

X-ray crystallographic study of 1aFe(II)

The structure is characterized by a strong disorder affecting the phenyl rings of the proximal strap, as shown on the right of the figure here below, where the carbon atoms of the two moieties have been differentiated with dark and light grey color code. Occupation parameters have been refined separately for the two disordered arms. Despite this molecule and solvent disorder modelisation, the structure is still affected by strongly distorted thermal ellipsoids, indicating that the disorder might be even more complex.

(C₈₉ H₆₈ Fe N₁₀ O₈, C₆ H₆); M = 1539.49. APEXII, Bruker-AXS diffractometer, Mo-K α radiation (λ = 0.71073 Å), T = 100(2) K; monoclinic C 2/c, a = 58.753(14), b = 12.399(3), c = 23.190(6) Å, β = 111.745(7) °, V = 15691(7) Å³, Z = 8, d = 1.303 g.cm⁻³, μ = 0.259 mm⁻¹. The structure was solved by direct methods using the SIR97 program [1], and then refined with full-matrix least-square methods based on F² (SHELX-97) [2] with the aid of the WINGX [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the BYPASS algorithm [4], implemented as the SQUEEZE option in PLATON [5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F² with 17723 unique intensities and 973 parameters converged at $\omega R(F^2)$ = 0.2823 ($R(F)$ = 0.1239) for 12032 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. 1999, 32, 115-119.

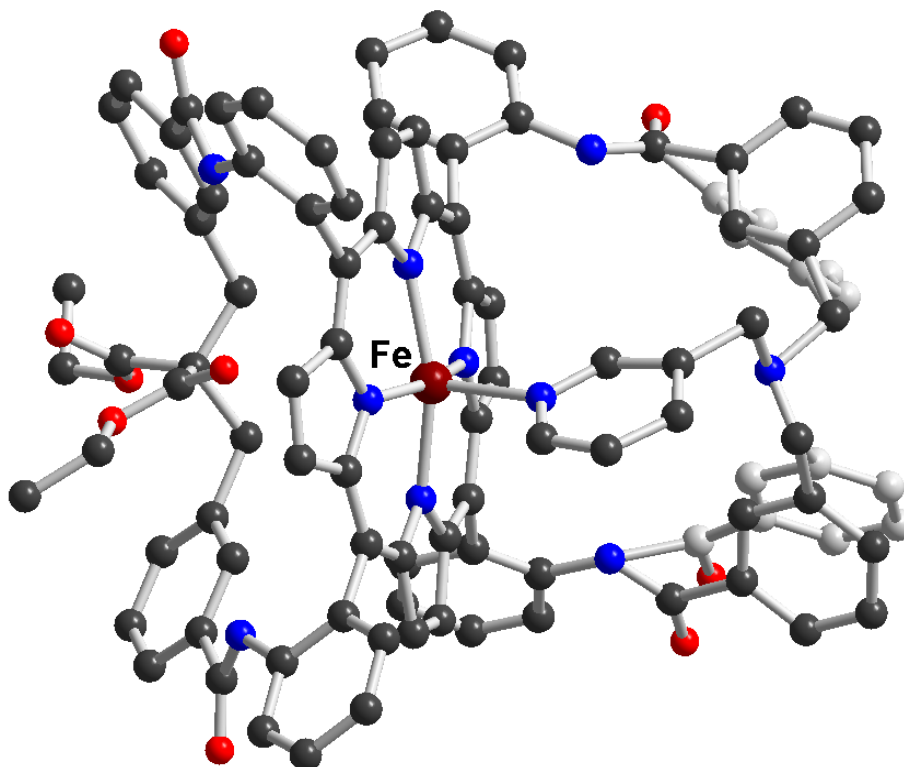
[2] SHELX97 - Programs for Crystal Structure Analysis (Release 97-2). G. M. Sheldrick, Institut für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838.

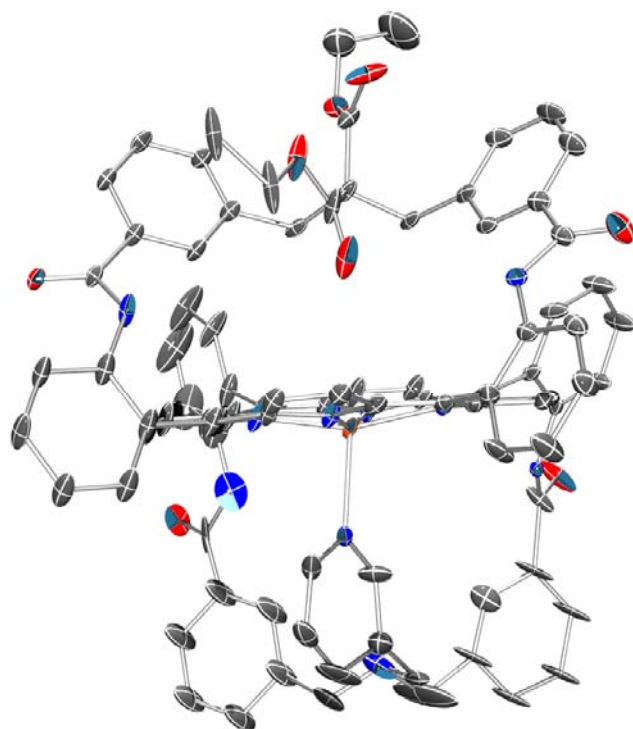
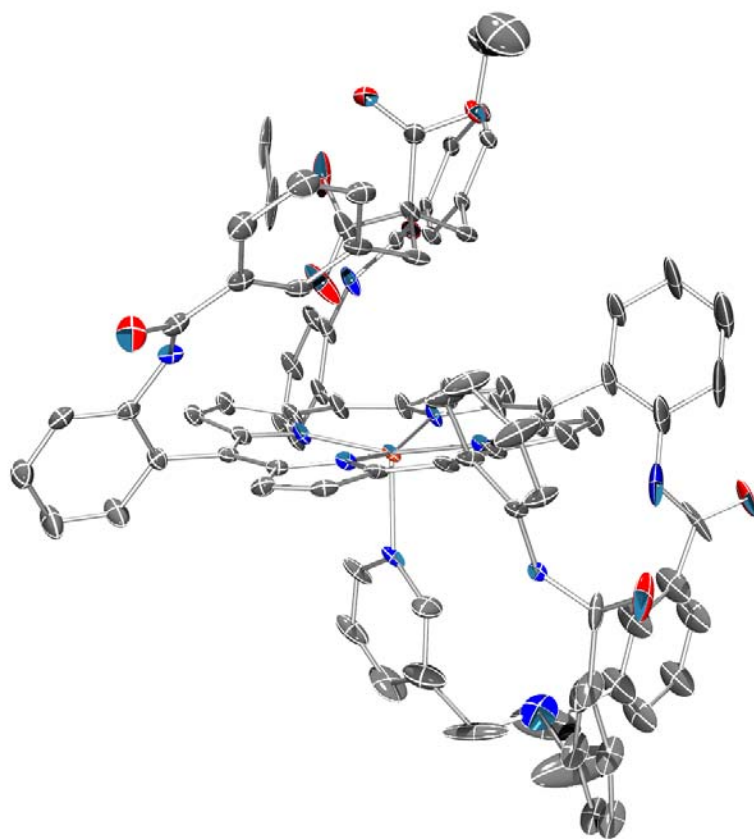
[4] Sluis, P. v.d. & Spek, A. L. (1990) Acta Cryst. A46, 194-201.

[5] A. L. Spek, Acta Crystallogr., Sect A 1990, 46, C34.

Ball & Stick side view of 1aFe(II), with the proximal strap disordered over two positions



ORTEP side views of 1aFe(II).



Structural data

Empirical formula	C89 H68 Fe N10 O8, C6 H6
Formula weight	1539.49
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, C 2/c
Unit cell dimensions	a = 58.753(14) Å, alpha = 90 ° b = 12.399(3) Å, beta = 111.745(7) ° c = 23.190(6) Å, gamma = 90 °
Volume	15691(7) Å ³
Z, Calculated density	8 , 1.303 (g.cm ⁻³)
Absorption coefficient	0.259 mm ⁻¹
F(000)	6432
Crystal size	0.3 x 0.21 x 0.17 mm
Theta range for data collection	2.93 to 27.6 °
h_min, h_max	-75 , 75
k_min, k_max	-15 , 14
l_min, l_max	-18 , 30
Reflections collected / unique	68315 / 17723 [R(int) = 0.0606]
Completeness to theta_max	0.973
Absorption correction type	multi-scan
Max. and min. transmission	0.957 , 0.705
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	17723 / 6 / 973
Goodness-of-fit	1.025
Final R indices [I>2sigma(I)]	R1 = 0.1239, wR2 = 0.2823
R indices (all data)	R1 = 0.1625, wR2 = 0.3037
Largest diff. peak and hole	1.617 and -1.024 e.Å ⁻³

Atomic coordinates and equivalent isotropic displacement parameters (Å² x 10³). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Fe1	0.625622(14)	0.02374(5)	0.10925(3)	0.02373(19)
N1	0.64489(9)	-0.0219(4)	0.0549(2)	0.0349(11)
N2	0.60170(9)	-0.1055(3)	0.0748(2)	0.0293(10)
N3	0.59956(8)	0.0935(3)	0.13843(18)	0.0256(9)
N4	0.64290(9)	0.1738(3)	0.12143(19)	0.0273(9)
C1	0.66430(12)	0.0316(4)	0.0472(3)	0.0388(15)
C2	0.67520(14)	-0.0361(5)	0.0144(3)	0.0476(17)
H2	0.6885	-0.0177	0.0026	0.057
C3	0.66294(13)	-0.1312(5)	0.0034(3)	0.0469(17)
H3	0.6665	-0.1926	-0.0164	0.056
C4	0.64344(12)	-0.1219(4)	0.0275(3)	0.0367(14)
C5	0.62477(13)	-0.1994(4)	0.0199(3)	0.0398(15)
C6	0.60453(11)	-0.1879(4)	0.0378(2)	0.0319(12)
C7	0.58371(11)	-0.2604(4)	0.0215(3)	0.0348(13)

H7	0.5814	-0.3244	-0.0026	0.042
C8	0.56815 (11)	-0.2202 (4)	0.0470 (3)	0.0331 (12)
H8	0.5527	-0.2496	0.043	0.04
C9	0.57944 (11)	-0.1241 (4)	0.0814 (2)	0.0302 (12)
C10	0.56946 (10)	-0.0585 (4)	0.1156 (2)	0.0261 (11)
C11	0.57918 (9)	0.0412 (4)	0.1423 (2)	0.0260 (11)
C12	0.56837 (10)	0.1093 (4)	0.1760 (2)	0.0298 (11)
H12	0.5547	0.092	0.1866	0.036
C13	0.58125 (10)	0.2014 (4)	0.1893 (2)	0.0299 (12)
H13	0.5782	0.2616	0.2107	0.036
C14	0.60067 (10)	0.1925 (4)	0.1655 (2)	0.0280 (11)
C15	0.61745 (11)	0.2747 (4)	0.1671 (2)	0.0301 (12)
C16	0.63686 (11)	0.2666 (4)	0.1456 (2)	0.0300 (12)
C17	0.65260 (14)	0.3544 (4)	0.1420 (3)	0.0457 (17)
H17	0.6523	0.4259	0.1564	0.055
C18	0.66764 (14)	0.3167 (5)	0.1147 (3)	0.0475 (18)
H18	0.68	0.3562	0.1065	0.057
C19	0.66131 (12)	0.2037 (4)	0.1003 (3)	0.0354 (13)
C20	0.67147 (12)	0.1378 (4)	0.0668 (3)	0.0363 (14)
C21	0.68859 (14)	0.1923 (5)	0.0403 (3)	0.0499 (18)
C22	0.67850 (17)	0.2348 (6)	-0.0188 (3)	0.069 (3)
H22	0.6615	0.2239	-0.0418	0.083
C23	0.6921 (2)	0.2927 (8)	-0.0460 (4)	0.102 (4)
H23	0.6844	0.32	-0.0869	0.122
C24	0.7162 (3)	0.3102 (11)	-0.0142 (6)	0.126 (6)
H24	0.7255	0.3511	-0.0325	0.152
C25	0.7273 (2)	0.2689 (8)	0.0441 (6)	0.103 (4)
H25	0.7443	0.2794	0.066	0.123
C26	0.71330 (17)	0.2104 (6)	0.0723 (5)	0.070 (2)
N5	0.72398 (14)	0.1686 (6)	0.1325 (4)	0.082 (2)
H5	0.7146	0.1516	0.1531	0.098
C27A	0.7487 (3)	0.1536 (11)	0.1597 (8)	0.070 (8)
O1A	0.7632 (2)	0.1957 (10)	0.1387 (7)	0.065 (4)
C28A	0.7537 (2)	0.0943 (12)	0.2140 (6)	0.091 (3)
C29A	0.74013 (18)	0.0905 (12)	0.2520 (7)	0.091 (3)
H29A	0.7252	0.1298	0.2411	0.109
C30A	0.7484 (2)	0.0293 (12)	0.3061 (6)	0.091 (3)
C31A	0.77018 (19)	-0.0282 (11)	0.3221 (6)	0.091 (3)
H31A	0.7758	-0.07	0.359	0.109
C32A	0.78371 (18)	-0.0244 (11)	0.2840 (6)	0.091 (3)
H32A	0.7986	-0.0636	0.2949	0.109
C33A	0.7754 (2)	0.0369 (12)	0.2300 (6)	0.091 (3)
H33A	0.7847	0.0394	0.2039	0.109
C27B	0.7456 (3)	0.1916 (18)	0.1821 (16)	0.172 (19)
O1B	0.7611 (4)	0.254 (2)	0.1816 (12)	0.242 (19)
C28B	0.7558 (2)	0.1304 (11)	0.2472 (5)	0.132 (5)
C29B	0.73880 (18)	0.0878 (11)	0.2697 (6)	0.132 (5)
H29B	0.7218	0.0914	0.2453	0.159
C30B	0.7467 (2)	0.0400 (11)	0.3281 (6)	0.132 (5)
C31B	0.7716 (2)	0.0347 (11)	0.3639 (5)	0.132 (5)
H31B	0.777	0.002	0.4037	0.159

C32B	0.78857 (18)	0.0773 (10)	0.3414 (6)	0.132 (5)
H32B	0.8056	0.0737	0.3658	0.159
C33B	0.7807 (2)	0.1252 (11)	0.2830 (5)	0.132 (5)
H33B	0.7923	0.1543	0.2676	0.159
C34	0.7275 (3)	-0.0283 (10)	0.3393 (6)	0.169 (8)
H34A	0.7181	-0.0883	0.313	0.202
H34B	0.7368	-0.0568	0.3814	0.202
C35	0.61160 (11)	0.3864 (4)	0.1832 (2)	0.0316 (12)
C36	0.58960 (14)	0.4338 (5)	0.1435 (3)	0.055 (2)
H36	0.5789	0.393	0.1097	0.066
C37	0.58316 (16)	0.5386 (6)	0.1524 (3)	0.074 (3)
H37	0.5683	0.5696	0.1253	0.089
C38	0.59913 (15)	0.5965 (6)	0.2020 (3)	0.070 (3)
H38	0.5953	0.6693	0.2075	0.084
C39	0.62037 (12)	0.5516 (5)	0.2435 (3)	0.0427 (16)
H39	0.6306	0.5922	0.278	0.051
C40	0.62668 (10)	0.4458 (4)	0.2344 (2)	0.0252 (11)
N6	0.64798 (7)	0.3956 (3)	0.27705 (18)	0.0213 (8)
H6	0.6481	0.3247	0.2785	0.026
C41	0.66801 (10)	0.4466 (4)	0.3154 (4)	0.0469 (18)
O2	0.67091 (8)	0.5444 (3)	0.3160 (3)	0.077 (2)
C42B	0.6897 (2)	0.3783 (11)	0.3462 (8)	0.0606 (18)
C43B	0.6944 (3)	0.2810 (15)	0.3609 (9)	0.0606 (18)
H43B	0.6805	0.2354	0.3435	0.073
C44B	0.7150 (3)	0.2264 (13)	0.3965 (9)	0.0606 (18)
C45B	0.7348 (3)	0.2787 (12)	0.3977 (8)	0.0606 (18)
H45B	0.7498	0.2399	0.4102	0.073
C46B	0.7351 (3)	0.3864 (11)	0.3819 (8)	0.0606 (18)
H46B	0.7501	0.4241	0.39	0.073
C47B	0.7119 (3)	0.4380 (12)	0.3529 (8)	0.0606 (18)
H47B	0.711	0.5101	0.3383	0.073
C42A	0.68371 (19)	0.3712 (8)	0.3699 (5)	0.072 (2)
C43A	0.6911 (2)	0.2730 (9)	0.3540 (4)	0.072 (2)
H43A	0.6849	0.2496	0.312	0.087
C44A	0.7077 (2)	0.2088 (7)	0.3995 (5)	0.072 (2)
C45A	0.71676 (16)	0.2429 (6)	0.4610 (5)	0.072 (2)
H45A	0.728	0.199	0.4921	0.087
C46A	0.70931 (17)	0.3412 (7)	0.4769 (4)	0.072 (2)
H46A	0.7155	0.3645	0.5189	0.087
C47A	0.69279 (17)	0.4054 (6)	0.4313 (5)	0.072 (2)
H47A	0.6877	0.4725	0.4422	0.087
C48	0.7225 (5)	0.1227 (12)	0.4012 (8)	0.289 (17)
H48A	0.7183	0.0881	0.4344	0.347
H48B	0.7406	0.1228	0.4151	0.347
N7	0.71223 (15)	0.0502 (6)	0.3421 (4)	0.088 (3)
N8	0.64906 (9)	-0.0672 (3)	0.1892 (2)	0.0307 (10)
C49	0.6932 (2)	0.0052 (11)	0.3581 (4)	0.138 (7)
H49A	0.6831	0.0632	0.3659	0.165
H49B	0.7002	-0.0389	0.3962	0.165
C50	0.67599 (18)	-0.0720 (8)	0.2985 (4)	0.081 (3)
C51	0.66264 (14)	-0.0195 (6)	0.2425 (3)	0.062 (2)

H51	0.6634	0.0571	0.2425	0.075
C52	0.64901 (14)	-0.1754 (5)	0.1865 (3)	0.0485 (18)
H52	0.639	-0.2075	0.1483	0.058
C53	0.66166 (17)	-0.2418 (7)	0.2323 (4)	0.067 (3)
H53	0.6608	-0.318	0.2276	0.08
C54	0.6767 (2)	-0.1906 (10)	0.2893 (7)	0.115 (5)
H54	0.6874	-0.2337	0.3221	0.138
C60	0.54601 (10)	-0.0927 (4)	0.1217 (3)	0.0305 (11)
C61	0.52390 (10)	-0.0359 (4)	0.0928 (2)	0.0300 (11)
C62	0.50268 (11)	-0.0645 (5)	0.1028 (3)	0.0371 (13)
H62	0.488	-0.0246	0.0836	0.045
C63	0.50311 (12)	-0.1517 (5)	0.1408 (3)	0.0468 (16)
H63	0.4886	-0.1729	0.147	0.056
C64	0.52484 (12)	-0.2079 (6)	0.1699 (4)	0.063 (2)
H64	0.5254	-0.2655	0.1974	0.076
C65	0.54559 (12)	-0.1804 (6)	0.1591 (4)	0.0540 (19)
H65	0.56	-0.2221	0.1776	0.065
N9	0.52447 (8)	0.0512 (4)	0.0546 (2)	0.0315 (10)
H9	0.533	0.0414	0.0308	0.038
C66	0.51333 (11)	0.1496 (5)	0.0502 (3)	0.0376 (13)
O3	0.49681 (9)	0.1671 (4)	0.0698 (3)	0.0589 (13)
C67	0.52336 (11)	0.2357 (4)	0.0211 (3)	0.0357 (13)
C68	0.54653 (11)	0.2300 (4)	0.0175 (2)	0.0314 (12)
H68	0.5566	0.1695	0.0354	0.038
C69	0.55567 (11)	0.3089 (4)	-0.0111 (2)	0.0336 (13)
C70	0.54084 (13)	0.3996 (5)	-0.0352 (3)	0.0445 (16)
H70	0.5465	0.4554	-0.0547	0.053
C71	0.51775 (14)	0.4078 (5)	-0.0305 (3)	0.0530 (18)
H71	0.5081	0.4702	-0.0463	0.064
C72	0.50872 (13)	0.3267 (5)	-0.0034 (3)	0.0480 (16)
H72	0.4929	0.3327	-0.0016	0.058
C73	0.58085 (11)	0.2962 (4)	-0.0151 (2)	0.0334 (13)
H73A	0.5916	0.2564	0.022	0.04
H73B	0.588	0.3687	-0.0141	0.04
C74	0.62603 (12)	-0.3003 (4)	-0.0154 (3)	0.0395 (15)
C75	0.62128 (12)	-0.2934 (4)	-0.0789 (3)	0.0399 (15)
C76	0.62390 (13)	-0.3852 (4)	-0.1113 (3)	0.0423 (16)
H76	0.6207	-0.3807	-0.1545	0.051
C77	0.63103 (14)	-0.4817 (5)	-0.0806 (3)	0.0491 (18)
H77	0.6329	-0.5433	-0.1029	0.059
C78	0.63560 (14)	-0.4904 (5)	-0.0177 (3)	0.0491 (18)
H78	0.6406	-0.5573	0.0032	0.059
C79	0.63271 (13)	-0.3997 (4)	0.0145 (3)	0.0438 (16)
H79	0.6353	-0.4055	0.0574	0.053
N10	0.61401 (11)	-0.1925 (4)	-0.1083 (2)	0.0412 (13)
H10	0.6024	-0.1579	-0.1003	0.049
C80	0.62307 (9)	-0.1432 (4)	-0.1477 (2)	0.0256 (11)
O4	0.63407 (7)	-0.1912 (3)	-0.17520 (16)	0.0309 (8)
C81	0.61807 (9)	-0.0247 (4)	-0.1557 (2)	0.0260 (11)
C82	0.61567 (11)	0.0415 (4)	-0.1091 (2)	0.0299 (12)
H82	0.6171	0.0105	-0.0705	0.036

C83	0.61120 (10)	0.1514 (4)	-0.1186 (2)	0.0278 (11)
C84	0.60978 (10)	0.1959 (4)	-0.1745 (2)	0.0304 (12)
H84	0.6071	0.2712	-0.1814	0.037
C85	0.61224 (11)	0.1309 (5)	-0.2207 (2)	0.0340 (13)
H85	0.6111	0.1623	-0.259	0.041
C86	0.61636 (10)	0.0204 (5)	-0.2116 (2)	0.0299 (11)
H86	0.618	-0.0233	-0.2435	0.036
C87	0.60798 (11)	0.2206 (4)	-0.0680 (2)	0.0323 (13)
H87A	0.6152	0.2924	-0.0686	0.039
H87B	0.6173	0.1872	-0.0273	0.039
C88	0.58065 (11)	0.2362 (4)	-0.0740 (2)	0.0307 (12)
C89	0.56608 (11)	0.3041 (5)	-0.1297 (2)	0.0369 (13)
O5	0.54378 (10)	0.2964 (5)	-0.1572 (2)	0.0750 (19)
O6	0.57906 (8)	0.3804 (3)	-0.14148 (19)	0.0396 (10)
C90	0.5673 (2)	0.4533 (8)	-0.1899 (5)	0.087 (3)
H90A	0.5524	0.419	-0.2201	0.105
H90B	0.5784	0.4713	-0.2118	0.105
C91	0.5602 (3)	0.5553 (10)	-0.1651 (7)	0.144 (6)
H91A	0.5518	0.6042	-0.1997	0.216
H91B	0.575	0.5905	-0.1363	0.216
H91C	0.5492	0.5375	-0.1434	0.216
C92	0.56999 (14)	0.1218 (5)	-0.0770 (3)	0.0473 (17)
O7	0.57340 (13)	0.0674 (4)	-0.0325 (3)	0.078 (2)
O8A	0.55815 (10)	0.0871 (4)	-0.1345 (3)	0.0678 (17)
C93A	0.5545 (3)	-0.0354 (16)	-0.1304 (10)	0.077 (5)
H93A	0.5409	-0.0517	-0.1161	0.093
H93B	0.5697	-0.071	-0.1024	0.093
C94A	0.5480 (3)	-0.0697 (12)	-0.1997 (9)	0.077 (5)
H94A	0.5456	-0.148	-0.2035	0.116
H94B	0.5615	-0.0494	-0.2129	0.116
H94C	0.533	-0.0332	-0.226	0.116
O8B	0.55815 (10)	0.0871 (4)	-0.1345 (3)	0.0678 (17)
C93B	0.5470 (4)	-0.016 (2)	-0.1547 (9)	0.085 (6)
H93C	0.5369	-0.0368	-0.1306	0.102
H93D	0.5598	-0.0716	-0.1484	0.102
C94B	0.5307 (3)	-0.0068 (16)	-0.2253 (8)	0.085 (6)
H94D	0.5232	-0.0769	-0.2406	0.127
H94E	0.5408	0.0154	-0.2485	0.127
H94F	0.5178	0.047	-0.2309	0.127
C100	0.76818 (19)	0.3934 (12)	0.3723 (6)	0.098 (3)
H100	0.7842	0.3732	0.399	0.118
C101	0.7544 (2)	0.4625 (12)	0.3937 (5)	0.098 (3)
H101	0.761	0.4895	0.4349	0.118
C102	0.7309 (2)	0.4921 (11)	0.3547 (6)	0.098 (3)
H102	0.7215	0.5393	0.3692	0.118
C103	0.72122 (19)	0.4526 (11)	0.2943 (6)	0.098 (3)
H103	0.7052	0.4729	0.2676	0.118
C104	0.7350 (2)	0.3836 (12)	0.2730 (5)	0.098 (3)
H104	0.7284	0.3566	0.2317	0.118
C105	0.7585 (2)	0.3540 (11)	0.3120 (6)	0.098 (3)
H105	0.7679	0.3068	0.2974	0.118

C110	0.7768 (3)	0.2885 (17)	0.4358 (10)	0.141 (5)
H110	0.7664	0.3269	0.4516	0.169
C111	0.7792 (3)	0.3221 (14)	0.3811 (10)	0.141 (5)
H111	0.7704	0.3835	0.3596	0.169
C112	0.7944 (4)	0.2659 (18)	0.3579 (8)	0.141 (5)
H112	0.796	0.2889	0.3205	0.169
C113	0.8072 (3)	0.1761 (17)	0.3893 (10)	0.141 (5)
H113	0.8176	0.1377	0.3735	0.169
C114	0.8048 (3)	0.1425 (14)	0.4440 (10)	0.141 (5)
H114	0.8136	0.0811	0.4655	0.169
C115	0.7896 (4)	0.1987 (18)	0.4672 (8)	0.141 (5)
H115	0.7879	0.1757	0.5046	0.169

Anisotropic displacement parameters (Å²)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 \left[h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} \right].$$

Atom	U11	U22	U33	U23	U13	U12
Fe1	0.0430 (4)	0.0145 (3)	0.0195 (3)	-0.0010 (3)	0.0183 (3)	-0.0044 (3)
N1	0.062 (3)	0.024 (2)	0.033 (2)	-0.0093 (19)	0.034 (2)	-0.021 (2)
N2	0.049 (3)	0.020 (2)	0.027 (2)	-0.0032 (17)	0.023 (2)	-0.0102 (19)
N3	0.041 (3)	0.017 (2)	0.0195 (19)	-0.0005 (16)	0.0122 (19)	0.0022 (18)
N4	0.049 (3)	0.016 (2)	0.021 (2)	-0.0047 (16)	0.018 (2)	-0.0038 (19)
C1	0.071 (4)	0.028 (3)	0.034 (3)	-0.013 (2)	0.038 (3)	-0.026 (3)
C2	0.083 (5)	0.031 (3)	0.052 (4)	-0.022 (3)	0.051 (4)	-0.027 (3)
C3	0.073 (5)	0.034 (3)	0.056 (4)	-0.025 (3)	0.050 (4)	-0.028 (3)
C4	0.064 (4)	0.022 (3)	0.042 (3)	-0.013 (2)	0.040 (3)	-0.018 (3)
C5	0.072 (4)	0.025 (3)	0.038 (3)	-0.010 (2)	0.038 (3)	-0.021 (3)
C6	0.058 (4)	0.020 (2)	0.028 (3)	-0.003 (2)	0.028 (3)	-0.007 (2)
C7	0.054 (4)	0.022 (3)	0.033 (3)	-0.006 (2)	0.022 (3)	-0.013 (2)
C8	0.044 (3)	0.024 (3)	0.033 (3)	0.001 (2)	0.016 (3)	-0.006 (2)
C9	0.046 (3)	0.020 (2)	0.025 (2)	0.004 (2)	0.012 (2)	-0.006 (2)
C10	0.033 (3)	0.022 (2)	0.020 (2)	0.0054 (19)	0.005 (2)	0.002 (2)
C11	0.031 (3)	0.025 (3)	0.019 (2)	0.004 (2)	0.006 (2)	0.005 (2)
C12	0.030 (3)	0.038 (3)	0.020 (2)	-0.003 (2)	0.006 (2)	0.007 (2)
C13	0.038 (3)	0.029 (3)	0.017 (2)	-0.001 (2)	0.005 (2)	0.015 (2)
C14	0.044 (3)	0.024 (3)	0.011 (2)	0.0004 (19)	0.006 (2)	0.004 (2)
C15	0.059 (4)	0.019 (2)	0.013 (2)	-0.0009 (19)	0.014 (2)	0.002 (2)
C16	0.057 (4)	0.019 (2)	0.016 (2)	-0.0036 (19)	0.016 (2)	-0.005 (2)
C17	0.096 (5)	0.019 (3)	0.036 (3)	-0.011 (2)	0.039 (3)	-0.018 (3)
C18	0.094 (5)	0.024 (3)	0.044 (3)	-0.018 (3)	0.048 (4)	-0.026 (3)
C19	0.059 (4)	0.022 (3)	0.032 (3)	-0.009 (2)	0.026 (3)	-0.017 (3)
C20	0.060 (4)	0.026 (3)	0.035 (3)	-0.011 (2)	0.031 (3)	-0.022 (3)
C21	0.079 (5)	0.034 (3)	0.059 (4)	-0.028 (3)	0.052 (4)	-0.036 (3)

C22	0.112 (7)	0.074 (5)	0.044 (4)	-0.027 (4)	0.055 (4)	-0.065 (5)
C23	0.158 (10)	0.109 (8)	0.073 (6)	-0.039 (5)	0.084 (7)	-0.103 (8)
C24	0.174 (12)	0.147 (11)	0.092 (8)	-0.048 (8)	0.090 (9)	-0.124 (10)
C25	0.105 (8)	0.092 (7)	0.138 (10)	-0.056 (7)	0.076 (8)	-0.086 (7)
C26	0.090 (6)	0.047 (4)	0.090 (6)	-0.026 (4)	0.054 (5)	-0.046 (4)
N5	0.061 (4)	0.059 (4)	0.129 (7)	-0.015 (5)	0.040 (5)	-0.042 (4)
C27A	0.14 (2)	0.009 (6)	0.118 (15)	0.011 (7)	0.123 (17)	0.015 (8)
O1A	0.059 (7)	0.058 (7)	0.109 (10)	0.025 (7)	0.068 (8)	-0.003 (6)
C28A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C29A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C30A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C31A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C32A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C33A	0.053 (4)	0.115 (7)	0.128 (7)	0.070 (6)	0.061 (5)	0.052 (4)
C27B	0.035 (9)	0.056 (14)	0.33 (4)	0.11 (2)	-0.043 (16)	-0.035 (9)
O1B	0.166 (19)	0.19 (2)	0.21 (2)	0.160 (19)	-0.118 (17)	-0.157 (18)
C28B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C29B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C30B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C31B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C32B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C33B	0.123 (8)	0.074 (5)	0.102 (7)	0.048 (5)	-0.073 (6)	-0.074 (5)
C34	0.240 (17)	0.158 (12)	0.114 (10)	0.073 (9)	0.073 (11)	0.179 (13)
C35	0.055 (3)	0.020 (2)	0.016 (2)	-0.0015 (19)	0.009 (2)	0.009 (2)
C36	0.083 (5)	0.033 (3)	0.021 (3)	-0.007 (2)	-0.013 (3)	0.015 (3)
C37	0.090 (6)	0.044 (4)	0.046 (4)	-0.010 (3)	-0.025 (4)	0.032 (4)
C38	0.082 (5)	0.035 (4)	0.053 (4)	-0.021 (3)	-0.024 (4)	0.031 (4)
C39	0.051 (4)	0.030 (3)	0.028 (3)	-0.011 (2)	-0.007 (3)	0.017 (3)
C40	0.038 (3)	0.021 (2)	0.018 (2)	-0.0021 (19)	0.013 (2)	0.004 (2)
N6	0.028 (2)	0.0151 (19)	0.023 (2)	0.0008 (16)	0.0121 (17)	0.0035 (16)
C41	0.017 (3)	0.016 (3)	0.099 (6)	0.007 (3)	0.011 (3)	-0.001 (2)
O2	0.034 (2)	0.015 (2)	0.162 (6)	0.011 (3)	0.010 (3)	-0.0020 (18)
C42B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C43B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C44B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C45B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C46B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C47B	0.045 (3)	0.040 (3)	0.083 (5)	0.000 (3)	0.007 (3)	-0.009 (3)
C42A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C43A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C44A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C45A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C46A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C47A	0.036 (3)	0.029 (3)	0.113 (6)	0.035 (4)	-0.017 (3)	0.012 (3)
C48	0.45 (4)	0.096 (10)	0.144 (14)	-0.008 (10)	-0.096 (18)	0.164 (17)
N7	0.071 (5)	0.064 (5)	0.106 (7)	0.022 (5)	0.006 (5)	0.035 (4)
N8	0.048 (3)	0.022 (2)	0.034 (2)	0.0106 (19)	0.029 (2)	0.010 (2)
C49	0.168 (12)	0.195 (14)	0.031 (4)	0.036 (6)	0.014 (6)	0.153 (12)
C50	0.102 (7)	0.095 (7)	0.060 (5)	0.035 (5)	0.044 (5)	0.058 (6)
C51	0.070 (5)	0.052 (4)	0.050 (4)	0.030 (4)	0.003 (4)	0.010 (4)
C52	0.090 (5)	0.021 (3)	0.056 (4)	0.019 (3)	0.053 (4)	0.018 (3)

C53	0.087 (6)	0.051 (4)	0.090 (6)	0.046 (5)	0.064 (5)	0.040 (4)
C54	0.092 (7)	0.103 (9)	0.149 (11)	0.108 (9)	0.044 (8)	0.052 (7)
C60	0.035 (3)	0.025 (3)	0.035 (3)	0.003 (2)	0.017 (2)	0.001 (2)
C61	0.033 (3)	0.026 (3)	0.024 (2)	-0.006 (2)	0.002 (2)	0.002 (2)
C62	0.030 (3)	0.036 (3)	0.035 (3)	-0.006 (3)	0.001 (2)	0.004 (2)
C63	0.035 (3)	0.049 (4)	0.058 (4)	0.010 (3)	0.020 (3)	0.004 (3)
C64	0.041 (4)	0.059 (5)	0.099 (6)	0.042 (4)	0.037 (4)	0.015 (3)
C65	0.040 (4)	0.048 (4)	0.078 (5)	0.038 (4)	0.028 (4)	0.022 (3)
N9	0.038 (3)	0.028 (2)	0.023 (2)	-0.0001 (18)	0.0047 (19)	0.0062 (19)
C66	0.034 (3)	0.032 (3)	0.034 (3)	-0.006 (2)	-0.001 (2)	0.007 (2)
O3	0.054 (3)	0.038 (3)	0.086 (4)	0.006 (3)	0.028 (3)	0.011 (2)
C67	0.044 (3)	0.024 (3)	0.029 (3)	-0.007 (2)	0.002 (2)	0.002 (2)
C68	0.047 (3)	0.022 (3)	0.017 (2)	-0.004 (2)	0.002 (2)	0.007 (2)
C69	0.061 (4)	0.018 (2)	0.016 (2)	-0.0059 (19)	0.008 (2)	0.005 (2)
C70	0.061 (4)	0.025 (3)	0.034 (3)	0.001 (2)	0.001 (3)	0.003 (3)
C71	0.063 (5)	0.021 (3)	0.058 (4)	0.005 (3)	0.003 (4)	0.016 (3)
C72	0.046 (4)	0.030 (3)	0.056 (4)	-0.002 (3)	0.005 (3)	0.008 (3)
C73	0.066 (4)	0.016 (2)	0.015 (2)	-0.0012 (19)	0.011 (2)	0.006 (2)
C74	0.067 (4)	0.026 (3)	0.044 (3)	-0.014 (2)	0.043 (3)	-0.023 (3)
C75	0.067 (4)	0.025 (3)	0.045 (3)	-0.012 (2)	0.041 (3)	-0.021 (3)
C76	0.080 (5)	0.025 (3)	0.041 (3)	-0.011 (2)	0.044 (3)	-0.016 (3)
C77	0.097 (5)	0.020 (3)	0.053 (4)	-0.015 (3)	0.053 (4)	-0.017 (3)
C78	0.093 (5)	0.022 (3)	0.049 (4)	-0.009 (3)	0.046 (4)	-0.018 (3)
C79	0.079 (5)	0.024 (3)	0.045 (3)	-0.011 (3)	0.043 (3)	-0.023 (3)
N10	0.076 (4)	0.019 (2)	0.051 (3)	-0.010 (2)	0.050 (3)	-0.014 (2)
C80	0.031 (3)	0.028 (3)	0.020 (2)	-0.008 (2)	0.012 (2)	-0.012 (2)
O4	0.039 (2)	0.035 (2)	0.0241 (18)	-0.0006 (16)	0.0179 (16)	-0.0014 (17)
C81	0.034 (3)	0.026 (2)	0.023 (2)	-0.007 (2)	0.015 (2)	-0.017 (2)
C82	0.054 (3)	0.022 (3)	0.018 (2)	-0.0034 (19)	0.017 (2)	-0.012 (2)
C83	0.040 (3)	0.021 (2)	0.023 (2)	-0.004 (2)	0.011 (2)	-0.015 (2)
C84	0.041 (3)	0.025 (3)	0.027 (3)	0.002 (2)	0.014 (2)	-0.009 (2)
C85	0.046 (3)	0.040 (3)	0.022 (2)	0.001 (2)	0.018 (2)	-0.016 (3)
C86	0.037 (3)	0.035 (3)	0.020 (2)	-0.006 (2)	0.014 (2)	-0.014 (2)
C87	0.059 (4)	0.017 (2)	0.016 (2)	-0.0020 (19)	0.008 (2)	-0.009 (2)
C88	0.056 (4)	0.020 (2)	0.020 (2)	-0.005 (2)	0.018 (2)	-0.013 (2)
C89	0.040 (3)	0.050 (4)	0.021 (3)	-0.002 (2)	0.011 (2)	-0.012 (3)
O5	0.066 (3)	0.104 (5)	0.032 (2)	0.029 (3)	-0.009 (2)	-0.039 (3)
O6	0.050 (2)	0.027 (2)	0.041 (2)	0.0122 (18)	0.017 (2)	-0.0019 (18)
C90	0.104 (8)	0.082 (7)	0.077 (6)	0.031 (5)	0.035 (6)	0.025 (6)
C91	0.163 (13)	0.092 (9)	0.174 (14)	0.058 (9)	0.060 (11)	0.066 (9)
C92	0.087 (5)	0.026 (3)	0.055 (4)	-0.016 (3)	0.056 (4)	-0.019 (3)
O7	0.169 (6)	0.021 (2)	0.092 (4)	0.000 (2)	0.102 (4)	-0.003 (3)
O8A	0.076 (3)	0.069 (3)	0.087 (4)	-0.060 (3)	0.063 (3)	-0.052 (3)
C93A	0.053 (7)	0.052 (7)	0.159 (14)	-0.081 (8)	0.077 (9)	-0.045 (6)
C94A	0.053 (7)	0.052 (7)	0.159 (14)	-0.081 (8)	0.077 (9)	-0.045 (6)
O8B	0.076 (3)	0.069 (3)	0.087 (4)	-0.060 (3)	0.063 (3)	-0.052 (3)
C93B	0.057 (8)	0.102 (11)	0.108 (11)	-0.076 (10)	0.046 (8)	-0.047 (8)
C94B	0.057 (8)	0.102 (11)	0.108 (11)	-0.076 (10)	0.046 (8)	-0.047 (8)
C100	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)
C101	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)
C102	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)

C103	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)
C104	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)
C105	0.085 (6)	0.094 (7)	0.089 (6)	-0.002 (5)	0.001 (5)	-0.031 (5)
C110	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)
C111	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)
C112	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)
C113	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)
C114	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)
C115	0.125 (10)	0.157 (13)	0.146 (12)	-0.034 (9)	0.059 (9)	-0.038 (8)

Bond lengths [Å]

Fe1	-	N1	=	2.061 (4)
Fe1	-	N3	=	2.078 (4)
Fe1	-	N2	=	2.086 (4)
Fe1	-	N4	=	2.088 (4)
Fe1	-	N8	=	2.171 (4)
N1	-	C4	=	1.381 (7)
N1	-	C1	=	1.386 (7)
N2	-	C6	=	1.383 (6)
N2	-	C9	=	1.391 (7)
N3	-	C14	=	1.370 (6)
N3	-	C11	=	1.393 (7)
N4	-	C16	=	1.383 (6)
N4	-	C19	=	1.393 (7)
C1	-	C20	=	1.406 (7)
C1	-	C2	=	1.433 (8)
C2	-	C3	=	1.356 (8)
C2	-	H2	=	0.95
C3	-	C4	=	1.454 (8)
C3	-	H3	=	0.95
C4	-	C5	=	1.419 (7)
C5	-	C6	=	1.405 (8)
C5	-	C74	=	1.512 (7)
C6	-	C7	=	1.451 (8)
C7	-	C8	=	1.354 (8)
C7	-	H7	=	0.95
C8	-	C9	=	1.451 (7)
C8	-	H8	=	0.95
C9	-	C10	=	1.407 (7)
C10	-	C11	=	1.405 (7)
C10	-	C60	=	1.498 (7)
C11	-	C12	=	1.447 (7)
C12	-	C13	=	1.341 (8)
C12	-	H12	=	0.95
C13	-	C14	=	1.445 (8)
C13	-	H13	=	0.95
C14	-	C15	=	1.410 (8)
C15	-	C16	=	1.406 (8)
C15	-	C35	=	1.507 (7)
C16	-	C17	=	1.450 (8)

C17 - C18 = 1.347(9)
C17 - H17 = 0.95
C18 - C19 = 1.457(7)
C18 - H18 = 0.95
C19 - C20 = 1.404(8)
C20 - C21 = 1.517(7)
C21 - C26 = 1.382(11)
C21 - C22 = 1.381(11)
C22 - C23 = 1.385(9)
C22 - H22 = 0.95
C23 - C24 = 1.352(16)
C23 - H23 = 0.95
C24 - C25 = 1.365(17)
C24 - H24 = 0.95
C25 - C26 = 1.423(11)
C25 - H25 = 0.95
C26 - N5 = 1.401(12)
N5 - C27A = 1.366(18)
N5 - C27B = 1.393(18)
N5 - H5 = 0.88
C27A - O1A = 1.242(18)
C27A - C28A = 1.391(17)
C28A - C29A = 1.39
C28A - C33A = 1.39
C29A - C30A = 1.39
C29A - H29A = 0.95
C30A - C31A = 1.39
C30A - C34 = 1.820(16)
C31A - C32A = 1.39
C31A - H31A = 0.95
C32A - C33A = 1.39
C32A - H32A = 0.95
C33A - H33A = 0.95
C27B - O1B = 1.19(2)
C27B - C28B = 1.60(3)
C28B - C29B = 1.39
C28B - C33B = 1.39
C29B - C30B = 1.39
C29B - H29B = 0.95
C30B - C31B = 1.39
C30B - C34 = 1.509(16)
C31B - C32B = 1.39
C31B - H31B = 0.95
C32B - C33B = 1.39
C32B - H32B = 0.95
C33B - H33B = 0.95
C34 - N7 = 1.341(12)
C34 - H34A = 0.99
C34 - H34B = 0.99
C35 - C40 = 1.399(7)
C35 - C36 = 1.408(8)

C36 - C37 = 1.391(9)
C36 - H36 = 0.95
C37 - C38 = 1.384(10)
C37 - H37 = 0.95
C38 - C39 = 1.380(8)
C38 - H38 = 0.95
C39 - C40 = 1.400(7)
C39 - H39 = 0.95
C40 - N6 = 1.419(6)
N6 - C41 = 1.341(7)
N6 - H6 = 0.88
C41 - O2 = 1.223(7)
C41 - C42B = 1.475(14)
C41 - C42A = 1.568(9)
C42B - C43B = 1.26(2)
C42B - C47B = 1.46(2)
C43B - C44B = 1.37(2)
C43B - H43B = 0.95
C44B - C45B = 1.33(2)
C44B - C48 = 1.351(19)
C45B - C46B = 1.39(2)
C45B - H45B = 0.95
C46B - C47B = 1.43(2)
C46B - H46B = 0.95
C47B - H47B = 0.95
C42A - C43A = 1.39
C42A - C47A = 1.39
C43A - C44A = 1.39
C43A - H43A = 0.95
C44A - C48 = 1.370(18)
C44A - C45A = 1.39
C45A - C46A = 1.39
C45A - H45A = 0.95
C46A - C47A = 1.39
C46A - H46A = 0.95
C47A - H47A = 0.95
C48 - N7 = 1.561(18)
C48 - H48A = 0.99
C48 - H48B = 0.99
N7 - C49 = 1.416(16)
N8 - C51 = 1.335(9)
N8 - C52 = 1.343(7)
C49 - C50 = 1.678(14)
C49 - H49A = 0.99
C49 - H49B = 0.99
C50 - C51 = 1.405(10)
C50 - C54 = 1.489(16)
C51 - H51 = 0.95
C52 - C53 = 1.333(10)
C52 - H52 = 0.95
C53 - C54 = 1.436(16)

C53 - H53 = 0.95
C54 - H54 = 0.95
C60 - C65 = 1.397(8)
C60 - C61 = 1.409(7)
C61 - C62 = 1.395(8)
C61 - N9 = 1.404(7)
C62 - C63 = 1.391(9)
C62 - H62 = 0.95
C63 - C64 = 1.390(9)
C63 - H63 = 0.95
C64 - C65 = 1.375(9)
C64 - H64 = 0.95
C65 - H65 = 0.95
N9 - C66 = 1.371(7)
N9 - H9 = 0.88
C66 - O3 = 1.234(8)
C66 - C67 = 1.496(9)
C67 - C68 = 1.396(8)
C67 - C72 = 1.405(8)
C68 - C69 = 1.395(8)
C68 - H68 = 0.95
C69 - C70 = 1.405(8)
C69 - C73 = 1.524(9)
C70 - C71 = 1.404(10)
C70 - H70 = 0.95
C71 - C72 = 1.391(10)
C71 - H71 = 0.95
C72 - H72 = 0.95
C73 - C88 = 1.552(7)
C73 - H73A = 0.99
C73 - H73B = 0.99
C74 - C75 = 1.395(8)
C74 - C79 = 1.398(9)
C75 - C76 = 1.404(8)
C75 - N10 = 1.414(8)
C76 - C77 = 1.375(9)
C76 - H76 = 0.95
C77 - C78 = 1.387(9)
C77 - H77 = 0.95
C78 - C79 = 1.396(8)
C78 - H78 = 0.95
C79 - H79 = 0.95
N10 - C80 = 1.361(6)
N10 - H10 = 0.88
C80 - O4 = 1.220(6)
C80 - C81 = 1.496(7)
C81 - C86 = 1.381(7)
C81 - C82 = 1.405(7)
C82 - C83 = 1.391(7)
C82 - H82 = 0.95
C83 - C84 = 1.383(7)

C83 - C87 = 1.520(7)
C84 - C85 = 1.389(8)
C84 - H84 = 0.95
C85 - C86 = 1.393(8)
C85 - H85 = 0.95
C86 - H86 = 0.95
C87 - C88 = 1.571(8)
C87 - H87A = 0.99
C87 - H87B = 0.99
C88 - C89 = 1.513(8)
C88 - C92 = 1.542(7)
C89 - O5 = 1.230(7)
C89 - O6 = 1.306(7)
O6 - C90 = 1.407(9)
C90 - C91 = 1.511(16)
C90 - H90A = 0.99
C90 - H90B = 0.99
C91 - H91A = 0.98
C91 - H91B = 0.98
C91 - H91C = 0.98
C92 - O7 = 1.186(8)
C92 - O8A = 1.325(8)
O8A - C93A = 1.54(2)
C93A - C94A = 1.57(2)
C93A - H93A = 0.99
C93A - H93B = 0.99
C94A - H94A = 0.98
C94A - H94B = 0.98
C94A - H94C = 0.98
C93B - C94B = 1.56(2)
C93B - H93C = 0.99
C93B - H93D = 0.99
C94B - H94D = 0.98
C94B - H94E = 0.98
C94B - H94F = 0.98
C100 - C101 = 1.39
C100 - C105 = 1.39
C100 - H100 = 0.95
C101 - C102 = 1.39
C101 - H101 = 0.95
C102 - C103 = 1.39
C102 - H102 = 0.95
C103 - C104 = 1.39
C103 - H103 = 0.95
C104 - C105 = 1.39
C104 - H104 = 0.95
C105 - H105 = 0.95
C110 - C111 = 1.39
C110 - C115 = 1.39
C110 - H110 = 0.95
C111 - C112 = 1.39

C111 - H111 = 0.95
C112 - C113 = 1.39
C112 - H112 = 0.95
C113 - C114 = 1.39
C113 - H113 = 0.95
C114 - C115 = 1.39
C114 - H114 = 0.95
C115 - H115 = 0.95

Angles [°]

N1 - Fe1 - N3 = 162.06 (19)
N1 - Fe1 - N2 = 89.97 (17)
N3 - Fe1 - N2 = 88.35 (17)
N1 - Fe1 - N4 = 88.72 (16)
N3 - Fe1 - N4 = 88.00 (17)
N2 - Fe1 - N4 = 164.03 (18)
N1 - Fe1 - N8 = 93.54 (18)
N3 - Fe1 - N8 = 104.39 (16)
N2 - Fe1 - N8 = 93.00 (18)
N4 - Fe1 - N8 = 102.97 (18)
C4 - N1 - C1 = 106.5 (4)
C4 - N1 - Fe1 = 124.9 (3)
C1 - N1 - Fe1 = 127.7 (3)
C6 - N2 - C9 = 106.3 (4)
C6 - N2 - Fe1 = 125.9 (4)
C9 - N2 - Fe1 = 127.8 (3)
C14 - N3 - C11 = 106.5 (4)
C14 - N3 - Fe1 = 127.3 (4)
C11 - N3 - Fe1 = 125.6 (3)
C16 - N4 - C19 = 105.7 (4)
C16 - N4 - Fe1 = 127.7 (4)
C19 - N4 - Fe1 = 126.2 (3)
N1 - C1 - C20 = 124.7 (5)
N1 - C1 - C2 = 109.8 (5)
C20 - C1 - C2 = 125.5 (5)
C3 - C2 - C1 = 107.4 (5)
C3 - C2 - H2 = 126.3
C1 - C2 - H2 = 126.3
C2 - C3 - C4 = 107.3 (5)
C2 - C3 - H3 = 126.3
C4 - C3 - H3 = 126.3
N1 - C4 - C5 = 125.4 (5)
N1 - C4 - C3 = 108.9 (5)
C5 - C4 - C3 = 125.5 (5)
C6 - C5 - C4 = 126.4 (5)
C6 - C5 - C74 = 117.5 (5)
C4 - C5 - C74 = 116.0 (5)
N2 - C6 - C5 = 124.6 (5)
N2 - C6 - C7 = 109.6 (5)

C5 - C6 - C7 = 125.7 (5)
C8 - C7 - C6 = 107.3 (5)
C8 - C7 - H7 = 126.3
C6 - C7 - H7 = 126.3
C7 - C8 - C9 = 107.3 (5)
C7 - C8 - H8 = 126.3
C9 - C8 - H8 = 126.3
N2 - C9 - C10 = 124.9 (5)
N2 - C9 - C8 = 109.4 (5)
C10 - C9 - C8 = 125.7 (5)
C11 - C10 - C9 = 124.8 (5)
C11 - C10 - C60 = 116.4 (5)
C9 - C10 - C60 = 118.7 (5)
N3 - C11 - C10 = 126.8 (5)
N3 - C11 - C12 = 108.8 (4)
C10 - C11 - C12 = 124.3 (5)
C13 - C12 - C11 = 107.4 (5)
C13 - C12 - H12 = 126.3
C11 - C12 - H12 = 126.3
C12 - C13 - C14 = 107.7 (5)
C12 - C13 - H13 = 126.1
C14 - C13 - H13 = 126.1
N3 - C14 - C15 = 125.1 (5)
N3 - C14 - C13 = 109.5 (5)
C15 - C14 - C13 = 125.4 (5)
C16 - C15 - C14 = 126.2 (5)
C16 - C15 - C35 = 116.3 (5)
C14 - C15 - C35 = 116.7 (5)
N4 - C16 - C15 = 124.5 (5)
N4 - C16 - C17 = 109.6 (5)
C15 - C16 - C17 = 125.8 (5)
C18 - C17 - C16 = 108.1 (5)
C18 - C17 - H17 = 126
C16 - C17 - H17 = 126
C17 - C18 - C19 = 106.6 (5)
C17 - C18 - H18 = 126.7
C19 - C18 - H18 = 126.7
N4 - C19 - C20 = 125.8 (5)
N4 - C19 - C18 = 109.9 (5)
C20 - C19 - C18 = 124.2 (5)
C19 - C20 - C1 = 125.8 (5)
C19 - C20 - C21 = 116.5 (5)
C1 - C20 - C21 = 116.8 (5)
C26 - C21 - C22 = 116.7 (6)
C26 - C21 - C20 = 125.3 (7)
C22 - C21 - C20 = 117.8 (7)
C21 - C22 - C23 = 122.8 (9)
C21 - C22 - H22 = 118.6
C23 - C22 - H22 = 118.6
C24 - C23 - C22 = 120.0 (10)
C24 - C23 - H23 = 120

C22 - C23 - H23 = 120
 C23 - C24 - C25 = 119.8(8)
 C23 - C24 - H24 = 120.1
 C25 - C24 - H24 = 120.1
 C24 - C25 - C26 = 120.2(10)
 C24 - C25 - H25 = 119.9
 C26 - C25 - H25 = 119.9
 C21 - C26 - N5 = 117.9(7)
 C21 - C26 - C25 = 120.4(10)
 N5 - C26 - C25 = 121.6(9)
 C27A - N5 - C26 = 121.2(9)
 C27B - N5 - C26 = 133.0(12)
 C27A - N5 - H5 = 119.4
 C27B - N5 - H5 = 99.5
 C26 - N5 - H5 = 119.4
 O1A - C27A - N5 = 121.9(14)
 O1A - C27A - C28A = 129.3(17)
 N5 - C27A - C28A = 108.6(11)
 C29A - C28A - C33A = 120
 C29A - C28A - C27A = 128.0(8)
 C33A - C28A - C27A = 112.0(8)
 C30A - C29A - C28A = 120
 C30A - C29A - H29A = 120
 C28A - C29A - H29A = 120
 C31A - C30A - C29A = 120
 C31A - C30A - C34 = 112.6(6)
 C29A - C30A - C34 = 122.1(7)
 C30A - C31A - C32A = 120
 C30A - C31A - H31A = 120
 C32A - C31A - H31A = 120
 C33A - C32A - C31A = 120
 C33A - C32A - H32A = 120
 C31A - C32A - H32A = 120
 C32A - C33A - C28A = 120
 C32A - C33A - H33A = 120
 C28A - C33A - H33A = 120
 O1B - C27B - N5 = 126(3)
 O1B - C27B - C28B = 107.3(15)
 N5 - C27B - C28B = 126.2(14)
 C29B - C28B - C33B = 120
 C29B - C28B - C27B = 117.9(12)
 C33B - C28B - C27B = 121.9(11)
 C28B - C29B - C30B = 120
 C28B - C29B - H29B = 120
 C30B - C29B - H29B = 120
 C29B - C30B - C31B = 120
 C29B - C30B - C34 = 113.9(9)
 C31B - C30B - C34 = 124.0(8)
 C32B - C31B - C30B = 120
 C32B - C31B - H31B = 120
 C30B - C31B - H31B = 120

C31B - C32B - C33B = 120
 C31B - C32B - H32B = 120
 C33B - C32B - H32B = 120
 C32B - C33B - C28B = 120
 C32B - C33B - H33B = 120
 C28B - C33B - H33B = 120
 N7 - C34 - C30B = 99.1 (12)
 N7 - C34 - C30A = 107.7 (10)
 N7 - C34 - H34A = 110.2
 C30B - C34 - H34A = 126.8
 C30A - C34 - H34A = 110.2
 N7 - C34 - H34B = 110.2
 C30B - C34 - H34B = 101.2
 C30A - C34 - H34B = 110.2
 H34A - C34 - H34B = 108.5
 C40 - C35 - C36 = 118.4 (5)
 C40 - C35 - C15 = 124.3 (5)
 C36 - C35 - C15 = 117.3 (5)
 C37 - C36 - C35 = 121.8 (6)
 C37 - C36 - H36 = 119.1
 C35 - C36 - H36 = 119.1
 C38 - C37 - C36 = 118.0 (6)
 C38 - C37 - H37 = 121
 C36 - C37 - H37 = 121
 C39 - C38 - C37 = 122.0 (6)
 C39 - C38 - H38 = 119
 C37 - C38 - H38 = 119
 C38 - C39 - C40 = 119.6 (5)
 C38 - C39 - H39 = 120.2
 C40 - C39 - H39 = 120.2
 C35 - C40 - C39 = 120.1 (5)
 C35 - C40 - N6 = 118.6 (4)
 C39 - C40 - N6 = 121.3 (5)
 C41 - N6 - C40 = 125.8 (4)
 C41 - N6 - H6 = 117.1
 C40 - N6 - H6 = 117.1
 O2 - C41 - N6 = 124.0 (6)
 O2 - C41 - C42B = 118.1 (7)
 N6 - C41 - C42B = 116.0 (7)
 O2 - C41 - C42A = 122.9 (7)
 N6 - C41 - C42A = 111.2 (6)
 C43B - C42B - C47B = 111.1 (14)
 C43B - C42B - C41 = 138.3 (14)
 C47B - C42B - C41 = 109.8 (11)
 C42B - C43B - C44B = 134.2 (16)
 C42B - C43B - H43B = 112.9
 C44B - C43B - H43B = 112.9
 C45B - C44B - C48 = 101.8 (19)
 C45B - C44B - C43B = 110.2 (15)
 C48 - C44B - C43B = 135.4 (16)
 C44B - C45B - C46B = 124.3 (15)

C44B - C45B - H45B = 117.9
C46B - C45B - H45B = 117.9
C45B - C46B - C47B = 116.9(13)
C45B - C46B - H46B = 121.6
C47B - C46B - H46B = 121.6
C46B - C47B - C42B = 118.9(13)
C46B - C47B - H47B = 120.5
C42B - C47B - H47B = 120.5
C43A - C42A - C47A = 120
C43A - C42A - C41 = 117.2(7)
C47A - C42A - C41 = 122.2(7)
C42A - C43A - C44A = 120
C42A - C43A - H43A = 120
C44A - C43A - H43A = 120
C48 - C44A - C45A = 102.1(10)
C48 - C44A - C43A = 136.5(10)
C45A - C44A - C43A = 120
C46A - C45A - C44A = 120
C46A - C45A - H45A = 120
C44A - C45A - H45A = 120
C47A - C46A - C45A = 120
C47A - C46A - H46A = 120
C45A - C46A - H46A = 120
C46A - C47A - C42A = 120
C46A - C47A - H47A = 120
C42A - C47A - H47A = 120
C44B - C48 - N7 = 117.9(12)
C44A - C48 - N7 = 112.9(12)
C44B - C48 - H48A = 107.8
C44A - C48 - H48A = 91.1
N7 - C48 - H48A = 107.8
C44B - C48 - H48B = 107.8
C44A - C48 - H48B = 127.2
N7 - C48 - H48B = 107.8
H48A - C48 - H48B = 107.2
C34 - N7 - C49 = 109.5(9)
C34 - N7 - C48 = 114.3(11)
C49 - N7 - C48 = 94.8(14)
C51 - N8 - C52 = 118.5(6)
C51 - N8 - Fe1 = 122.2(4)
C52 - N8 - Fe1 = 119.2(5)
N7 - C49 - C50 = 107.6(8)
N7 - C49 - H49A = 110.2
C50 - C49 - H49A = 110.2
N7 - C49 - H49B = 110.2
C50 - C49 - H49B = 110.2
H49A - C49 - H49B = 108.5
C51 - C50 - C54 = 111.2(9)
C51 - C50 - C49 = 117.2(8)
C54 - C50 - C49 = 129.9(8)
N8 - C51 - C50 = 126.0(8)

N8 - C51 - H51 = 117
 C50 - C51 - H51 = 117
 C53 - C52 - N8 = 126.1(8)
 C53 - C52 - H52 = 117
 N8 - C52 - H52 = 117
 C52 - C53 - C54 = 115.6(8)
 C52 - C53 - H53 = 122.2
 C54 - C53 - H53 = 122.2
 C53 - C54 - C50 = 121.9(8)
 C53 - C54 - H54 = 119.1
 C50 - C54 - H54 = 119.1
 C65 - C60 - C61 = 117.3(5)
 C65 - C60 - C10 = 120.5(5)
 C61 - C60 - C10 = 122.1(5)
 C62 - C61 - N9 = 122.1(5)
 C62 - C61 - C60 = 121.1(5)
 N9 - C61 - C60 = 116.8(5)
 C63 - C62 - C61 = 119.7(5)
 C63 - C62 - H62 = 120.1
 C61 - C62 - H62 = 120.1
 C64 - C63 - C62 = 119.7(6)
 C64 - C63 - H63 = 120.2
 C62 - C63 - H63 = 120.2
 C65 - C64 - C63 = 120.3(6)
 C65 - C64 - H64 = 119.9
 C63 - C64 - H64 = 119.9
 C64 - C65 - C60 = 121.8(6)
 C64 - C65 - H65 = 119.1
 C60 - C65 - H65 = 119.1
 C66 - N9 - C61 = 127.6(5)
 C66 - N9 - H9 = 116.2
 C61 - N9 - H9 = 116.2
 O3 - C66 - N9 = 123.2(6)
 O3 - C66 - C67 = 122.4(5)
 N9 - C66 - C67 = 114.4(5)
 C68 - C67 - C72 = 118.7(6)
 C68 - C67 - C66 = 123.2(5)
 C72 - C67 - C66 = 118.1(6)
 C69 - C68 - C67 = 123.3(5)
 C69 - C68 - H68 = 118.4
 C67 - C68 - H68 = 118.4
 C68 - C69 - C70 = 117.3(6)
 C68 - C69 - C73 = 120.7(5)
 C70 - C69 - C73 = 122.1(5)
 C71 - C70 - C69 = 120.1(6)
 C71 - C70 - H70 = 119.9
 C69 - C70 - H70 = 119.9
 C72 - C71 - C70 = 121.5(6)
 C72 - C71 - H71 = 119.2
 C70 - C71 - H71 = 119.2
 C71 - C72 - C67 = 119.0(6)

C71 - C72 - H72 = 120.5
C67 - C72 - H72 = 120.5
C69 - C73 - C88 = 114.3 (5)
C69 - C73 - H73A = 108.7
C88 - C73 - H73A = 108.7
C69 - C73 - H73B = 108.7
C88 - C73 - H73B = 108.7
H73A - C73 - H73B = 107.6
C75 - C74 - C79 = 119.2 (5)
C75 - C74 - C5 = 119.3 (5)
C79 - C74 - C5 = 121.4 (5)
C74 - C75 - C76 = 119.8 (6)
C74 - C75 - N10 = 118.0 (5)
C76 - C75 - N10 = 122.2 (5)
C77 - C76 - C75 = 120.0 (5)
C77 - C76 - H76 = 120
C75 - C76 - H76 = 120
C76 - C77 - C78 = 121.0 (5)
C76 - C77 - H77 = 119.5
C78 - C77 - H77 = 119.5
C77 - C78 - C79 = 119.1 (6)
C77 - C78 - H78 = 120.5
C79 - C78 - H78 = 120.5
C78 - C79 - C74 = 120.8 (6)
C78 - C79 - H79 = 119.6
C74 - C79 - H79 = 119.6
C80 - N10 - C75 = 126.7 (5)
C80 - N10 - H10 = 116.6
C75 - N10 - H10 = 116.6
O4 - C80 - N10 = 123.2 (5)
O4 - C80 - C81 = 122.1 (4)
N10 - C80 - C81 = 114.7 (4)
C86 - C81 - C82 = 119.5 (5)
C86 - C81 - C80 = 117.3 (4)
C82 - C81 - C80 = 123.2 (4)
C83 - C82 - C81 = 121.2 (5)
C83 - C82 - H82 = 119.4
C81 - C82 - H82 = 119.4
C84 - C83 - C82 = 118.8 (5)
C84 - C83 - C87 = 121.1 (5)
C82 - C83 - C87 = 120.1 (4)
C83 - C84 - C85 = 120.2 (5)
C83 - C84 - H84 = 119.9
C85 - C84 - H84 = 119.9
C84 - C85 - C86 = 121.1 (5)
C84 - C85 - H85 = 119.4
C86 - C85 - H85 = 119.4
C81 - C86 - C85 = 119.2 (5)
C81 - C86 - H86 = 120.4
C85 - C86 - H86 = 120.4
C83 - C87 - C88 = 114.6 (4)

C83 - C87 - H87A = 108.6
C88 - C87 - H87A = 108.6
C83 - C87 - H87B = 108.6
C88 - C87 - H87B = 108.6
H87A - C87 - H87B = 107.6
C89 - C88 - C92 = 112.4 (5)
C89 - C88 - C73 = 107.6 (5)
C92 - C88 - C73 = 110.5 (4)
C89 - C88 - C87 = 112.4 (4)
C92 - C88 - C87 = 106.0 (5)
C73 - C88 - C87 = 107.9 (4)
O5 - C89 - O6 = 122.7 (6)
O5 - C89 - C88 = 123.8 (5)
O6 - C89 - C88 = 113.1 (5)
C89 - O6 - C90 = 118.7 (6)
O6 - C90 - C91 = 110.9 (9)
O6 - C90 - H90A = 109.5
C91 - C90 - H90A = 109.5
O6 - C90 - H90B = 109.5
C91 - C90 - H90B = 109.5
H90A - C90 - H90B = 108
C90 - C91 - H91A = 109.5
C90 - C91 - H91B = 109.5
H91A - C91 - H91B = 109.5
C90 - C91 - H91C = 109.5
H91A - C91 - H91C = 109.5
H91B - C91 - H91C = 109.5
O7 - C92 - O8A = 123.2 (6)
O7 - C92 - C88 = 123.3 (6)
O8A - C92 - C88 = 113.4 (5)
C92 - O8A - C93A = 106.9 (9)
O8A - C93A - C94A = 101.0 (14)
O8A - C93A - H93A = 111.6
C94A - C93A - H93A = 111.6
O8A - C93A - H93B = 111.6
C94A - C93A - H93B = 111.6
H93A - C93A - H93B = 109.4
C93A - C94A - H94A = 109.5
C93A - C94A - H94B = 109.5
H94A - C94A - H94B = 109.5
C93A - C94A - H94C = 109.5
H94A - C94A - H94C = 109.5
H94B - C94A - H94C = 109.5
C94B - C93B - H93C = 110.1
C94B - C93B - H93D = 110.1
H93C - C93B - H93D = 108.5
C93B - C94B - H94D = 109.5
C93B - C94B - H94E = 109.5
H94D - C94B - H94E = 109.5
C93B - C94B - H94F = 109.5
H94D - C94B - H94F = 109.5

H94E - C94B - H94F = 109.5
 C101 - C100 - C105 = 120
 C101 - C100 - H100 = 120
 C105 - C100 - H100 = 120
 C100 - C101 - C102 = 120
 C100 - C101 - H101 = 120
 C102 - C101 - H101 = 120
 C103 - C102 - C101 = 120
 C103 - C102 - H102 = 120
 C101 - C102 - H102 = 120
 C104 - C103 - C102 = 120
 C104 - C103 - H103 = 120
 C102 - C103 - H103 = 120
 C103 - C104 - C105 = 120
 C103 - C104 - H104 = 120
 C105 - C104 - H104 = 120
 C104 - C105 - C100 = 120
 C104 - C105 - H105 = 120
 C100 - C105 - H105 = 120
 C111 - C110 - C115 = 120
 C111 - C110 - H110 = 120
 C115 - C110 - H110 = 120
 C110 - C111 - C112 = 120
 C110 - C111 - H111 = 120
 C112 - C111 - H111 = 120
 C113 - C112 - C111 = 120
 C113 - C112 - H112 = 120
 C111 - C112 - H112 = 120
 C112 - C113 - C114 = 120
 C112 - C113 - H113 = 120
 C114 - C113 - H113 = 120
 C113 - C114 - C115 = 120
 C113 - C114 - H114 = 120
 C115 - C114 - H114 = 120
 C114 - C115 - C110 = 120
 C114 - C115 - H115 = 120
 C110 - C115 - H115 = 120

Torsion angles [°]

N3 - Fe1 - N1 - C4 = -101.5 (7)
 N2 - Fe1 - N1 - C4 = -17.0 (5)
 N4 - Fe1 - N1 - C4 = 178.9 (5)
 N8 - Fe1 - N1 - C4 = 76.0 (5)
 N3 - Fe1 - N1 - C1 = 90.4 (8)
 N2 - Fe1 - N1 - C1 = 174.9 (5)
 N4 - Fe1 - N1 - C1 = 10.9 (5)
 N8 - Fe1 - N1 - C1 = -92.0 (5)
 N1 - Fe1 - N2 - C6 = 8.4 (5)
 N3 - Fe1 - N2 - C6 = 170.5 (4)

N4	-	Fe1	-	N2	-	C6	=	93.6(8)
N8	-	Fe1	-	N2	-	C6	=	-85.2(4)
N1	-	Fe1	-	N2	-	C9	=	-168.2(4)
N3	-	Fe1	-	N2	-	C9	=	-6.1(4)
N4	-	Fe1	-	N2	-	C9	=	-82.9(7)
N8	-	Fe1	-	N2	-	C9	=	98.2(4)
N1	-	Fe1	-	N3	-	C14	=	-91.3(7)
N2	-	Fe1	-	N3	-	C14	=	-176.1(4)
N4	-	Fe1	-	N3	-	C14	=	-11.7(4)
N8	-	Fe1	-	N3	-	C14	=	91.2(4)
N1	-	Fe1	-	N3	-	C11	=	98.7(6)
N2	-	Fe1	-	N3	-	C11	=	13.8(4)
N4	-	Fe1	-	N3	-	C11	=	178.3(4)
N8	-	Fe1	-	N3	-	C11	=	-78.8(4)
N1	-	Fe1	-	N4	-	C16	=	167.3(4)
N3	-	Fe1	-	N4	-	C16	=	5.0(4)
N2	-	Fe1	-	N4	-	C16	=	81.9(7)
N8	-	Fe1	-	N4	-	C16	=	-99.3(4)
N1	-	Fe1	-	N4	-	C19	=	-5.1(5)
N3	-	Fe1	-	N4	-	C19	=	-167.4(5)
N2	-	Fe1	-	N4	-	C19	=	-90.5(8)
N8	-	Fe1	-	N4	-	C19	=	88.2(5)
C4	-	N1	-	C1	-	C20	=	177.8(6)
Fe1	-	N1	-	C1	-	C20	=	-12.4(9)
C4	-	N1	-	C1	-	C2	=	0.1(7)
Fe1	-	N1	-	C1	-	C2	=	169.9(5)
N1	-	C1	-	C2	-	C3	=	-1.5(8)
C20	-	C1	-	C2	-	C3	=	-179.2(7)
C1	-	C2	-	C3	-	C4	=	2.2(8)
C1	-	N1	-	C4	-	C5	=	-174.1(6)
Fe1	-	N1	-	C4	-	C5	=	15.7(9)
C1	-	N1	-	C4	-	C3	=	1.3(7)
Fe1	-	N1	-	C4	-	C3	=	-168.9(4)
C2	-	C3	-	C4	-	N1	=	-2.2(8)
C2	-	C3	-	C4	-	C5	=	173.2(7)
N1	-	C4	-	C5	-	C6	=	0.8(11)
C3	-	C4	-	C5	-	C6	=	-173.8(7)
N1	-	C4	-	C5	-	C74	=	175.9(6)
C3	-	C4	-	C5	-	C74	=	1.3(10)
C9	-	N2	-	C6	-	C5	=	-179.9(5)
Fe1	-	N2	-	C6	-	C5	=	3.0(8)
C9	-	N2	-	C6	-	C7	=	-0.8(6)
Fe1	-	N2	-	C6	-	C7	=	-177.9(4)
C4	-	C5	-	C6	-	N2	=	-10.9(10)
C74	-	C5	-	C6	-	N2	=	174.1(5)
C4	-	C5	-	C6	-	C7	=	170.1(6)
C74	-	C5	-	C6	-	C7	=	-4.9(9)
N2	-	C6	-	C7	-	C8	=	1.8(6)
C5	-	C6	-	C7	-	C8	=	-179.1(6)
C6	-	C7	-	C8	-	C9	=	-2.0(6)
C6	-	N2	-	C9	-	C10	=	-179.8(5)

Fe1 - N2 - C9 - C10 = -2.7 (7)
 C6 - N2 - C9 - C8 = -0.4 (6)
 Fe1 - N2 - C9 - C8 = 176.7 (3)
 C7 - C8 - C9 - N2 = 1.6 (6)
 C7 - C8 - C9 - C10 = -179.1 (5)
 N2 - C9 - C10 - C11 = 7.4 (8)
 C8 - C9 - C10 - C11 = -171.9 (5)
 N2 - C9 - C10 - C60 = -176.2 (5)
 C8 - C9 - C10 - C60 = 4.6 (8)
 C14 - N3 - C11 - C10 = 173.7 (5)
 Fe1 - N3 - C11 - C10 = -14.5 (7)
 C14 - N3 - C11 - C12 = -3.2 (5)
 Fe1 - N3 - C11 - C12 = 168.6 (3)
 C9 - C10 - C11 - N3 = 1.9 (8)
 C60 - C10 - C11 - N3 = -174.7 (5)
 C9 - C10 - C11 - C12 = 178.3 (5)
 C60 - C10 - C11 - C12 = 1.7 (7)
 N3 - C11 - C12 - C13 = 2.7 (6)
 C10 - C11 - C12 - C13 = -174.3 (5)
 C11 - C12 - C13 - C14 = -1.1 (6)
 C11 - N3 - C14 - C15 = -174.7 (5)
 Fe1 - N3 - C14 - C15 = 13.7 (7)
 C11 - N3 - C14 - C13 = 2.5 (5)
 Fe1 - N3 - C14 - C13 = -169.0 (3)
 C12 - C13 - C14 - N3 = -0.9 (6)
 C12 - C13 - C14 - C15 = 176.3 (5)
 N3 - C14 - C15 - C16 = -5.1 (8)
 C13 - C14 - C15 - C16 = 178.1 (5)
 N3 - C14 - C15 - C35 = 164.1 (4)
 C13 - C14 - C15 - C35 = -12.7 (7)
 C19 - N4 - C16 - C15 = 174.1 (5)
 Fe1 - N4 - C16 - C15 = 0.4 (7)
 C19 - N4 - C16 - C17 = -2.7 (6)
 Fe1 - N4 - C16 - C17 = -176.3 (4)
 C14 - C15 - C16 - N4 = -2.4 (8)
 C35 - C15 - C16 - N4 = -171.6 (5)
 C14 - C15 - C16 - C17 = 173.8 (5)
 C35 - C15 - C16 - C17 = 4.6 (8)
 N4 - C16 - C17 - C18 = 1.4 (7)
 C15 - C16 - C17 - C18 = -175.3 (6)
 C16 - C17 - C18 - C19 = 0.4 (8)
 C16 - N4 - C19 - C20 = -173.5 (6)
 Fe1 - N4 - C19 - C20 = 0.3 (9)
 C16 - N4 - C19 - C18 = 2.9 (6)
 Fe1 - N4 - C19 - C18 = 176.7 (4)
 C17 - C18 - C19 - N4 = -2.1 (8)
 C17 - C18 - C19 - C20 = 174.4 (6)
 N4 - C19 - C20 - C1 = 1.9 (11)
 C18 - C19 - C20 - C1 = -174.0 (7)
 N4 - C19 - C20 - C21 = 171.1 (6)
 C18 - C19 - C20 - C21 = -4.8 (10)

N1 - C1 - C20 - C19 = 4.4(11)
 C2 - C1 - C20 - C19 = -178.3(7)
 N1 - C1 - C20 - C21 = -164.8(6)
 C2 - C1 - C20 - C21 = 12.6(10)
 C19 - C20 - C21 - C26 = 84.4(9)
 C1 - C20 - C21 - C26 = -105.4(8)
 C19 - C20 - C21 - C22 = -90.4(7)
 C1 - C20 - C21 - C22 = 79.8(8)
 C26 - C21 - C22 - C23 = 0.2(12)
 C20 - C21 - C22 - C23 = 175.5(8)
 C21 - C22 - C23 - C24 = -0.5(15)
 C22 - C23 - C24 - C25 = 1.3(18)
 C23 - C24 - C25 - C26 = -1.9(19)
 C22 - C21 - C26 - N5 = 179.7(7)
 C20 - C21 - C26 - N5 = 4.9(11)
 C22 - C21 - C26 - C25 = -0.8(11)
 C20 - C21 - C26 - C25 = -175.7(7)
 C24 - C25 - C26 - C21 = 1.7(15)
 C24 - C25 - C26 - N5 = -178.9(10)
 C21 - C26 - N5 - C27A = 159.9(10)
 C25 - C26 - N5 - C27A = -19.5(15)
 C21 - C26 - N5 - C27B = -162(3)
 C25 - C26 - N5 - C27B = 19(3)
 C27B - N5 - C27A - O1A = -107(3)
 C26 - N5 - C27A - O1A = 15(2)
 C27B - N5 - C27A - C28A = 68(2)
 C26 - N5 - C27A - C28A = -169.6(10)
 O1A - C27A - C28A - C29A = 146.7(14)
 N5 - C27A - C28A - C29A = -28(2)
 O1A - C27A - C28A - C33A = -31(2)
 N5 - C27A - C28A - C33A = 154.1(10)
 C33A - C28A - C29A - C30A = 0
 C27A - C28A - C29A - C30A = -177.6(18)
 C28A - C29A - C30A - C31A = 0
 C28A - C29A - C30A - C34 = -152.4(13)
 C29A - C30A - C31A - C32A = 0
 C34 - C30A - C31A - C32A = 154.9(12)
 C30A - C31A - C32A - C33A = 0
 C31A - C32A - C33A - C28A = 0
 C29A - C28A - C33A - C32A = 0
 C27A - C28A - C33A - C32A = 178.0(16)
 C27A - N5 - C27B - O1B = 78(6)
 C26 - N5 - C27B - O1B = -4(6)
 C27A - N5 - C27B - C28B = -95(3)
 C26 - N5 - C27B - C28B = -176.4(19)
 O1B - C27B - C28B - C29B = 155(3)
 N5 - C27B - C28B - C29B = -32(4)
 O1B - C27B - C28B - C33B = -21(4)
 N5 - C27B - C28B - C33B = 153(3)
 C33B - C28B - C29B - C30B = 0
 C27B - C28B - C29B - C30B = -175.8(19)

$C28B - C29B - C30B - C31B = 0$
 $C28B - C29B - C30B - C34 = -164.3(13)$
 $C29B - C30B - C31B - C32B = 0$
 $C34 - C30B - C31B - C32B = 162.6(14)$
 $C30B - C31B - C32B - C33B = 0$
 $C31B - C32B - C33B - C28B = 0$
 $C29B - C28B - C33B - C32B = 0$
 $C27B - C28B - C33B - C32B = 176(2)$
 $C29B - C30B - C34 - N7 = -69.6(12)$
 $C31B - C30B - C34 - N7 = 126.9(11)$
 $C29B - C30B - C34 - C30A = 53(2)$
 $C31B - C30B - C34 - C30A = -110(3)$
 $C31A - C30A - C34 - N7 = 156.8(10)$
 $C29A - C30A - C34 - N7 = -49.0(15)$
 $C31A - C30A - C34 - C30B = 96(2)$
 $C29A - C30A - C34 - C30B = -110(3)$
 $C16 - C15 - C35 - C40 = -70.0(7)$
 $C14 - C15 - C35 - C40 = 119.8(6)$
 $C16 - C15 - C35 - C36 = 109.3(7)$
 $C14 - C15 - C35 - C36 = -60.9(7)$
 $C40 - C35 - C36 - C37 = 2.8(11)$
 $C15 - C35 - C36 - C37 = -176.5(7)$
 $C35 - C36 - C37 - C38 = 0.1(14)$
 $C36 - C37 - C38 - C39 = -2.8(15)$
 $C37 - C38 - C39 - C40 = 2.6(14)$
 $C36 - C35 - C40 - C39 = -3.1(9)$
 $C15 - C35 - C40 - C39 = 176.2(6)$
 $C36 - C35 - C40 - N6 = 175.5(5)$
 $C15 - C35 - C40 - N6 = -5.2(8)$
 $C38 - C39 - C40 - C35 = 0.5(10)$
 $C38 - C39 - C40 - N6 = -178.1(7)$
 $C35 - C40 - N6 - C41 = 156.9(6)$
 $C39 - C40 - N6 - C41 = -24.6(8)$
 $C40 - N6 - C41 - O2 = -4.0(11)$
 $C40 - N6 - C41 - C42B = -168.0(9)$
 $C40 - N6 - C41 - C42A = 161.0(7)$
 $O2 - C41 - C42B - C43B = 172(2)$
 $N6 - C41 - C42B - C43B = -23(3)$
 $C42A - C41 - C42B - C43B = 64(3)$
 $O2 - C41 - C42B - C47B = -20.0(18)$
 $N6 - C41 - C42B - C47B = 145.0(12)$
 $C42A - C41 - C42B - C47B = -128(2)$
 $C47B - C42B - C43B - C44B = 21(4)$
 $C41 - C42B - C43B - C44B = -170.3(19)$
 $C42B - C43B - C44B - C45B = -26(3)$
 $C42B - C43B - C44B - C48 = -160(3)$
 $C48 - C44B - C45B - C46B = 166.6(18)$
 $C43B - C44B - C45B - C46B = 18(3)$
 $C44B - C45B - C46B - C47B = -11(3)$
 $C45B - C46B - C47B - C42B = 5(3)$
 $C43B - C42B - C47B - C46B = -8(3)$

C41 - C42B - C47B - C46B = 179.9(14)
O2 - C41 - C42A - C43A = -139.4(8)
N6 - C41 - C42A - C43A = 55.4(8)
C42B - C41 - C42A - C43A = -50.2(16)
O2 - C41 - C42A - C47A = 32.1(13)
N6 - C41 - C42A - C47A = -133.1(7)
C42B - C41 - C42A - C47A = 121(2)
C47A - C42A - C43A - C44A = 0
C41 - C42A - C43A - C44A = 171.7(9)
C42A - C43A - C44A - C48 = -164(2)
C42A - C43A - C44A - C45A = 0
C48 - C44A - C45A - C46A = 168.7(16)
C43A - C44A - C45A - C46A = 0
C44A - C45A - C46A - C47A = 0
C45A - C46A - C47A - C42A = 0
C43A - C42A - C47A - C46A = 0
C41 - C42A - C47A - C46A = -171.2(10)
C45B - C44B - C48 - C44A = 171(4)
C43B - C44B - C48 - C44A = -53(3)
C45B - C44B - C48 - N7 = -107(2)
C43B - C44B - C48 - N7 = 28(4)
C45A - C44A - C48 - C44B = -87(3)
C43A - C44A - C48 - C44B = 79(3)
C45A - C44A - C48 - N7 = 165.0(16)
C43A - C44A - C48 - N7 = -29(3)
C30B - C34 - N7 - C49 = -174.9(9)
C30A - C34 - N7 - C49 = 170.6(10)
C30B - C34 - N7 - C48 = -69.9(16)
C30A - C34 - N7 - C48 = -84.5(16)
C44B - C48 - N7 - C34 = 150(2)
C44A - C48 - N7 - C34 = 173.5(17)
C44B - C48 - N7 - C49 = -96(2)
C44A - C48 - N7 - C49 = -73(2)
N1 - Fe1 - N8 - C51 = 116.7(5)
N3 - Fe1 - N8 - C51 = -64.1(5)
N2 - Fe1 - N8 - C51 = -153.2(5)
N4 - Fe1 - N8 - C51 = 27.1(5)
N1 - Fe1 - N8 - C52 = -66.9(4)
N3 - Fe1 - N8 - C52 = 112.3(4)
N2 - Fe1 - N8 - C52 = 23.2(4)
N4 - Fe1 - N8 - C52 = -156.4(4)
C34 - N7 - C49 - C50 = -67.4(10)
C48 - N7 - C49 - C50 = 174.6(7)
N7 - C49 - C50 - C51 = -66.4(10)
N7 - C49 - C50 - C54 = 97.2(12)
C52 - N8 - C51 - C50 = -4.5(12)
Fe1 - N8 - C51 - C50 = 172.0(7)
C54 - C50 - C51 - N8 = 9.5(13)
C49 - C50 - C51 - N8 = 176.1(8)
C51 - N8 - C52 - C53 = -0.9(10)
Fe1 - N8 - C52 - C53 = -177.4(6)

N8 - C52 - C53 - C54 = -0.3 (11)
 C52 - C53 - C54 - C50 = 6.4 (14)
 C51 - C50 - C54 - C53 = -10.3 (14)
 C49 - C50 - C54 - C53 = -174.7 (10)
 C11 - C10 - C60 - C65 = -111.5 (6)
 C9 - C10 - C60 - C65 = 71.7 (7)
 C11 - C10 - C60 - C61 = 65.6 (7)
 C9 - C10 - C60 - C61 = -111.1 (6)
 C65 - C60 - C61 - C62 = 1.9 (8)
 C10 - C60 - C61 - C62 = -175.3 (5)
 C65 - C60 - C61 - N9 = -179.1 (6)
 C10 - C60 - C61 - N9 = 3.6 (7)
 N9 - C61 - C62 - C63 = 179.8 (5)
 C60 - C61 - C62 - C63 = -1.3 (8)
 C61 - C62 - C63 - C64 = 1.7 (10)
 C62 - C63 - C64 - C65 = -2.7 (12)
 C63 - C64 - C65 - C60 = 3.4 (13)
 C61 - C60 - C65 - C64 = -3.0 (11)
 C10 - C60 - C65 - C64 = 174.3 (7)
 C62 - C61 - N9 - C66 = 39.8 (8)
 C60 - C61 - N9 - C66 = -139.2 (6)
 C61 - N9 - C66 - O3 = -16.2 (9)
 C61 - N9 - C66 - C67 = 162.1 (5)
 O3 - C66 - C67 - C68 = 158.0 (6)
 N9 - C66 - C67 - C68 = -20.3 (7)
 O3 - C66 - C67 - C72 = -21.8 (8)
 N9 - C66 - C67 - C72 = 159.9 (5)
 C72 - C67 - C68 - C69 = -2.0 (8)
 C66 - C67 - C68 - C69 = 178.2 (5)
 C67 - C68 - C69 - C70 = 2.3 (8)
 C67 - C68 - C69 - C73 = -178.3 (5)
 C68 - C69 - C70 - C71 = -0.6 (8)
 C73 - C69 - C70 - C71 = 179.9 (5)
 C69 - C70 - C71 - C72 = -1.3 (10)
 C70 - C71 - C72 - C67 = 1.5 (10)
 C68 - C67 - C72 - C71 = 0.0 (9)
 C66 - C67 - C72 - C71 = 179.8 (6)
 C68 - C69 - C73 - C88 = 89.6 (6)
 C70 - C69 - C73 - C88 = -91.0 (6)
 C6 - C5 - C74 - C75 = 106.5 (7)
 C4 - C5 - C74 - C75 = -69.1 (8)
 C6 - C5 - C74 - C79 = -75.8 (8)
 C4 - C5 - C74 - C79 = 108.6 (7)
 C79 - C74 - C75 - C76 = -1.7 (9)
 C5 - C74 - C75 - C76 = 176.0 (6)
 C79 - C74 - C75 - N10 = 178.6 (6)
 C5 - C74 - C75 - N10 = -3.7 (9)
 C74 - C75 - C76 - C77 = 0.3 (10)
 N10 - C75 - C76 - C77 = 180.0 (6)
 C75 - C76 - C77 - C78 = 0.4 (11)
 C76 - C77 - C78 - C79 = 0.4 (11)

C77 - C78 - C79 - C74 = -1.9(11)
C75 - C74 - C79 - C78 = 2.5(10)
C5 - C74 - C79 - C78 = -175.1(6)
C74 - C75 - N10 - C80 = 132.7(6)
C76 - C75 - N10 - C80 = -47.1(9)
C75 - N10 - C80 - O4 = 19.7(9)
C75 - N10 - C80 - C81 = -161.4(5)
O4 - C80 - C81 - C86 = 27.3(7)
N10 - C80 - C81 - C86 = -151.6(5)
O4 - C80 - C81 - C82 = -151.2(5)
N10 - C80 - C81 - C82 = 29.9(7)
C86 - C81 - C82 - C83 = 1.1(8)
C80 - C81 - C82 - C83 = 179.5(5)
C81 - C82 - C83 - C84 = -1.8(8)
C81 - C82 - C83 - C87 = 178.3(5)
C82 - C83 - C84 - C85 = 1.5(8)
C87 - C83 - C84 - C85 = -178.6(5)
C83 - C84 - C85 - C86 = -0.6(9)
C82 - C81 - C86 - C85 = -0.1(8)
C80 - C81 - C86 - C85 = -178.7(5)
C84 - C85 - C86 - C81 = -0.1(8)
C84 - C83 - C87 - C88 = 86.2(6)
C82 - C83 - C87 - C88 = -93.9(6)
C69 - C73 - C88 - C89 = 63.7(6)
C69 - C73 - C88 - C92 = -59.4(6)
C69 - C73 - C88 - C87 = -174.9(4)
C83 - C87 - C88 - C89 = -68.3(6)
C83 - C87 - C88 - C92 = 54.8(5)
C83 - C87 - C88 - C73 = 173.2(4)
C92 - C88 - C89 - O5 = 33.0(8)
C73 - C88 - C89 - O5 = -88.9(7)
C87 - C88 - C89 - O5 = 152.5(6)
C92 - C88 - C89 - O6 = -154.3(5)
C73 - C88 - C89 - O6 = 83.7(6)
C87 - C88 - C89 - O6 = -34.9(6)
O5 - C89 - O6 - C90 = -3.6(10)
C88 - C89 - O6 - C90 = -176.4(6)
C89 - O6 - C90 - C91 = 96.4(11)
C89 - C88 - C92 - O7 = -156.6(7)
C73 - C88 - C92 - O7 = -36.4(9)
C87 - C88 - C92 - O7 = 80.3(7)
C89 - C88 - C92 - O8A = 28.1(7)
C73 - C88 - C92 - O8A = 148.3(5)
C87 - C88 - C92 - O8A = -95.1(6)
O7 - C92 - O8A - C93A = -9.5(11)
C88 - C92 - O8A - C93A = 165.9(8)
C92 - O8A - C93A - C94A = -163.6(9)
C105 - C100 - C101 - C102 = 0
C100 - C101 - C102 - C103 = 0
C101 - C102 - C103 - C104 = 0
C102 - C103 - C104 - C105 = 0

$C103 - C104 - C105 - C100 = 0$
 $C101 - C100 - C105 - C104 = 0$
 $C115 - C110 - C111 - C112 = 0$
 $C110 - C111 - C112 - C113 = 0$
 $C111 - C112 - C113 - C114 = 0$
 $C112 - C113 - C114 - C115 = 0$
 $C113 - C114 - C115 - C110 = 0$
 $C111 - C110 - C115 - C114 = 0$