -0.3893(2) 0.8709(2) 0.52393(6) 0.062(7) Uiso 1 d R .
H10F H -0.4861(2) 0.8734(2) 0.52874(6) 0.075 Uiso 1 calc R .
C106 C -0.1529(2) 0.5989(2) 0.54963(6) 0.061(7) Uiso 1 d R .
H10G H -0.0821(2) 0.5706(2) 0.53330(6) 0.073 Uiso 1 calc R .
C107 C -0.3047(2) 0.5795(2) 0.54532(6) 0.078(8) Uiso 1 d R .
H10H H -0.3514(2) 0.5347(2) 0.52650(6) 0.094 Uiso 1 calc R .
C108 C -0.3607(2) 0.6342(2) 0.57685(6) 0.071(8) Uiso 1 d R .
H10I H -0.4568(2) 0.6378(2) 0.58257(6) 0.085 Uiso 1 calc R .
C109 C -0.2549(2) 0.6941(2) 0.59740(6) 0.069(7) Uiso 1 d R .
H10J H -0.2682(2) 0.7406(2) 0.61948(6) 0.083 Uiso 1 calc R .
C110 C -0.1354(2) 0.6734(2) 0.58071(6) 0.071(7) Uiso 1 d R .
H11A H -0.0488(2) 0.7034(2) 0.58907(6) 0.085 Uiso 1 calc R .
C111 C -0.3180(2) 0.9872(2) 0.57941(6) 0.044(7) Uiso 1 d R .
C112 C -0.2422(2) 1.0662(2) 0.63791(6) 0.055(6) Uiso 1 d R .
H11B H -0.3197(2) 1.0283(2) 0.64917(6) 0.066 Uiso 1 calc R .
C113 C -0.2621(2) 1.1998(2) 0.63634(6) 0.106(10) Uiso 1 d R .
C114 C -0.2667(2) 1.3724(2) 0.61281(6) 0.204(15) Uiso 1 d R .
H11C H -0.2474(2) 1.4161(2) 0.59114(6) 0.305 Uiso 1 calc R .
H11D H -0.2140(2) 1.4009(2) 0.63288(6) 0.305 Uiso 1 calc R .
H11E H -0.3604(2) 1.3791(2) 0.61867(6) 0.305 Uiso 1 calc R .
C115 C -0.1084(2) 1.0518(2) 0.66295(6) 0.090(8) Uiso 1 d R .
H11F H -0.1210(2) 1.0893(2) 0.68645(6) 0.109 Uiso 1 calc R .
H11G H -0.0320(2) 1.0866(2) 0.65079(6) 0.109 Uiso 1 calc R .
C116 C -0.2049(2) 0.8657(2) 0.70320(6) 0.106(9) Uiso 1 d R .
H11H H -0.1912(2) 0.9108(2) 0.72523(6) 0.127 Uiso 1 calc R .
H11I H -0.2936(2) 0.8827(2) 0.69366(6) 0.127 Uiso 1 calc R .
C117 C -0.1946(2) 0.7382(2) 0.71237(6) 0.093(8) Uiso 1 d R .
C118 C -0.0970(2) 0.7167(2) 0.73874(6) 0.249(20) Uiso 1 d R .
H11J H -0.0487(2) 0.7770(2) 0.74889(6) 0.299 Uiso 1 calc R .
C119 C -0.0717(2) 0.6050(2) 0.74994(6) 0.225(17) Uiso 1 d R .
H11K H -0.0064(2) 0.5905(2) 0.76759(6) 0.270 Uiso 1 calc R .
C120 C -0.1440(2) 0.5148(2) 0.73477(6) 0.216(17) Uiso 1 d R .
H12B H -0.1271(2) 0.4401(2) 0.74227(6) 0.260 Uiso 1 calc R .
C121 C -0.2416(2) 0.5364(2) 0.70839(6) 0.221(17) Uiso 1 d R .
H12C H -0.2899(2) 0.4761(2) 0.69824(6) 0.265 Uiso 1 calc R .
C122 C -0.2669(2) 0.6481(2) 0.69719(6) 0.152(12) Uiso 1 d R .
H12D H -0.3322(2) 0.6625(2) 0.67955(6) 0.182 Uiso 1 calc R .

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S1 0.060(5) 0.066(4) 0.070(4) 0.002(3) 0.007(4) -0.017(4)
O1 0.006(10) 0.103(12) 0.083(12) -0.008(9) -0.002(10) -0.018(10)
O2 0.121(17) 0.088(13) 0.107(13) 0.027(10) -0.052(12) 0.005(13)
O3 0.084(15) 0.113(14) 0.119(16) 0.006(11) -0.037(13) -0.009(12)
Fe2 0.024(2) 0.044(2) 0.069(2) 0.000(2) 0.001(2) 0.003(3)
S101 0.039(5) 0.094(5) 0.092(5) 0.015(4) 0.009(4) 0.023(4)
N101 0.017(12) 0.074(12) 0.054(11) 0.019(9) -0.006(11) 0.008(10)
O101 0.045(12) 0.068(10) 0.101(13) -0.035(9) 0.024(10) 0.007(10)
O102 0.214(23) 0.101(13) 0.172(17) -0.037(13) 0.060(17) 0.030(16)
O103 0.082(13) 0.027(7) 0.165(14) -0.010(10) -0.038(12) -0.004(11)

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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
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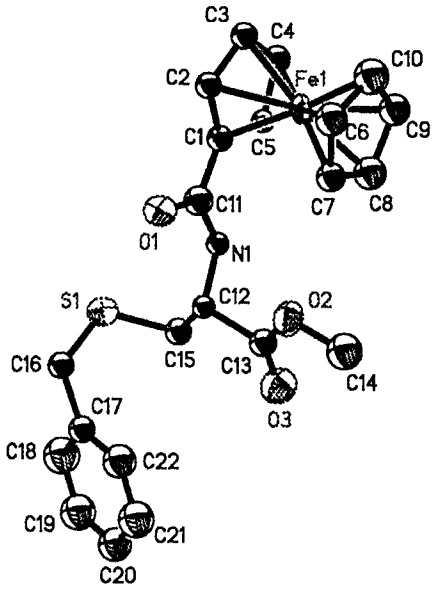
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C2
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C7
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O1
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C17
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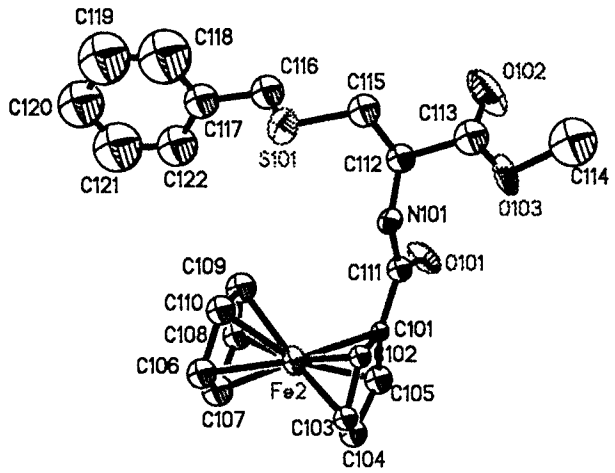
C20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C106
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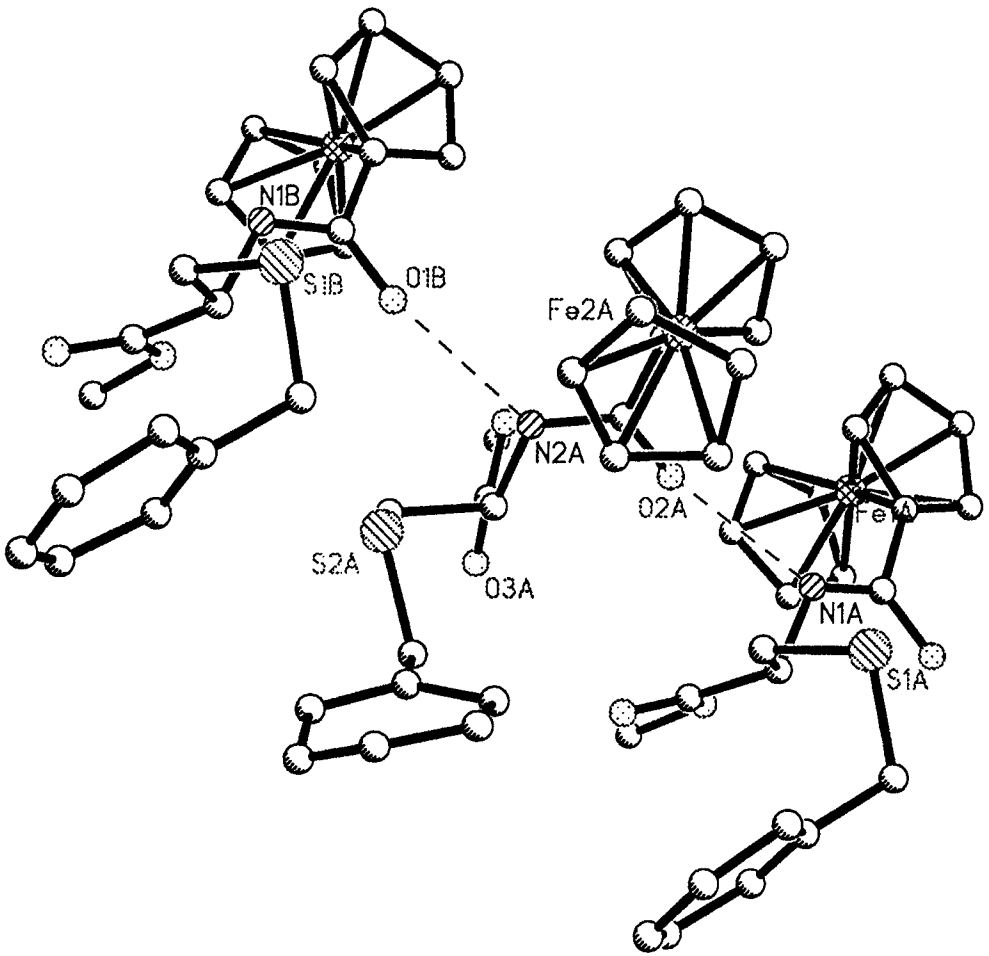
C103
C104


N1B
S1B
O1B
Fe2A
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S1A

BK3 AT -150 C

Space Group and Cell Dimensions Triclinic, P -1
a 7.03910(0) b 10.79221(0) c 11.16900(0)
alpha 108.07100(0) beta 107.95700(0) gamma 103.89600(0)
Volume 712.48(0)A**3

Empirical formula : Fe O2 N3 C17 H13

Cell dimensions were obtained from5655 reflections with 2Theta angle
in the range 3.00 - 57.50 degrees.

Crystal dimensions : 0.10 X 0.15 X 0.20 mm

FW = 347.15 Z = 2 F(000) = 356.75

Dcalc 1.618Mg.m-3, mu 1.07mm-1, lambda 0.70930A, 2Theta(max) 57.2

The intensity data were collected on a Siemens diffractometer,
using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -9 9; Kmin,max 0 14; Lmin,max -15 14
No. of reflections measured 8405
No. of unique reflections 3644
No. of reflections with Inet > 2.5sigma(Inet) 3090
Merging R-value on intensities 0.015
An empirical absorption correction was applied

The last least squares cycle was calculated with
36 atoms, 260 parameters and 3090 out of 3644 reflections.
Weights based on statistics were used.
The weight modifier K in KFo**2 is 0.000200

The residuals are as follows :--
For significant reflections, RF 0.030, Rw 0.036 GoF 1.51
For all reflections, RF 0.030, Rw 0.036.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.001.

In the last D-map, the deepest hole was -0.320e/A**3,
and the highest peak 0.420e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland,.J.-P., Lee, F.L. and White, P.S.
(1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)
Kynoch Press, Birmingham, England.

The following references may also be relevant.

3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot
Program, Technical Report ORNL-5138, Oak Ridge

4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.

DISANG -- The NRCVAX Distance and Angle Program

The Space Group is P -1 Centrosymmetric
The Equivalent Positions are:
1) x y z

The Lattice is Primitive. There are no Centring Vectors

BK3 AT -150 C 3-Sep-1996
The following Atoms are from the CD File
* Indicates that there are Symmetry Equivalents of an atom.

Name	x	y	z
Fe	0.48918(3)	0.65286(2)	0.33058(2)
O1	0.89651(20)	0.91365(12)	0.26791(12)
O2	0.70451(20)	0.69869(12)	0.08470(12)
N1	0.74417(24)	0.76648(15)	0.00360(14)
N2	0.92715(25)	0.78006(16)	-0.01586(16)
N3	0.91731(24)	0.83477(16)	-0.10586(16)
C1	0.76721(27)	0.71017(17)	0.30742(17)
C2	0.67471(28)	0.56017(18)	0.25742(18)
C3	0.66260(30)	0.52972(19)	0.37024(19)
C4	0.74447(29)	0.65948(20)	0.48907(19)
C5	0.81033(28)	0.77142(19)	0.45183(18)
C6	0.24329(30)	0.66007(20)	0.39239(21)
C7	0.31202(30)	0.77660(19)	0.36139(19)
C8	0.28456(30)	0.72427(21)	0.22103(20)
C9	0.19932(30)	0.57501(21)	0.16560(20)
C10	0.17233(30)	0.53505(20)	0.27055(21)
C11	0.80271(27)	0.79061(17)	0.22840(17)
C12	0.72445(27)	0.85454(17)	-0.14545(17)
C13	0.64093(30)	0.90941(18)	-0.23872(18)
C14	0.44013(31)	0.91382(18)	-0.25960(19)
C15	0.32215(30)	0.86441(19)	-0.19036(18)
C16	0.40239(29)	0.81209(18)	-0.09699(18)
C17	0.60773(27)	0.80905(16)	-0.07557(16)
H2	0.62651(357)	0.49280(235)	0.16577(233)
H3	0.60283(332)	0.43979(223)	0.36700(205)
H4	0.75194(332)	0.66863(214)	0.57950(218)
H5	0.86773(337)	0.86453(230)	0.50538(217)
H6	0.24364(326)	0.66152(213)	0.47498(215)
H7	0.37160(347)	0.87390(235)	0.42454(221)
H8	0.32334(362)	0.77792(245)	0.17654(230)
H9	0.17258(365)	0.51434(251)	0.07849(240)
H10	0.11492(365)	0.44298(249)	0.25930(227)
H13	0.72169(348)	0.93903(225)	-0.28098(219)
H14	0.36450(364)	0.94401(233)	-0.32998(228)
H15	0.18596(350)	0.86601(216)	-0.20724(210)
H16	0.32220(374)	0.77750(242)	-0.05172(239)

Fe-C1	2.0273(17)	C4-C5	1.417(3)
Fe-C2	2.0377(17)	C4-H4	0.967(21)
Fe-C3	2.0648(18)	C5-H5	0.902(22)
Fe-C4	2.0655(19)	C6-C7	1.420(3)
Fe-C5	2.0566(18)	C6-C10	1.428(3)
Fe-C6	2.0607(18)	C6-H6	0.917(21)
Fe-C7	2.0583(18)	C7-C8	1.423(3)
Fe-C8	2.0487(19)	C7-H7	0.961(22)
Fe-C9	2.0401(19)	C8-C9	1.423(3)
Fe-C10	2.0560(19)	C8-H8	0.918(24)
O1-C11	1.1956(21)	C9-C10	1.417(3)
O2-N1	1.3794(19)	C9-H9	0.918(23)
O2-C11	1.4271(20)	C10-H10	0.930(24)
N1-N2	1.3526(21)	C12-C13	1.398(3)
N1-C17	1.3623(23)	C12-C17	1.4017(24)
N2-N3	1.3072(22)	C13-C14	1.375(3)
N3-C12	1.3826(23)	C13-H13	0.906(22)
C1-C2	1.4370(24)	C14-C15	1.418(3)
C1-C5	1.4390(24)	C14-H14	0.996(23)

C1-C11	1.4499(25)	C15-C16	1.371(3)
C2-C3	1.419(3)	C15-H15	0.924(22)
C2-H2	0.947(23)	C16-C17	1.4007(25)
C3-C4	1.429(3)	C16-H16	0.952(24)
C3-H3	0.945(22)		

C1-Fe-C2	41.40(7)	C2-C3-C4	108.29(16)
C1-Fe-C3	68.50(7)	C2-C3-H3	126.3(12)
C1-Fe-C4	68.36(7)	C4-C3-H3	125.3(12)
C1-Fe-C5	41.26(7)	Fe-C4-C3	69.73(11)
C1-Fe-C6	162.22(7)	Fe-C4-C5	69.55(10)
C1-Fe-C7	125.31(7)	Fe-C4-H4	126.2(12)
C1-Fe-C8	107.57(8)	C3-C4-C5	108.76(16)
C1-Fe-C9	120.56(8)	C3-C4-H4	125.2(12)
C1-Fe-C10	155.60(8)	C5-C4-H4	126.0(12)
C2-Fe-C3	40.46(7)	Fe-C5-C1	68.28(10)
C2-Fe-C4	68.45(7)	Fe-C5-C4	70.23(11)
C2-Fe-C5	69.37(7)	Fe-C5-H5	126.1(13)
C2-Fe-C6	155.55(8)	C1-C5-C4	107.22(16)
C2-Fe-C7	161.25(7)	C1-C5-H5	124.3(13)
C2-Fe-C8	123.34(8)	C4-C5-H5	128.5(13)
C2-Fe-C9	105.37(8)	Fe-C6-C7	69.74(10)
C2-Fe-C10	119.33(7)	Fe-C6-C10	69.52(11)
C3-Fe-C4	40.48(8)	Fe-C6-H6	125.8(13)
C3-Fe-C5	68.31(7)	C7-C6-C10	107.92(17)
C3-Fe-C6	121.69(8)	C7-C6-H6	127.7(13)
C3-Fe-C7	157.81(8)	C10-C6-H6	124.4(13)
C3-Fe-C8	159.53(8)	Fe-C7-C6	69.92(10)
C3-Fe-C9	122.56(8)	Fe-C7-C8	69.36(10)
C3-Fe-C10	106.61(8)	Fe-C7-H7	124.7(13)
C4-Fe-C5	40.22(7)	C6-C7-C8	108.08(17)
C4-Fe-C6	108.96(8)	C6-C7-H7	126.3(13)
C4-Fe-C7	123.44(8)	C8-C7-H7	125.6(13)
C4-Fe-C8	158.58(8)	Fe-C8-C7	70.09(10)
C4-Fe-C9	159.78(8)	Fe-C8-C9	69.30(11)
C4-Fe-C10	124.36(8)	Fe-C8-H8	123.3(14)
C5-Fe-C6	125.38(8)	C7-C8-C9	107.87(17)
C5-Fe-C7	109.36(7)	C7-C8-H8	125.6(14)
C5-Fe-C8	122.87(8)	C9-C8-H8	126.5(14)
C5-Fe-C9	157.60(8)	Fe-C9-C8	69.95(11)
C5-Fe-C10	161.18(8)	Fe-C9-C10	70.37(11)
C6-Fe-C7	40.34(8)	Fe-C9-H9	123.0(14)
C6-Fe-C8	68.12(8)	C8-C9-C10	108.23(17)
C6-Fe-C9	68.25(8)	C8-C9-H9	126.4(14)
C6-Fe-C10	40.60(8)	C10-C9-H9	125.3(14)
C7-Fe-C8	40.55(8)	Fe-C10-C6	69.88(11)
C7-Fe-C9	68.31(8)	Fe-C10-C9	69.16(11)
C7-Fe-C10	68.09(8)	Fe-C10-H10	127.6(14)
C8-Fe-C9	40.74(8)	C6-C10-C9	107.91(17)
C8-Fe-C10	68.20(8)	C6-C10-H10	127.2(13)
C9-Fe-C10	40.47(8)	C9-C10-H10	124.9(13)
N1-O2-C11	112.51(12)	O1-C11-O2	121.30(16)
O2-N1-N2	118.72(14)	O1-C11-C1	129.44(16)
O2-N1-C17	127.53(14)	O2-C11-C1	109.25(14)
N2-N1-C17	113.27(14)	N3-C12-C13	130.01(16)
N1-N2-N3	106.95(14)	N3-C12-C17	109.38(15)
N2-N3-C12	108.65(14)	C13-C12-C17	120.61(16)
Fe-C1-C2	69.69(10)	C12-C13-C14	116.98(17)
Fe-C1-C5	70.47(10)	C12-C13-H13	118.2(14)
Fe-C1-C11	122.99(12)	C14-C13-H13	124.8(14)
C2-C1-C5	108.22(15)	C13-C14-C15	121.68(17)
C2-C1-C11	127.53(15)	C13-C14-H14	121.8(13)
C5-C1-C11	124.17(15)	C15-C14-H14	116.3(13)
Fe-C2-C1	68.91(10)	C14-C15-C16	122.27(17)
Fe-C2-C3	70.80(10)	C14-C15-H15	120.6(13)
Fe-C2-H2	124.5(13)	C16-C15-H15	117.1(13)
C1-C2-C3	107.51(16)	C15-C16-C17	115.63(16)
C1-C2-H2	127.1(13)	C15-C16-H16	122.2(14)
C3-C2-H2	125.4(13)	C17-C16-H16	122.1(14)
Fe-C3-C2	68.74(10)	N1-C17-C12	101.72(14)
Fe-C3-C4	69.79(10)	N1-C17-C16	135.46(16)

Fe-C3-H3 124.3(12) C12-C17-C16 122.81(16)

BK3 AT -150 C 3-Sep-1996

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Fe	0.48918(4)	0.65286(3)	0.33058(3)	1.283(12)
O1	0.89651(21)	0.91365(12)	0.26791(13)	1.78 (6)
O2	0.70451(20)	0.69869(13)	0.08470(12)	1.62 (6)
N1	0.74417(24)	0.76648(15)	0.00360(15)	1.53 (7)
N2	0.9272 (3)	0.78006(16)	-0.01586(16)	1.78 (8)
N3	0.91731(25)	0.83477(16)	-0.10586(16)	1.76 (8)
C1	0.7672 (3)	0.71017(18)	0.30742(17)	1.39 (7)
C2	0.6747 (3)	0.56017(18)	0.25742(19)	1.48 (8)
C3	0.6626 (3)	0.52972(20)	0.37024(20)	1.75 (9)
C4	0.7445 (3)	0.65948(20)	0.48907(20)	1.80 (9)
C5	0.8103 (3)	0.77142(19)	0.45183(18)	1.58 (8)
C6	0.2433 (3)	0.66007(21)	0.39239(21)	1.88 (9)
C7	0.3120 (3)	0.77660(20)	0.36139(20)	1.79 (9)
C8	0.2846 (3)	0.72427(21)	0.22103(20)	1.94 (9)
C9	0.1993 (3)	0.57501(21)	0.16560(20)	2.06 (9)
C10	0.1723 (3)	0.53505(21)	0.27055(22)	2.03 (9)
C11	0.8027 (3)	0.79061(18)	0.22840(17)	1.40 (8)
C12	0.7245 (3)	0.85454(17)	-0.14545(18)	1.44 (8)
C13	0.6409 (3)	0.90941(19)	-0.23872(19)	1.68 (9)
C14	0.4401 (3)	0.91382(19)	-0.25960(19)	1.75 (9)
C15	0.3222 (3)	0.86441(19)	-0.19036(19)	1.66 (8)
C16	0.4024 (3)	0.81209(18)	-0.09699(18)	1.55 (8)
C17	0.6077 (3)	0.80905(17)	-0.07557(17)	1.31 (8)
H2	0.627 (4)	0.4928 (24)	0.1658 (23)	2.2 (4)
H3	0.603 (3)	0.4398 (22)	0.3670 (21)	1.5 (4)
H4	0.752 (3)	0.6686 (21)	0.5795 (22)	1.8 (4)
H5	0.868 (3)	0.8645 (23)	0.5054 (22)	1.6 (4)
H6	0.244 (3)	0.6615 (21)	0.4750 (22)	1.6 (4)
H7	0.372 (3)	0.8739 (24)	0.4245 (22)	2.0 (4)
H8	0.323 (4)	0.7779 (25)	0.1765 (23)	2.4 (5)
H9	0.173 (4)	0.514 (3)	0.0785 (24)	2.4 (5)
H10	0.115 (4)	0.4430 (25)	0.2593 (23)	2.3 (5)
H13	0.722 (3)	0.9390 (23)	-0.2810 (22)	2.1 (4)
H14	0.365 (4)	0.9440 (23)	-0.3300 (23)	2.5 (5)
H15	0.186 (4)	0.8660 (22)	-0.2072 (21)	1.7 (4)
H16	0.322 (4)	0.7775 (24)	-0.0517 (24)	2.7 (5)

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Fe	1.479(13)	1.683(13)	1.603(13)	0.614(9)	0.453(10)	0.711(9)
O1	2.38 (7)	1.58 (6)	2.33 (6)	0.40 (5)	0.91 (6)	0.55 (5)
O2	2.58 (7)	1.78 (6)	1.60 (6)	0.49 (5)	0.82 (5)	0.75 (5)
N1	1.98 (8)	2.15 (7)	1.89 (7)	0.71 (6)	0.94 (6)	1.00 (6)
N2	2.15 (8)	2.50 (8)	2.38 (8)	1.08 (7)	1.12 (7)	1.01 (6)
N3	2.16 (8)	2.47 (8)	2.45 (8)	1.04 (6)	1.21 (7)	1.14 (7)
C1	1.57 (8)	1.68 (8)	1.74 (8)	0.59 (7)	0.48 (7)	0.56 (7)
C2	1.72 (9)	1.70 (8)	2.18 (9)	0.69 (7)	0.73 (7)	0.80 (7)
C3	2.04 (9)	2.25 (9)	2.62 (9)	1.00 (7)	0.78 (8)	1.39 (8)
C4	1.89 (9)	2.99 (10)	2.03 (9)	1.02 (8)	0.56 (7)	1.27 (8)
C5	1.63 (9)	2.20 (9)	1.62 (8)	0.54 (7)	0.35 (7)	0.58 (7)
C6	2.00 (9)	3.03 (10)	2.66 (10)	1.23 (8)	1.15 (8)	1.47 (8)
C7	2.15 (9)	2.30 (9)	2.48 (9)	1.20 (8)	0.87 (8)	0.95 (8)
C8	2.21 (10)	3.06 (10)	2.68 (10)	1.47 (8)	0.84 (8)	1.72 (8)
C9	1.92 (10)	2.89 (10)	2.12 (9)	1.10 (8)	0.08 (8)	0.53 (8)
C10	1.49 (9)	2.21 (9)	3.52 (11)	0.60 (7)	0.55 (8)	1.16 (8)
C11	1.50 (8)	1.89 (8)	1.71 (8)	0.72 (7)	0.63 (7)	0.42 (7)
C12	1.81 (9)	1.60 (8)	1.85 (8)	0.57 (7)	0.87 (7)	0.39 (7)
C13	2.43 (10)	2.02 (8)	2.27 (9)	0.82 (7)	1.34 (8)	0.93 (7)
C14	2.75 (10)	2.15 (9)	2.07 (9)	1.12 (8)	1.12 (8)	0.99 (7)
C15	1.83 (9)	2.13 (8)	2.11 (9)	0.82 (7)	0.83 (7)	0.52 (7)
C16	2.03 (9)	2.00 (8)	1.85 (8)	0.51 (7)	1.16 (7)	0.61 (7)
C17	2.03 (9)	1.30 (7)	1.38 (8)	0.50 (6)	0.71 (7)	0.30 (6)
H2	2.8(6)					
H3	1.9(5)					
H4	2.3(5)					
H5	2.1(5)					
H6	2.0(5)					
H7	2.5(5)					
H8	3.0(6)					
H9	3.0(6)					
H10	3.0(6)					
H13	2.6(6)					
H14	3.2(6)					
H15	2.2(5)					
H16	3.4(6)					

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)