Jonathan R. Frisch, Ryan McDonnell, Elena V. Rybak-Akimova, and Lawrence Que, Jr.

Factors Affecting the Carboxylate Shift Upon Formation of Nonheme Diiron-O2 Adducts

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'C72 H78 B F3 Fe2 N11 O6 P S'

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loop_

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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loop_

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

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_computing_publication_material 'Bruker SHELXTL'

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and

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

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_refine_ls_weighting_scheme calc

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'calc w=1/[\s^2^(Fo^2^)+(0.0277P)^2^+6.8346P] where P=(Fo^2^+2Fc^2^)/3'

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loop_

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Fe2 Fe 0.15961(2) 0.84911(3) 0.936645(13) 0.02362(10) Uani 1 1 d . . .

S1 S 0.11526(6) 0.71341(6) 0.21079(3) 0.0405(2) Uani 1 1 d . . .

P1 P 0.32357(5) 0.79822(5) 1.02154(3) 0.03006(18) Uani 1 1 d . . .

F1 F 0.15335(18) 0.70303(16) 0.12652(8) 0.0817(8) Uani 1 1 d . . .

F2 F 0.21044(15) 0.80823(16) 0.16888(8) 0.0741(7) Uani 1 1 d . . .

F3 F 0.25852(18) 0.6824(2) 0.18648(11) 0.1179(12) Uani 1 1 d . . .

O1 O 0.16432(12) 0.72748(11) 0.91575(6) 0.0264(4) Uani 1 1 d . . .

O2 O 0.31126(12) 0.70464(13) 1.00889(7) 0.0329(5) Uani 1 1 d . . .

O3 O 0.24890(12) 0.85555(13) 0.99910(7) 0.0321(5) Uani 1 1 d . . .

O4 O 0.0971(2) 0.62397(16) 0.20837(10) 0.0777(9) Uani 1 1 d . . .

O5 O 0.16539(17) 0.74259(18) 0.25648(8) 0.0652(8) Uani 1 1 d . . .

O6 O 0.04499(16) 0.76655(18) 0.18923(9) 0.0681(8) Uani 1 1 d . . .

N1 N 0.20746(15) 0.58063(15) 0.87211(8) 0.0281(5) Uani 1 1 d . . .

N2 N 0.05737(14) 0.85281(15) 0.86176(8) 0.0260(5) Uani 1 1 d . . .

N3 N 0.19337(15) 0.53689(15) 0.96303(8) 0.0311(6) Uani 1 1 d . . .

N4 N 0.12367(16) 0.41502(16) 0.93894(9) 0.0367(6) Uani 1 1 d . . .

N5 N 0.36925(15) 0.61181(15) 0.92268(8) 0.0304(6) Uani 1 1 d . . .

N6 N 0.43010(15) 0.60066(15) 0.86000(8) 0.0306(6) Uani 1 1 d . . .

N7 N 0.19659(14) 0.95391(15) 0.90026(8) 0.0272(5) Uani 1 1 d . . .

N8 N 0.19359(15) 1.02656(15) 0.83251(8) 0.0286(6) Uani 1 1 d . . .

N9 N 0.04350(14) 0.86964(15) 0.95486(8) 0.0266(5) Uani 1 1 d . . .

N10 N -0.09777(14) 0.89162(15) 0.93722(8) 0.0300(6) Uani 1 1 d . . .

N11 N 0.3291(2) 0.8047(2) 0.87881(14) 0.0631(9) Uani 1 1 d . . .

C1 C 0.13149(18) 0.71622(18) 0.86506(9) 0.0271(6) Uani 1 1 d . . .

H1A H 0.1721 0.7430 0.8476 0.033 Uiso 1 1 calc R . .

C2 C 0.12368(18) 0.62239(18) 0.85271(10) 0.0305(7) Uani 1 1 d . . .

H2A H 0.0794 0.5959 0.8670 0.037 Uiso 1 1 calc R . .

H2B H 0.1065 0.6149 0.8172 0.037 Uiso 1 1 calc R . .

C3 C 0.04548(18) 0.76110(17) 0.84979(10) 0.0283(7) Uani 1 1 d . . .

H3A H 0.0221 0.7540 0.8146 0.034 Uiso 1 1 calc R . .

H3B H 0.0044 0.7357 0.8669 0.034 Uiso 1 1 calc R . .

C4 C 0.1986(2) 0.48889(18) 0.88154(11) 0.0340(7) Uani 1 1 d . . .

H4A H 0.2538 0.4593 0.8837 0.041 Uiso 1 1 calc R . .

H4B H 0.1551 0.4628 0.8549 0.041 Uiso 1 1 calc R . .

C5 C 0.17177(19) 0.47986(19) 0.92796(11) 0.0320(7) Uani 1 1 d . . .

C6 C 0.15652(19) 0.5079(2) 0.99983(11) 0.0341(7) Uani 1 1 d . . .

C7 C 0.1566(2) 0.5442(2) 1.04453(11) 0.0420(8) Uani 1 1 d . . .

H7A H 0.1870 0.5955 1.0550 0.050 Uiso 1 1 calc R . .

C8 C 0.1107(2) 0.5026(3) 1.07298(12) 0.0520(10) Uani 1 1 d . . .

H8A H 0.1088 0.5259 1.1035 0.062 Uiso 1 1 calc R . .

C9 C 0.0671(2) 0.4268(3) 1.05753(14) 0.0580(11) Uani 1 1 d . . .

H9A H 0.0358 0.4001 1.0780 0.070 Uiso 1 1 calc R . .

C10 C 0.0674(2) 0.3890(2) 1.01409(13) 0.0510(9) Uani 1 1 d . . .

H10A H 0.0381 0.3369 1.0042 0.061 Uiso 1 1 calc R . .

C11 C 0.1130(2) 0.4316(2) 0.98534(12) 0.0382(8) Uani 1 1 d . . .

C12 C 0.0905(2) 0.3420(2) 0.90734(13) 0.0508(9) Uani 1 1 d . . .

H12A H 0.0567 0.3637 0.8759 0.061 Uiso 1 1 calc R . .

H12B H 0.0518 0.3077 0.9223 0.061 Uiso 1 1 calc R . .

C13 C 0.1622(3) 0.2853(2) 0.89875(16) 0.0710(12) Uani 1 1 d . . .

H13A H 0.1378 0.2379 0.8775 0.107 Uiso 1 1 calc R . .

H13B H 0.1948 0.2626 0.9297 0.107 Uiso 1 1 calc R . .

H13C H 0.2002 0.3190 0.8836 0.107 Uiso 1 1 calc R . .

C14 C 0.26971(18) 0.59557(19) 0.84248(10) 0.0308(7) Uani 1 1 d . . .

H14A H 0.2556 0.6491 0.8237 0.037 Uiso 1 1 calc R . .

H14B H 0.2680 0.5477 0.8195 0.037 Uiso 1 1 calc R . .

C15 C 0.35681(19) 0.60216(18) 0.87539(10) 0.0293(7) Uani 1 1 d . . .

C16 C 0.45833(19) 0.61717(19) 0.93980(11) 0.0331(7) Uani 1 1 d . . .

C17 C 0.5084(2) 0.6261(2) 0.98646(12) 0.0446(9) Uani 1 1 d . . .

H17A H 0.4835 0.6300 1.0135 0.054 Uiso 1 1 calc R . .

C18 C 0.5960(2) 0.6289(3) 0.99177(13) 0.0559(10) Uani 1 1 d . . .

H18A H 0.6318 0.6353 1.0233 0.067 Uiso 1 1 calc R . .

C19 C 0.6338(2) 0.6226(2) 0.95270(14) 0.0536(10) Uani 1 1 d . . .

H19A H 0.6944 0.6252 0.9582 0.064 Uiso 1 1 calc R . .

C20 C 0.5853(2) 0.6125(2) 0.90623(12) 0.0425(8) Uani 1 1 d . . .

H20A H 0.6108 0.6071 0.8795 0.051 Uiso 1 1 calc R . .

C21 C 0.49690(19) 0.61070(19) 0.90055(11) 0.0336(7) Uani 1 1 d . . .

C22 C 0.4373(2) 0.5890(2) 0.81003(11) 0.0369(8) Uani 1 1 d . . .

H22A H 0.3976 0.5431 0.7948 0.044 Uiso 1 1 calc R . .

H22B H 0.4962 0.5704 0.8101 0.044 Uiso 1 1 calc R . .

C23 C 0.4170(2) 0.6697(2) 0.78032(12) 0.0424(8) Uani 1 1 d . . .

H23A H 0.4220 0.6585 0.7472 0.064 Uiso 1 1 calc R . .

H23B H 0.4574 0.7148 0.7947 0.064 Uiso 1 1 calc R . .

H23C H 0.3586 0.6881 0.7798 0.064 Uiso 1 1 calc R . .

C24 C 0.09528(18) 0.90002(18) 0.82725(10) 0.0289(7) Uani 1 1 d . . .

H24A H 0.0499 0.9316 0.8042 0.035 Uiso 1 1 calc R . .

H24B H 0.1221 0.8593 0.8086 0.035 Uiso 1 1 calc R . .

C25 C 0.16099(17) 0.96131(18) 0.85363(10) 0.0252(6) Uani 1 1 d . . .

C26 C 0.25728(17) 1.01980(18) 0.91061(10) 0.0267(6) Uani 1 1 d . . .

C27 C 0.31297(18) 1.04311(19) 0.95396(11) 0.0335(7) Uani 1 1 d . . .

H27A H 0.3150 1.0119 0.9828 0.040 Uiso 1 1 calc R . .

C28 C 0.3649(2) 1.1129(2) 0.95348(12) 0.0430(8) Uani 1 1 d . . .

H28A H 0.4024 1.1311 0.9827 0.052 Uiso 1 1 calc R . .

C29 C 0.3635(2) 1.1576(2) 0.91058(13) 0.0463(9) Uani 1 1 d . . .

H29A H 0.4011 1.2047 0.9114 0.056 Uiso 1 1 calc R . .

C30 C 0.30943(19) 1.1352(2) 0.86736(12) 0.0393(8) Uani 1 1 d . . .

H30A H 0.3085 1.1658 0.8384 0.047 Uiso 1 1 calc R . .

C31 C 0.25598(18) 1.06536(19) 0.86831(10) 0.0301(7) Uani 1 1 d . . .

C32 C 0.1662(2) 1.0545(2) 0.78174(10) 0.0364(8) Uani 1 1 d . . .

H32A H 0.1446 1.0045 0.7612 0.044 Uiso 1 1 calc R . .

H32B H 0.2162 1.0776 0.7712 0.044 Uiso 1 1 calc R . .

C33 C 0.0976(2) 1.1215(2) 0.77484(12) 0.0461(9) Uani 1 1 d . . .

H33A H 0.0814 1.1383 0.7407 0.069 Uiso 1 1 calc R . .

H33B H 0.1191 1.1716 0.7947 0.069 Uiso 1 1 calc R . .

H33C H 0.0475 1.0984 0.7845 0.069 Uiso 1 1 calc R . .

C34 C -0.02182(18) 0.89327(19) 0.86861(10) 0.0297(7) Uani 1 1 d . . .

H34A H -0.0723 0.8662 0.8470 0.036 Uiso 1 1 calc R . .

H34B H -0.0219 0.9548 0.8605 0.036 Uiso 1 1 calc R . .

C35 C -0.02636(18) 0.88251(18) 0.92021(10) 0.0268(6) Uani 1 1 d . . .

C36 C 0.01643(18) 0.87143(17) 0.99799(10) 0.0271(7) Uani 1 1 d . . .

C37 C 0.06302(19) 0.86131(19) 1.04516(10) 0.0330(7) Uani 1 1 d . . .

H37A H 0.1224 0.8485 1.0525 0.040 Uiso 1 1 calc R . .

C38 C 0.0189(2) 0.8708(2) 1.08121(11) 0.0376(8) Uani 1 1 d . . .

H38A H 0.0489 0.8653 1.1141 0.045 Uiso 1 1 calc R . .

C39 C -0.0681(2) 0.8881(2) 1.07020(12) 0.0407(8) Uani 1 1 d . . .

H39A H -0.0960 0.8952 1.0959 0.049 Uiso 1 1 calc R . .

C40 C -0.1159(2) 0.8954(2) 1.02312(11) 0.0392(8) Uani 1 1 d . . .

H40A H -0.1758 0.9057 1.0158 0.047 Uiso 1 1 calc R . .

C41 C -0.07129(18) 0.88672(19) 0.98735(10) 0.0307(7) Uani 1 1 d . . .

C42 C -0.18739(18) 0.8999(2) 0.90989(11) 0.0371(8) Uani 1 1 d . . .

H42A H -0.2238 0.8622 0.9246 0.044 Uiso 1 1 calc R . .

H42B H -0.1921 0.8803 0.8763 0.044 Uiso 1 1 calc R . .

C43 C -0.2201(2) 0.9894(2) 0.90893(12) 0.0465(9) Uani 1 1 d . . .

H43A H -0.2796 0.9913 0.8901 0.070 Uiso 1 1 calc R . .

H43B H -0.1848 1.0270 0.8940 0.070 Uiso 1 1 calc R . .

H43C H -0.2175 1.0086 0.9420 0.070 Uiso 1 1 calc R . .

C44 C 0.3436(2) 0.8085(2) 1.08554(11) 0.0501(9) Uani 1 1 d . . .

H44A H 0.2939 0.7880 1.0966 0.075 Uiso 1 1 calc R . .

H44B H 0.3541 0.8688 1.0945 0.075 Uiso 1 1 calc R . .

H44C H 0.3940 0.7745 1.1007 0.075 Uiso 1 1 calc R . .

C45 C 0.4168(2) 0.8359(2) 1.00436(15) 0.0588(11) Uani 1 1 d . . .

H45A H 0.4087 0.8306 0.9693 0.088 Uiso 1 1 calc R . .

H45B H 0.4664 0.8017 1.0206 0.088 Uiso 1 1 calc R . .

H45C H 0.4266 0.8960 1.0138 0.088 Uiso 1 1 calc R . .

C46 C 0.61571(18) 0.62172(18) 0.31058(10) 0.0280(7) Uani 1 1 d . . .

C47 C 0.60697(19) 0.6681(2) 0.35136(11) 0.0359(7) Uani 1 1 d . . .

H47A H 0.6273 0.7253 0.3550 0.043 Uiso 1 1 calc R . .

C48 C 0.5697(2) 0.6337(2) 0.38672(11) 0.0448(9) Uani 1 1 d . . .

H48A H 0.5651 0.6676 0.4137 0.054 Uiso 1 1 calc R . .

C49 C 0.5395(2) 0.5510(2) 0.38284(12) 0.0442(9) Uani 1 1 d . . .

H49A H 0.5147 0.5272 0.4071 0.053 Uiso 1 1 calc R . .

C50 C 0.54605(19) 0.5032(2) 0.34309(11) 0.0395(8) Uani 1 1 d . . .

H50A H 0.5253 0.4461 0.3397 0.047 Uiso 1 1 calc R . .

C51 C 0.58288(18) 0.53842(19) 0.30792(10) 0.0325(7) Uani 1 1 d . . .

H51A H 0.5859 0.5043 0.2808 0.039 Uiso 1 1 calc R . .

C52 C 0.59359(18) 0.64385(17) 0.21439(10) 0.0257(6) Uani 1 1 d . . .

C53 C 0.50457(19) 0.64134(19) 0.20820(11) 0.0346(7) Uani 1 1 d . . .

H53A H 0.4815 0.6504 0.2356 0.041 Uiso 1 1 calc R . .

C54 C 0.4486(2) 0.6262(2) 0.16390(11) 0.0380(8) Uani 1 1 d . . .

H54A H 0.3886 0.6251 0.1616 0.046 Uiso 1 1 calc R . .

C55 C 0.4795(2) 0.61268(19) 0.12301(11) 0.0358(7) Uani 1 1 d . . .

H55A H 0.4416 0.6015 0.0926 0.043 Uiso 1 1 calc R . .

C56 C 0.5664(2) 0.6158(2) 0.12750(11) 0.0376(8) Uani 1 1 d . . .

H56A H 0.5888 0.6073 0.0998 0.045 Uiso 1 1 calc R . .

C57 C 0.62164(19) 0.63136(19) 0.17184(10) 0.0323(7) Uani 1 1 d . . .

H57A H 0.6813 0.6337 0.1735 0.039 Uiso 1 1 calc R . .

C58 C 0.75114(18) 0.61615(18) 0.26647(10) 0.0283(7) Uani 1 1 d . . .

C59 C 0.77251(19) 0.53075(19) 0.27891(10) 0.0324(7) Uani 1 1 d . . .

H59A H 0.7362 0.4983 0.2941 0.039 Uiso 1 1 calc R . .

C60 C 0.8454(2) 0.4919(2) 0.26972(11) 0.0383(8) Uani 1 1 d . . .

H60A H 0.8573 0.4337 0.2783 0.046 Uiso 1 1 calc R . .

C61 C 0.8999(2) 0.5373(2) 0.24835(11) 0.0398(8) Uani 1 1 d . . .

H61A H 0.9487 0.5104 0.2415 0.048 Uiso 1 1 calc R . .

C62 C 0.88300(19) 0.6225(2) 0.23693(11) 0.0368(8) Uani 1 1 d . . .

H62A H 0.9209 0.6549 0.2229 0.044 Uiso 1 1 calc R . .

C63 C 0.81049(18) 0.6600(2) 0.24614(10) 0.0326(7) Uani 1 1 d . . .

H63A H 0.8003 0.7187 0.2383 0.039 Uiso 1 1 calc R . .

C64 C 0.67382(18) 0.76521(18) 0.27673(10) 0.0292(7) Uani 1 1 d . . .

C65 C 0.7409(2) 0.7964(2) 0.31327(11) 0.0383(8) Uani 1 1 d . . .

H65A H 0.7809 0.7566 0.3310 0.046 Uiso 1 1 calc R . .

C66 C 0.7518(2) 0.8821(2) 0.32492(12) 0.0439(8) Uani 1 1 d . . .

H66A H 0.7984 0.8999 0.3501 0.053 Uiso 1 1 calc R . .

C67 C 0.6952(2) 0.9420(2) 0.30008(12) 0.0438(9) Uani 1 1 d . . .

H67A H 0.7018 1.0010 0.3081 0.053 Uiso 1 1 calc R . .

C68 C 0.6292(2) 0.9143(2) 0.26348(12) 0.0404(8) Uani 1 1 d . . .

H68A H 0.5900 0.9548 0.2457 0.049 Uiso 1 1 calc R . .

C69 C 0.61872(19) 0.82771(18) 0.25187(11) 0.0324(7) Uani 1 1 d . . .

H69A H 0.5725 0.8107 0.2262 0.039 Uiso 1 1 calc R . .

C70 C 0.1877(2) 0.7272(3) 0.17153(13) 0.0513(10) Uani 1 1 d . . .

C71 C 0.3374(2) 0.8419(2) 0.84619(15) 0.0459(9) Uani 1 1 d . . .

C72 C 0.3473(2) 0.8892(2) 0.80438(13) 0.0546(10) Uani 1 1 d . . .

H72C H 0.3506 0.9505 0.8118 0.082 Uiso 1 1 calc R . .

H72B H 0.2982 0.8783 0.7773 0.082 Uiso 1 1 calc R . .

H72A H 0.4000 0.8711 0.7955 0.082 Uiso 1 1 calc R . .

B1 B 0.6591(2) 0.6620(2) 0.26777(12) 0.0288(8) Uani 1 1 d . . .

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

Fe1 0.0257(2) 0.0287(2) 0.0237(2) -0.00292(18) 0.00498(17) 0.00128(18)

Fe2 0.0224(2) 0.0257(2) 0.0215(2) -0.00101(18) 0.00262(16) -0.00042(18)

S1 0.0507(5) 0.0439(5) 0.0306(4) 0.0070(4) 0.0170(4) 0.0035(4)

P1 0.0272(4) 0.0349(5) 0.0249(4) -0.0026(3) -0.0001(3) -0.0010(3)

F1 0.134(2) 0.0801(17) 0.0438(13) -0.0064(12) 0.0465(14) 0.0069(16)

F2 0.0796(17) 0.0792(17) 0.0764(16) 0.0083(13) 0.0443(13) -0.0165(13)

F3 0.095(2) 0.163(3) 0.115(2) 0.062(2) 0.0642(18) 0.084(2)

O1 0.0301(11) 0.0267(11) 0.0210(10) -0.0011(8) 0.0033(8) 0.0012(9)

O2 0.0367(12) 0.0341(12) 0.0251(11) -0.0040(9) 0.0016(9) -0.0005(10)

O3 0.0289(11) 0.0387(12) 0.0246(10) -0.0041(9) -0.0023(9) 0.0021(10)

O4 0.131(3) 0.0462(16) 0.0622(18) 0.0064(14) 0.0368(18) -0.0132(17)

O5 0.0774(19) 0.091(2) 0.0277(13) -0.0013(13) 0.0139(13) -0.0170(16)

O6 0.0527(16) 0.090(2) 0.0679(18) 0.0256(16) 0.0270(14) 0.0242(15)

N1 0.0313(14) 0.0271(13) 0.0262(13) -0.0025(10) 0.0073(11) 0.0010(11)

N2 0.0252(12) 0.0286(13) 0.0234(12) -0.0022(10) 0.0044(10) 0.0016(11)

N3 0.0341(14) 0.0306(14) 0.0281(14) -0.0001(11) 0.0063(11) -0.0005(11)

N4 0.0352(15) 0.0317(15) 0.0424(16) 0.0009(12) 0.0076(13) -0.0031(12)

N5 0.0296(14) 0.0363(15) 0.0259(13) -0.0008(11) 0.0077(11) 0.0038(11)

N6 0.0356(15) 0.0302(14) 0.0295(14) -0.0012(11) 0.0143(12) 0.0033(11)

N7 0.0263(13) 0.0292(14) 0.0259(13) -0.0006(11) 0.0053(11) -0.0007(11)

N8 0.0297(14) 0.0313(14) 0.0254(13) 0.0040(11) 0.0075(11) 0.0023(11)

N9 0.0237(13) 0.0316(14) 0.0242(13) -0.0002(10) 0.0049(10) -0.0009(10)

N10 0.0224(13) 0.0383(15) 0.0285(14) -0.0020(11) 0.0046(11) 0.0049(11)

N11 0.055(2) 0.055(2) 0.081(3) 0.0022(19) 0.0206(19) -0.0055(17)

C1 0.0300(16) 0.0307(16) 0.0196(14) -0.0015(12) 0.0038(12) 0.0004(13)

C2 0.0296(16) 0.0325(17) 0.0273(16) -0.0042(13) 0.0027(13) -0.0017(13)

C3 0.0270(16) 0.0292(16) 0.0264(15) -0.0037(13) 0.0019(13) -0.0017(13)

C4 0.0394(18) 0.0283(17) 0.0345(17) -0.0049(14) 0.0089(14) 0.0003(14)

C5 0.0326(17) 0.0291(17) 0.0340(17) 0.0005(14) 0.0071(14) 0.0017(14)

C6 0.0333(17) 0.0369(18) 0.0322(17) 0.0082(14) 0.0076(14) 0.0068(14)

C7 0.048(2) 0.046(2) 0.0314(18) 0.0078(15) 0.0077(16) 0.0073(16)

C8 0.060(2) 0.064(3) 0.036(2) 0.0158(18) 0.0183(18) 0.013(2)

C9 0.056(2) 0.071(3) 0.053(2) 0.025(2) 0.024(2) 0.003(2)

C10 0.048(2) 0.050(2) 0.058(2) 0.0169(19) 0.0172(19) -0.0041(18)

C11 0.0336(18) 0.0392(19) 0.0413(19) 0.0079(15) 0.0079(15) 0.0024(15)

C12 0.055(2) 0.037(2) 0.060(2) -0.0100(18) 0.0137(19) -0.0160(18)

C13 0.090(3) 0.037(2) 0.096(3) -0.011(2) 0.041(3) -0.005(2)

C14 0.0385(18) 0.0314(17) 0.0246(15) -0.0024(13) 0.0112(14) 0.0021(14)

C15 0.0361(17) 0.0248(16) 0.0293(16) -0.0002(13) 0.0122(14) 0.0052(13)

C16 0.0311(17) 0.0329(17) 0.0361(18) 0.0001(14) 0.0098(14) 0.0050(14)

C17 0.0363(19) 0.063(2) 0.0331(19) 0.0032(16) 0.0059(15) 0.0103(17)

C18 0.038(2) 0.085(3) 0.042(2) 0.002(2) 0.0044(17) 0.008(2)

C19 0.0293(19) 0.068(3) 0.063(3) 0.002(2) 0.0103(18) 0.0026(17)

C20 0.038(2) 0.047(2) 0.048(2) 0.0000(17) 0.0217(17) 0.0037(16)

C21 0.0356(18) 0.0299(17) 0.0368(18) 0.0017(14) 0.0114(15) 0.0041(14)

C22 0.046(2) 0.0360(18) 0.0343(18) -0.0022(14) 0.0215(15) 0.0037(15)

C23 0.052(2) 0.040(2) 0.0398(19) 0.0040(15) 0.0198(16) 0.0023(16)

C24 0.0312(16) 0.0337(17) 0.0202(15) 0.0014(13) 0.0026(12) 0.0031(13)

C25 0.0258(15) 0.0265(16) 0.0240(15) 0.0000(12) 0.0074(13) 0.0039(12)

C26 0.0242(15) 0.0272(16) 0.0293(16) -0.0021(13) 0.0071(13) 0.0009(12)

C27 0.0284(17) 0.0385(18) 0.0327(17) 0.0004(14) 0.0051(14) -0.0023(14)

C28 0.0321(18) 0.049(2) 0.046(2) -0.0049(17) 0.0046(16) -0.0097(16)

C29 0.0348(18) 0.045(2) 0.058(2) 0.0032(18) 0.0089(17) -0.0134(16)

C30 0.0340(18) 0.043(2) 0.044(2) 0.0092(16) 0.0140(15) -0.0042(15)

C31 0.0260(16) 0.0321(17) 0.0338(17) -0.0012(14) 0.0103(14) 0.0010(13)

C32 0.0400(19) 0.0429(19) 0.0274(17) 0.0100(14) 0.0102(14) -0.0009(15)

C33 0.047(2) 0.039(2) 0.048(2) 0.0132(16) 0.0023(17) 0.0008(16)

C34 0.0272(16) 0.0349(17) 0.0256(15) -0.0001(13) 0.0032(13) 0.0051(13)

C35 0.0244(15) 0.0266(16) 0.0273(16) -0.0017(12) 0.0020(13) 0.0014(12)

C36 0.0289(16) 0.0261(16) 0.0280(16) -0.0008(12) 0.0098(13) -0.0017(13)

C37 0.0321(17) 0.0379(18) 0.0275(16) -0.0007(14) 0.0042(13) -0.0011(14)

C38 0.044(2) 0.0406(19) 0.0283(17) 0.0015(14) 0.0092(15) -0.0004(15)

C39 0.051(2) 0.0392(19) 0.0388(19) 0.0009(15) 0.0237(17) 0.0026(16)

C40 0.0342(18) 0.046(2) 0.041(2) 0.0014(16) 0.0164(15) 0.0046(15)

C41 0.0291(17) 0.0336(17) 0.0292(16) -0.0001(13) 0.0065(13) -0.0004(14)

C42 0.0247(16) 0.047(2) 0.0368(18) -0.0072(15) 0.0021(14) 0.0009(15)

C43 0.0356(19) 0.052(2) 0.047(2) -0.0132(17) -0.0009(16) 0.0093(17)

C44 0.070(3) 0.043(2) 0.0286(18) -0.0076(15) -0.0082(17) 0.0125(18)

C45 0.034(2) 0.057(2) 0.086(3) 0.009(2) 0.0145(19) -0.0054(18)

C46 0.0241(15) 0.0311(17) 0.0260(15) 0.0043(13) 0.0000(12) 0.0036(13)

C47 0.0357(18) 0.0390(19) 0.0327(17) -0.0018(14) 0.0072(14) 0.0021(15)

C48 0.048(2) 0.058(2) 0.0303(18) -0.0009(16) 0.0126(16) 0.0072(18)

C49 0.0366(19) 0.061(2) 0.0362(19) 0.0145(17) 0.0109(15) -0.0004(17)

C50 0.0309(18) 0.0414(19) 0.042(2) 0.0115(16) -0.0008(15) -0.0030(15)

C51 0.0310(17) 0.0359(18) 0.0272(16) 0.0004(14) 0.0004(13) -0.0006(14)

C52 0.0310(16) 0.0176(14) 0.0291(16) 0.0018(12) 0.0081(13) 0.0017(12)

C53 0.0346(17) 0.0397(18) 0.0313(17) 0.0038(14) 0.0116(14) 0.0058(15)

C54 0.0291(17) 0.045(2) 0.0373(19) 0.0077(15) 0.0033(15) 0.0012(15)

C55 0.0401(19) 0.0349(18) 0.0274(17) 0.0023(14) -0.0023(14) 0.0002(15)

C56 0.043(2) 0.044(2) 0.0250(16) 0.0000(14) 0.0084(15) 0.0054(16)

C57 0.0304(16) 0.0367(18) 0.0306(17) 0.0023(14) 0.0087(14) 0.0023(14)

C58 0.0296(16) 0.0287(16) 0.0232(15) -0.0041(12) -0.0010(13) 0.0000(13)

C59 0.0304(17) 0.0331(17) 0.0303(17) -0.0034(13) 0.0002(13) 0.0004(14)

C60 0.0380(19) 0.0322(18) 0.0358(18) -0.0080(14) -0.0089(15) 0.0089(15)

C61 0.0281(17) 0.051(2) 0.0355(18) -0.0194(16) -0.0026(14) 0.0057(16)

C62 0.0286(17) 0.048(2) 0.0325(17) -0.0087(15) 0.0033(14) -0.0041(15)

C63 0.0319(17) 0.0324(17) 0.0313(16) -0.0005(14) 0.0029(13) 0.0012(14)

C64 0.0313(17) 0.0299(17) 0.0278(16) -0.0002(13) 0.0099(13) -0.0006(13)

C65 0.0429(19) 0.0320(18) 0.0376(18) 0.0000(14) 0.0049(15) 0.0010(15)

C66 0.054(2) 0.039(2) 0.0386(19) -0.0095(16) 0.0109(17) -0.0094(17)

C67 0.058(2) 0.0267(18) 0.055(2) -0.0062(16) 0.0306(19) -0.0037(17)

C68 0.047(2) 0.0284(18) 0.054(2) 0.0093(16) 0.0281(18) 0.0090(15)

C69 0.0305(17) 0.0316(17) 0.0378(18) 0.0032(14) 0.0132(14) 0.0027(14)

C70 0.059(2) 0.058(3) 0.043(2) 0.0127(19) 0.0248(18) 0.023(2)

C71 0.0333(19) 0.036(2) 0.068(3) -0.0096(19) 0.0129(18) -0.0028(16)

C72 0.050(2) 0.051(2) 0.064(3) -0.002(2) 0.0139(19) -0.0031(19)

B1 0.0310(18) 0.0289(19) 0.0265(18) 0.0004(15) 0.0067(15) 0.0026(15)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Fe1 O2 2.0018(19) . ?

Fe1 O1 2.0146(18) . ?

Fe1 N3 2.104(2) . ?

Fe1 N5 2.123(2) . ?

Fe1 N1 2.322(2) . ?

Fe2 O1 1.9994(18) . ?

Fe2 O3 2.0082(18) . ?

Fe2 N9 2.076(2) . ?

Fe2 N7 2.098(2) . ?

Fe2 N2 2.367(2) . ?

S1 O6 1.420(3) . ?

S1 O4 1.427(3) . ?

S1 O5 1.434(2) . ?

S1 C70 1.806(4) . ?

P1 O2 1.509(2) . ?

P1 O3 1.514(2) . ?

P1 C45 1.782(3) . ?

P1 C44 1.782(3) . ?

F1 C70 1.326(4) . ?

F2 C70 1.326(4) . ?

F3 C70 1.319(4) . ?

O1 C1 1.426(3) . ?

N1 C14 1.471(3) . ?

N1 C4 1.472(4) . ?

N1 C2 1.482(4) . ?

N2 C24 1.471(3) . ?

N2 C34 1.475(3) . ?

N2 C3 1.476(3) . ?

N3 C5 1.323(4) . ?

N3 C6 1.395(4) . ?

N4 C5 1.355(4) . ?

N4 C11 1.395(4) . ?

N4 C12 1.473(4) . ?

N5 C15 1.322(3) . ?

N5 C16 1.402(4) . ?

N6 C15 1.350(4) . ?

N6 C21 1.388(4) . ?

N6 C22 1.466(4) . ?

N7 C25 1.322(3) . ?

N7 C26 1.402(3) . ?

N8 C25 1.351(3) . ?

N8 C31 1.390(4) . ?

N8 C32 1.474(3) . ?

N9 C35 1.324(3) . ?

N9 C36 1.396(3) . ?

N10 C35 1.354(3) . ?

N10 C41 1.392(4) . ?

N10 C42 1.473(4) . ?

N11 C71 1.129(4) . ?

C1 C2 1.507(4) . ?

C1 C3 1.520(4) . ?

C1 H1A 1.0000 . ?

C2 H2A 0.9900 . ?

C2 H2B 0.9900 . ?

C3 H3A 0.9900 . ?

C3 H3B 0.9900 . ?

C4 C5 1.490(4) . ?

C4 H4A 0.9900 . ?

C4 H4B 0.9900 . ?

C6 C7 1.393(4) . ?

C6 C11 1.396(4) . ?

C7 C8 1.380(5) . ?

C7 H7A 0.9500 . ?

C8 C9 1.395(5) . ?

C8 H8A 0.9500 . ?

C9 C10 1.371(5) . ?

C9 H9A 0.9500 . ?

C10 C11 1.391(4) . ?

C10 H10A 0.9500 . ?

C12 C13 1.519(5) . ?

C12 H12A 0.9900 . ?

C12 H12B 0.9900 . ?

C13 H13A 0.9800 . ?

C13 H13B 0.9800 . ?

C13 H13C 0.9800 . ?

C14 C15 1.494(4) . ?

C14 H14A 0.9900 . ?

C14 H14B 0.9900 . ?

C16 C17 1.389(4) . ?

C16 C21 1.403(4) . ?

C17 C18 1.381(5) . ?

C17 H17A 0.9500 . ?

C18 C19 1.390(5) . ?

C18 H18A 0.9500 . ?

C19 C20 1.378(5) . ?

C19 H19A 0.9500 . ?

C20 C21 1.391(4) . ?

C20 H20A 0.9500 . ?

C22 C23 1.512(4) . ?

C22 H22A 0.9900 . ?

C22 H22B 0.9900 . ?

C23 H23A 0.9800 . ?

C23 H23B 0.9800 . ?

C23 H23C 0.9800 . ?

C24 C25 1.492(4) . ?

C24 H24A 0.9900 . ?

C24 H24B 0.9900 . ?

C26 C27 1.392(4) . ?

C26 C31 1.395(4) . ?

C27 C28 1.375(4) . ?

C27 H27A 0.9500 . ?

C28 C29 1.403(5) . ?

C28 H28A 0.9500 . ?

C29 C30 1.374(4) . ?

C29 H29A 0.9500 . ?

C30 C31 1.394(4) . ?

C30 H30A 0.9500 . ?

C32 C33 1.501(4) . ?

C32 H32A 0.9900 . ?

C32 H32B 0.9900 . ?

C33 H33A 0.9800 . ?

C33 H33B 0.9800 . ?

C33 H33C 0.9800 . ?

C34 C35 1.497(4) . ?

C34 H34A 0.9900 . ?

C34 H34B 0.9900 . ?

C36 C37 1.385(4) . ?

C36 C41 1.391(4) . ?

C37 C38 1.385(4) . ?

C37 H37A 0.9500 . ?

C38 C39 1.387(4) . ?

C38 H38A 0.9500 . ?

C39 C40 1.384(4) . ?

C39 H39A 0.9500 . ?

C40 C41 1.383(4) . ?

C40 H40A 0.9500 . ?

C42 C43 1.493(4) . ?

C42 H42A 0.9900 . ?

C42 H42B 0.9900 . ?

C43 H43A 0.9800 . ?

C43 H43B 0.9800 . ?

C43 H43C 0.9800 . ?

C44 H44A 0.9800 . ?

C44 H44B 0.9800 . ?

C44 H44C 0.9800 . ?

C45 H45A 0.9800 . ?

C45 H45B 0.9800 . ?

C45 H45C 0.9800 . ?

C46 C51 1.401(4) . ?

C46 C47 1.403(4) . ?

C46 B1 1.663(4) . ?

C47 C48 1.394(4) . ?

C47 H47A 0.9500 . ?

C48 C49 1.376(5) . ?

C48 H48A 0.9500 . ?

C49 C50 1.381(5) . ?

C49 H49A 0.9500 . ?

C50 C51 1.391(4) . ?

C50 H50A 0.9500 . ?

C51 H51A 0.9500 . ?

C52 C53 1.400(4) . ?

C52 C57 1.402(4) . ?

C52 B1 1.657(4) . ?

C53 C54 1.387(4) . ?

C53 H53A 0.9500 . ?

C54 C55 1.385(4) . ?

C54 H54A 0.9500 . ?

C55 C56 1.372(4) . ?

C55 H55A 0.9500 . ?

C56 C57 1.384(4) . ?

C56 H56A 0.9500 . ?

C57 H57A 0.9500 . ?

C58 C59 1.403(4) . ?

C58 C63 1.405(4) . ?

C58 B1 1.653(4) . ?

C59 C60 1.398(4) . ?

C59 H59A 0.9500 . ?

C60 C61 1.376(4) . ?

C60 H60A 0.9500 . ?

C61 C62 1.383(4) . ?

C61 H61A 0.9500 . ?

C62 C63 1.384(4) . ?

C62 H62A 0.9500 . ?

C63 H63A 0.9500 . ?

C64 C69 1.395(4) . ?

C64 C65 1.398(4) . ?

C64 B1 1.642(4) . ?

C65 C66 1.382(4) . ?

C65 H65A 0.9500 . ?

C66 C67 1.380(5) . ?

C66 H66A 0.9500 . ?

C67 C68 1.371(5) . ?

C67 H67A 0.9500 . ?

C68 C69 1.395(4) . ?

C68 H68A 0.9500 . ?

C69 H69A 0.9500 . ?

C71 C72 1.443(5) . ?

C72 H72C 0.9800 . ?

C72 H72B 0.9800 . ?

C72 H72A 0.9800 . ?

loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O2 Fe1 O1 102.38(8) . . ?

O2 Fe1 N3 107.84(9) . . ?

O1 Fe1 N3 104.56(9) . . ?

O2 Fe1 N5 100.57(9) . . ?

O1 Fe1 N5 128.17(8) . . ?

N3 Fe1 N5 111.50(9) . . ?

O2 Fe1 N1 174.87(8) . . ?

O1 Fe1 N1 79.23(8) . . ?

N3 Fe1 N1 76.25(9) . . ?

N5 Fe1 N1 74.80(9) . . ?

O1 Fe2 O3 104.01(8) . . ?

O1 Fe2 N9 108.69(9) . . ?

O3 Fe2 N9 105.57(8) . . ?

O1 Fe2 N7 124.14(8) . . ?

O3 Fe2 N7 99.88(9) . . ?

N9 Fe2 N7 112.22(9) . . ?

O1 Fe2 N2 79.75(8) . . ?

O3 Fe2 N2 175.43(8) . . ?

N9 Fe2 N2 75.32(8) . . ?

N7 Fe2 N2 75.72(8) . . ?

O6 S1 O4 114.82(19) . . ?

O6 S1 O5 115.22(18) . . ?

O4 S1 O5 114.87(17) . . ?

O6 S1 C70 103.03(16) . . ?

O4 S1 C70 103.95(18) . . ?

O5 S1 C70 102.53(17) . . ?

O2 P1 O3 115.28(12) . . ?

O2 P1 C45 109.06(16) . . ?

O3 P1 C45 108.84(15) . . ?

O2 P1 C44 108.30(14) . . ?

O3 P1 C44 108.24(14) . . ?

C45 P1 C44 106.79(19) . . ?

C1 O1 Fe2 112.81(15) . . ?

C1 O1 Fe1 115.12(15) . . ?

Fe2 O1 Fe1 123.39(9) . . ?

P1 O2 Fe1 131.47(12) . . ?

P1 O3 Fe2 132.44(12) . . ?

C14 N1 C4 111.6(2) . . ?

C14 N1 C2 113.4(2) . . ?

C4 N1 C2 112.2(2) . . ?

C14 N1 Fe1 108.34(17) . . ?

C4 N1 Fe1 106.79(17) . . ?

C2 N1 Fe1 103.93(16) . . ?

C24 N2 C34 112.3(2) . . ?

C24 N2 C3 112.6(2) . . ?

C34 N2 C3 112.2(2) . . ?

C24 N2 Fe2 107.77(16) . . ?

C34 N2 Fe2 109.23(16) . . ?

C3 N2 Fe2 102.07(16) . . ?

C5 N3 C6 105.4(2) . . ?

C5 N3 Fe1 115.72(19) . . ?

C6 N3 Fe1 138.5(2) . . ?

C5 N4 C11 106.4(3) . . ?

C5 N4 C12 125.7(3) . . ?

C11 N4 C12 127.9(3) . . ?

C15 N5 C16 105.0(2) . . ?

C15 N5 Fe1 114.72(19) . . ?

C16 N5 Fe1 137.76(19) . . ?

C15 N6 C21 106.9(2) . . ?

C15 N6 C22 126.2(3) . . ?

C21 N6 C22 126.8(3) . . ?

C25 N7 C26 105.2(2) . . ?

C25 N7 Fe2 117.29(19) . . ?

C26 N7 Fe2 137.25(18) . . ?

C25 N8 C31 106.9(2) . . ?

C25 N8 C32 127.0(2) . . ?

C31 N8 C32 126.0(2) . . ?

C35 N9 C36 105.5(2) . . ?

C35 N9 Fe2 119.48(19) . . ?

C36 N9 Fe2 134.99(19) . . ?

C35 N10 C41 106.3(2) . . ?

C35 N10 C42 128.8(2) . . ?

C41 N10 C42 124.9(2) . . ?

O1 C1 C2 110.3(2) . . ?

O1 C1 C3 109.1(2) . . ?

C2 C1 C3 111.3(2) . . ?

O1 C1 H1A 108.7 . . ?

C2 C1 H1A 108.7 . . ?

C3 C1 H1A 108.7 . . ?

N1 C2 C1 108.9(2) . . ?

N1 C2 H2A 109.9 . . ?

C1 C2 H2A 109.9 . . ?

N1 C2 H2B 109.9 . . ?

C1 C2 H2B 109.9 . . ?

H2A C2 H2B 108.3 . . ?

N2 C3 C1 108.8(2) . . ?

N2 C3 H3A 109.9 . . ?

C1 C3 H3A 109.9 . . ?

N2 C3 H3B 109.9 . . ?

C1 C3 H3B 109.9 . . ?

H3A C3 H3B 108.3 . . ?

N1 C4 C5 108.3(2) . . ?

N1 C4 H4A 110.0 . . ?

C5 C4 H4A 110.0 . . ?

N1 C4 H4B 110.0 . . ?

C5 C4 H4B 110.0 . . ?

H4A C4 H4B 108.4 . . ?

N3 C5 N4 113.2(3) . . ?

N3 C5 C4 121.8(3) . . ?

N4 C5 C4 125.1(3) . . ?

C7 C6 N3 130.1(3) . . ?

C7 C6 C11 120.8(3) . . ?

N3 C6 C11 109.1(3) . . ?

C8 C7 C6 117.3(3) . . ?

C8 C7 H7A 121.4 . . ?

C6 C7 H7A 121.4 . . ?

C7 C8 C9 120.9(3) . . ?

C7 C8 H8A 119.5 . . ?

C9 C8 H8A 119.5 . . ?

C10 C9 C8 122.9(3) . . ?

C10 C9 H9A 118.6 . . ?

C8 C9 H9A 118.6 . . ?

C9 C10 C11 116.0(4) . . ?

C9 C10 H10A 122.0 . . ?

C11 C10 H10A 122.0 . . ?

C10 C11 N4 131.9(3) . . ?

C10 C11 C6 122.1(3) . . ?

N4 C11 C6 105.9(3) . . ?

N4 C12 C13 111.8(3) . . ?

N4 C12 H12A 109.3 . . ?

C13 C12 H12A 109.3 . . ?

N4 C12 H12B 109.3 . . ?

C13 C12 H12B 109.3 . . ?

H12A C12 H12B 107.9 . . ?

C12 C13 H13A 109.5 . . ?

C12 C13 H13B 109.5 . . ?

H13A C13 H13B 109.5 . . ?

C12 C13 H13C 109.5 . . ?

H13A C13 H13C 109.5 . . ?

H13B C13 H13C 109.5 . . ?

N1 C14 C15 108.3(2) . . ?

N1 C14 H14A 110.0 . . ?

C15 C14 H14A 110.0 . . ?

N1 C14 H14B 110.0 . . ?

C15 C14 H14B 110.0 . . ?

H14A C14 H14B 108.4 . . ?

N5 C15 N6 113.4(3) . . ?

N5 C15 C14 122.8(3) . . ?

N6 C15 C14 123.8(3) . . ?

C17 C16 N5 130.8(3) . . ?

C17 C16 C21 120.2(3) . . ?

N5 C16 C21 109.0(3) . . ?

C18 C17 C16 117.1(3) . . ?

C18 C17 H17A 121.5 . . ?

C16 C17 H17A 121.5 . . ?

C17 C18 C19 122.4(3) . . ?

C17 C18 H18A 118.8 . . ?

C19 C18 H18A 118.8 . . ?

C20 C19 C18 121.4(3) . . ?

C20 C19 H19A 119.3 . . ?

C18 C19 H19A 119.3 . . ?

C19 C20 C21 116.5(3) . . ?

C19 C20 H20A 121.7 . . ?

C21 C20 H20A 121.7 . . ?

N6 C21 C20 131.9(3) . . ?

N6 C21 C16 105.7(3) . . ?

C20 C21 C16 122.4(3) . . ?

N6 C22 C23 112.5(2) . . ?

N6 C22 H22A 109.1 . . ?

C23 C22 H22A 109.1 . . ?

N6 C22 H22B 109.1 . . ?

C23 C22 H22B 109.1 . . ?

H22A C22 H22B 107.8 . . ?

C22 C23 H23A 109.5 . . ?

C22 C23 H23B 109.5 . . ?

H23A C23 H23B 109.5 . . ?

C22 C23 H23C 109.5 . . ?

H23A C23 H23C 109.5 . . ?

H23B C23 H23C 109.5 . . ?

N2 C24 C25 110.0(2) . . ?

N2 C24 H24A 109.7 . . ?

C25 C24 H24A 109.7 . . ?

N2 C24 H24B 109.7 . . ?

C25 C24 H24B 109.7 . . ?

H24A C24 H24B 108.2 . . ?

N7 C25 N8 113.1(2) . . ?

N7 C25 C24 122.5(2) . . ?

N8 C25 C24 124.3(2) . . ?

C27 C26 C31 120.5(3) . . ?

C27 C26 N7 130.5(3) . . ?

C31 C26 N7 109.0(2) . . ?

C28 C27 C26 117.7(3) . . ?

C28 C27 H27A 121.2 . . ?

C26 C27 H27A 121.2 . . ?

C27 C28 C29 121.2(3) . . ?

C27 C28 H28A 119.4 . . ?

C29 C28 H28A 119.4 . . ?

C30 C29 C28 122.0(3) . . ?

C30 C29 H29A 119.0 . . ?

C28 C29 H29A 119.0 . . ?

C29 C30 C31 116.4(3) . . ?

C29 C30 H30A 121.8 . . ?

C31 C30 H30A 121.8 . . ?

N8 C31 C30 132.0(3) . . ?

N8 C31 C26 105.8(2) . . ?

C30 C31 C26 122.2(3) . . ?

N8 C32 C33 112.1(3) . . ?

N8 C32 H32A 109.2 . . ?

C33 C32 H32A 109.2 . . ?

N8 C32 H32B 109.2 . . ?

C33 C32 H32B 109.2 . . ?

H32A C32 H32B 107.9 . . ?

C32 C33 H33A 109.5 . . ?

C32 C33 H33B 109.5 . . ?

H33A C33 H33B 109.5 . . ?

C32 C33 H33C 109.5 . . ?

H33A C33 H33C 109.5 . . ?

H33B C33 H33C 109.5 . . ?

N2 C34 C35 108.9(2) . . ?

N2 C34 H34A 109.9 . . ?

C35 C34 H34A 109.9 . . ?

N2 C34 H34B 109.9 . . ?

C35 C34 H34B 109.9 . . ?

H34A C34 H34B 108.3 . . ?

N9 C35 N10 113.0(2) . . ?

N9 C35 C34 121.3(2) . . ?

N10 C35 C34 125.4(2) . . ?

C37 C36 C41 121.4(3) . . ?

C37 C36 N9 129.9(3) . . ?

C41 C36 N9 108.7(2) . . ?

C36 C37 C38 116.9(3) . . ?

C36 C37 H37A 121.6 . . ?

C38 C37 H37A 121.6 . . ?

C37 C38 C39 121.2(3) . . ?

C37 C38 H38A 119.4 . . ?

C39 C38 H38A 119.4 . . ?

C40 C39 C38 122.4(3) . . ?

C40 C39 H39A 118.8 . . ?

C38 C39 H39A 118.8 . . ?

C41 C40 C39 116.1(3) . . ?

C41 C40 H40A 121.9 . . ?

C39 C40 H40A 121.9 . . ?

C40 C41 C36 122.0(3) . . ?

C40 C41 N10 131.5(3) . . ?

C36 C41 N10 106.4(2) . . ?

N10 C42 C43 112.9(3) . . ?

N10 C42 H42A 109.0 . . ?

C43 C42 H42A 109.0 . . ?

N10 C42 H42B 109.0 . . ?

C43 C42 H42B 109.0 . . ?

H42A C42 H42B 107.8 . . ?

C42 C43 H43A 109.5 . . ?

C42 C43 H43B 109.5 . . ?

H43A C43 H43B 109.5 . . ?

C42 C43 H43C 109.5 . . ?

H43A C43 H43C 109.5 . . ?

H43B C43 H43C 109.5 . . ?

P1 C44 H44A 109.5 . . ?

P1 C44 H44B 109.5 . . ?

H44A C44 H44B 109.5 . . ?

P1 C44 H44C 109.5 . . ?

H44A C44 H44C 109.5 . . ?

H44B C44 H44C 109.5 . . ?

P1 C45 H45A 109.5 . . ?

P1 C45 H45B 109.5 . . ?

H45A C45 H45B 109.5 . . ?

P1 C45 H45C 109.5 . . ?

H45A C45 H45C 109.5 . . ?

H45B C45 H45C 109.5 . . ?

C51 C46 C47 114.5(3) . . ?

C51 C46 B1 122.0(3) . . ?

C47 C46 B1 123.4(3) . . ?

C48 C47 C46 122.8(3) . . ?

C48 C47 H47A 118.6 . . ?

C46 C47 H47A 118.6 . . ?

C49 C48 C47 120.5(3) . . ?

C49 C48 H48A 119.8 . . ?

C47 C48 H48A 119.8 . . ?

C48 C49 C50 118.8(3) . . ?

C48 C49 H49A 120.6 . . ?

C50 C49 H49A 120.6 . . ?

C49 C50 C51 120.2(3) . . ?

C49 C50 H50A 119.9 . . ?

C51 C50 H50A 119.9 . . ?

C50 C51 C46 123.2(3) . . ?

C50 C51 H51A 118.4 . . ?

C46 C51 H51A 118.4 . . ?

C53 C52 C57 114.4(3) . . ?

C53 C52 B1 122.0(2) . . ?

C57 C52 B1 123.6(3) . . ?

C54 C53 C52 123.0(3) . . ?

C54 C53 H53A 118.5 . . ?

C52 C53 H53A 118.5 . . ?

C55 C54 C53 120.4(3) . . ?

C55 C54 H54A 119.8 . . ?

C53 C54 H54A 119.8 . . ?

C56 C55 C54 118.3(3) . . ?

C56 C55 H55A 120.8 . . ?

C54 C55 H55A 120.8 . . ?

C55 C56 C57 120.8(3) . . ?

C55 C56 H56A 119.6 . . ?

C57 C56 H56A 119.6 . . ?

C56 C57 C52 123.0(3) . . ?

C56 C57 H57A 118.5 . . ?

C52 C57 H57A 118.5 . . ?

C59 C58 C63 114.8(3) . . ?

C59 C58 B1 125.1(3) . . ?

C63 C58 B1 119.7(3) . . ?

C60 C59 C58 122.2(3) . . ?

C60 C59 H59A 118.9 . . ?

C58 C59 H59A 118.9 . . ?

C61 C60 C59 120.4(3) . . ?

C61 C60 H60A 119.8 . . ?

C59 C60 H60A 119.8 . . ?

C60 C61 C62 119.4(3) . . ?

C60 C61 H61A 120.3 . . ?

C62 C61 H61A 120.3 . . ?

C61 C62 C63 119.4(3) . . ?

C61 C62 H62A 120.3 . . ?

C63 C62 H62A 120.3 . . ?

C62 C63 C58 123.7(3) . . ?

C62 C63 H63A 118.2 . . ?

C58 C63 H63A 118.2 . . ?

C69 C64 C65 114.8(3) . . ?

C69 C64 B1 123.9(3) . . ?

C65 C64 B1 121.1(3) . . ?

C66 C65 C64 123.3(3) . . ?

C66 C65 H65A 118.4 . . ?

C64 C65 H65A 118.4 . . ?

C67 C66 C65 120.3(3) . . ?

C67 C66 H66A 119.8 . . ?

C65 C66 H66A 119.8 . . ?

C68 C67 C66 118.3(3) . . ?

C68 C67 H67A 120.8 . . ?

C66 C67 H67A 120.8 . . ?

C67 C68 C69 121.1(3) . . ?

C67 C68 H68A 119.5 . . ?

C69 C68 H68A 119.5 . . ?

C68 C69 C64 122.2(3) . . ?

C68 C69 H69A 118.9 . . ?

C64 C69 H69A 118.9 . . ?

F3 C70 F2 107.3(4) . . ?

F3 C70 F1 107.0(3) . . ?

F2 C70 F1 106.0(3) . . ?

F3 C70 S1 111.7(2) . . ?

F2 C70 S1 112.1(2) . . ?

F1 C70 S1 112.4(3) . . ?

N11 C71 C72 179.6(5) . . ?

C71 C72 H72C 109.5 . . ?

C71 C72 H72B 109.5 . . ?

H72C C72 H72B 109.5 . . ?

C71 C72 H72A 109.5 . . ?

H72C C72 H72A 109.5 . . ?

H72B C72 H72A 109.5 . . ?

C64 B1 C58 109.4(2) . . ?

C64 B1 C52 110.4(2) . . ?

C58 B1 C52 106.5(2) . . ?

C64 B1 C46 109.2(2) . . ?

C58 B1 C46 112.5(2) . . ?

C52 B1 C46 108.8(2) . . ?

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_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

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_geom_torsion_atom_site_label_4

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_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

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O3 Fe2 O1 C1 -157.43(17) . . . . ?

N9 Fe2 O1 C1 90.46(18) . . . . ?

N7 Fe2 O1 C1 -44.9(2) . . . . ?

N2 Fe2 O1 C1 19.91(17) . . . . ?

O3 Fe2 O1 Fe1 -11.45(13) . . . . ?

N9 Fe2 O1 Fe1 -123.57(11) . . . . ?

N7 Fe2 O1 Fe1 101.06(12) . . . . ?

N2 Fe2 O1 Fe1 165.88(12) . . . . ?

O2 Fe1 O1 C1 161.99(17) . . . . ?

N3 Fe1 O1 C1 -85.61(18) . . . . ?

N5 Fe1 O1 C1 47.7(2) . . . . ?

N1 Fe1 O1 C1 -13.04(17) . . . . ?

O2 Fe1 O1 Fe2 16.72(13) . . . . ?

N3 Fe1 O1 Fe2 129.11(11) . . . . ?

N5 Fe1 O1 Fe2 -97.58(13) . . . . ?

N1 Fe1 O1 Fe2 -158.31(12) . . . . ?

O3 P1 O2 Fe1 40.5(2) . . . . ?

C45 P1 O2 Fe1 -82.2(2) . . . . ?

C44 P1 O2 Fe1 161.92(18) . . . . ?

O1 Fe1 O2 P1 -33.48(18) . . . . ?

N3 Fe1 O2 P1 -143.42(16) . . . . ?

N5 Fe1 O2 P1 99.73(17) . . . . ?

N1 Fe1 O2 P1 74.3(10) . . . . ?

O2 P1 O3 Fe2 -30.6(2) . . . . ?

C45 P1 O3 Fe2 92.3(2) . . . . ?

C44 P1 O3 Fe2 -152.02(18) . . . . ?

O1 Fe2 O3 P1 17.58(18) . . . . ?

N9 Fe2 O3 P1 131.94(16) . . . . ?

N7 Fe2 O3 P1 -111.51(17) . . . . ?

N2 Fe2 O3 P1 -127.4(9) . . . . ?

O2 Fe1 N1 C14 -3.4(10) . . . . ?

O1 Fe1 N1 C14 105.41(18) . . . . ?

N3 Fe1 N1 C14 -146.53(19) . . . . ?

N5 Fe1 N1 C14 -29.31(17) . . . . ?

O2 Fe1 N1 C4 116.9(9) . . . . ?

O1 Fe1 N1 C4 -134.30(18) . . . . ?

N3 Fe1 N1 C4 -26.23(18) . . . . ?

N5 Fe1 N1 C4 90.99(18) . . . . ?

O2 Fe1 N1 C2 -124.3(9) . . . . ?

O1 Fe1 N1 C2 -15.47(16) . . . . ?

N3 Fe1 N1 C2 92.59(18) . . . . ?

N5 Fe1 N1 C2 -150.18(18) . . . . ?

O1 Fe2 N2 C24 -107.54(17) . . . . ?

O3 Fe2 N2 C24 38.0(11) . . . . ?

N9 Fe2 N2 C24 139.87(18) . . . . ?

N7 Fe2 N2 C24 21.84(17) . . . . ?

O1 Fe2 N2 C34 130.24(19) . . . . ?

O3 Fe2 N2 C34 -84.2(10) . . . . ?

N9 Fe2 N2 C34 17.66(18) . . . . ?

N7 Fe2 N2 C34 -100.37(19) . . . . ?

O1 Fe2 N2 C3 11.27(16) . . . . ?

O3 Fe2 N2 C3 156.8(9) . . . . ?

N9 Fe2 N2 C3 -101.32(17) . . . . ?

N7 Fe2 N2 C3 140.65(17) . . . . ?

O2 Fe1 N3 C5 -164.7(2) . . . . ?

O1 Fe1 N3 C5 86.9(2) . . . . ?

N5 Fe1 N3 C5 -55.2(2) . . . . ?

N1 Fe1 N3 C5 12.1(2) . . . . ?

O2 Fe1 N3 C6 23.9(3) . . . . ?

O1 Fe1 N3 C6 -84.6(3) . . . . ?

N5 Fe1 N3 C6 133.4(3) . . . . ?

N1 Fe1 N3 C6 -159.4(3) . . . . ?

O2 Fe1 N5 C15 -154.8(2) . . . . ?

O1 Fe1 N5 C15 -39.7(2) . . . . ?

N3 Fe1 N5 C15 91.1(2) . . . . ?

N1 Fe1 N5 C15 22.9(2) . . . . ?

O2 Fe1 N5 C16 3.7(3) . . . . ?

O1 Fe1 N5 C16 118.8(3) . . . . ?

N3 Fe1 N5 C16 -110.4(3) . . . . ?

N1 Fe1 N5 C16 -178.6(3) . . . . ?

O1 Fe2 N7 C25 53.7(2) . . . . ?

O3 Fe2 N7 C25 168.25(19) . . . . ?

N9 Fe2 N7 C25 -80.3(2) . . . . ?

N2 Fe2 N7 C25 -13.03(19) . . . . ?

O1 Fe2 N7 C26 -119.5(3) . . . . ?

O3 Fe2 N7 C26 -5.0(3) . . . . ?

N9 Fe2 N7 C26 106.5(3) . . . . ?

N2 Fe2 N7 C26 173.7(3) . . . . ?

O1 Fe2 N9 C35 -79.5(2) . . . . ?

O3 Fe2 N9 C35 169.4(2) . . . . ?

N7 Fe2 N9 C35 61.6(2) . . . . ?

N2 Fe2 N9 C35 -5.9(2) . . . . ?

O1 Fe2 N9 C36 98.2(3) . . . . ?

O3 Fe2 N9 C36 -12.9(3) . . . . ?

N7 Fe2 N9 C36 -120.7(3) . . . . ?

N2 Fe2 N9 C36 171.8(3) . . . . ?

Fe2 O1 C1 C2 -171.05(18) . . . . ?

Fe1 O1 C1 C2 40.0(3) . . . . ?

Fe2 O1 C1 C3 -48.5(3) . . . . ?

Fe1 O1 C1 C3 162.53(17) . . . . ?

C14 N1 C2 C1 -78.0(3) . . . . ?

C4 N1 C2 C1 154.4(2) . . . . ?

Fe1 N1 C2 C1 39.4(2) . . . . ?

O1 C1 C2 N1 -53.9(3) . . . . ?

C3 C1 C2 N1 -175.2(2) . . . . ?

C24 N2 C3 C1 77.2(3) . . . . ?

C34 N2 C3 C1 -154.9(2) . . . . ?

Fe2 N2 C3 C1 -38.1(2) . . . . ?

O1 C1 C3 N2 59.3(3) . . . . ?

C2 C1 C3 N2 -178.8(2) . . . . ?

C14 N1 C4 C5 152.8(2) . . . . ?

C2 N1 C4 C5 -78.6(3) . . . . ?

Fe1 N1 C4 C5 34.6(3) . . . . ?

C6 N3 C5 N4 -0.3(3) . . . . ?

Fe1 N3 C5 N4 -174.44(19) . . . . ?

C6 N3 C5 C4 179.3(3) . . . . ?

Fe1 N3 C5 C4 5.2(4) . . . . ?

C11 N4 C5 N3 0.1(3) . . . . ?

C12 N4 C5 N3 -179.7(3) . . . . ?

C11 N4 C5 C4 -179.5(3) . . . . ?

C12 N4 C5 C4 0.8(5) . . . . ?

N1 C4 C5 N3 -29.2(4) . . . . ?

N1 C4 C5 N4 150.4(3) . . . . ?

C5 N3 C6 C7 -178.0(3) . . . . ?

Fe1 N3 C6 C7 -6.0(5) . . . . ?

C5 N3 C6 C11 0.4(3) . . . . ?

Fe1 N3 C6 C11 172.4(2) . . . . ?

N3 C6 C7 C8 176.9(3) . . . . ?

C11 C6 C7 C8 -1.3(5) . . . . ?

C6 C7 C8 C9 0.7(5) . . . . ?

C7 C8 C9 C10 0.5(6) . . . . ?

C8 C9 C10 C11 -1.0(5) . . . . ?

C9 C10 C11 N4 -176.3(3) . . . . ?

C9 C10 C11 C6 0.4(5) . . . . ?

C5 N4 C11 C10 177.3(3) . . . . ?

C12 N4 C11 C10 -3.0(6) . . . . ?

C5 N4 C11 C6 0.2(3) . . . . ?

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C21 N6 C15 C14 178.3(3) . . . . ?

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N1 C14 C15 N5 -13.6(4) . . . . ?

N1 C14 C15 N6 167.8(3) . . . . ?

C15 N5 C16 C17 -178.8(3) . . . . ?

Fe1 N5 C16 C17 21.4(5) . . . . ?

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Fe2 N2 C24 C25 -26.4(3) . . . . ?

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C25 N7 C26 C27 179.3(3) . . . . ?

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C26 C27 C28 C29 -1.7(5) . . . . ?

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C28 C29 C30 C31 -0.2(5) . . . . ?

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Fe2 N9 C35 N10 177.56(18) . . . . ?

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C66 C67 C68 C69 0.7(5) . . . . ?

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O4 S1 C70 F3 -60.6(4) . . . . ?

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O6 S1 C70 F1 -60.4(3) . . . . ?

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PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O3 O 0.22747(7) 0.49373(9) 0.56988(7) 0.0513(4) Uani 1 1 d . . .

O4 O 0.27255(9) 0.60461(9) 0.60628(8) 0.0626(5) Uani 1 1 d . . .

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C1 C 0.32867(10) 0.32170(13) 0.51059(9) 0.0406(6) Uani 1 1 d . . .

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C2 C 0.39297(11) 0.30245(14) 0.52586(10) 0.0474(6) Uani 1 1 d . . .

H2A H 0.3997 0.2561 0.5099 0.057 Uiso 1 1 calc R . .

H2B H 0.4168 0.3371 0.5093 0.057 Uiso 1 1 calc R . .

C3 C 0.31252(11) 0.32797(14) 0.44715(10) 0.0451(6) Uani 1 1 d . . .

H3A H 0.3389 0.3617 0.4329 0.054 Uiso 1 1 calc R . .

H3B H 0.3174 0.2820 0.4296 0.054 Uiso 1 1 calc R . .

C4 C 0.47513(11) 0.31109(14) 0.60318(12) 0.0560(7) Uani 1 1 d . . .

H4A H 0.4955 0.2873 0.5755 0.067 Uiso 1 1 calc R . .

H4B H 0.4889 0.2906 0.6406 0.067 Uiso 1 1 calc R . .

C5 C 0.48828(11) 0.38763(14) 0.60395(10) 0.0453(6) Uani 1 1 d . . .

C6 C 0.47872(11) 0.50017(14) 0.61764(10) 0.0468(6) Uani 1 1 d . . .

C7 C 0.46102(12) 0.56615(15) 0.63138(12) 0.0593(7) Uani 1 1 d . . .

H7A H 0.4239 0.5735 0.6419 0.071 Uiso 1 1 calc R . .

C8 C 0.49910(14) 0.62084(17) 0.62933(15) 0.0745(9) Uani 1 1 d . . .

H8A H 0.4883 0.6665 0.6392 0.089 Uiso 1 1 calc R . .

C9 C 0.55360(14) 0.61023(18) 0.61292(15) 0.0783(10) Uani 1 1 d . . .

H9A H 0.5785 0.6492 0.6112 0.094 Uiso 1 1 calc R . .

C10 C 0.57227(13) 0.54495(17) 0.59916(14) 0.0688(8) Uani 1 1 d . . .

H10E H 0.6091 0.5381 0.5879 0.083 Uiso 1 1 calc R . .

C11 C 0.53404(11) 0.48967(15) 0.60272(11) 0.0512(7) Uani 1 1 d . . .

C12 C 0.59100(12) 0.38246(18) 0.57851(13) 0.0711(9) Uani 1 1 d . . .

H12A H 0.5921 0.3331 0.5909 0.085 Uiso 1 1 calc R . .

H12B H 0.6267 0.4057 0.5976 0.085 Uiso 1 1 calc R . .

C13 C 0.5897(2) 0.3851(3) 0.51499(17) 0.1227(16) Uani 1 1 d . . .

H13A H 0.6240 0.3611 0.5055 0.184 Uiso 1 1 calc R . .

H13B H 0.5899 0.4340 0.5028 0.184 Uiso 1 1 calc R . .

H13C H 0.5544 0.3621 0.4960 0.184 Uiso 1 1 calc R . .

C14 C 0.38974(13) 0.23777(14) 0.61460(11) 0.0553(7) Uani 1 1 d . . .

H14A H 0.4230 0.2071 0.6291 0.066 Uiso 1 1 calc R . .

H14B H 0.3627 0.2111 0.5865 0.066 Uiso 1 1 calc R . .

C15 C 0.35890(11) 0.25975(14) 0.66215(10) 0.0459(6) Uani 1 1 d . . .

C16 C 0.31865(11) 0.32501(14) 0.71966(10) 0.0469(6) Uani 1 1 d . . .

C17 C 0.29878(12) 0.37952(16) 0.74976(11) 0.0565(7) Uani 1 1 d . . .

H17A H 0.3022 0.4268 0.7389 0.068 Uiso 1 1 calc R . .

C18 C 0.27363(14) 0.36177(18) 0.79661(13) 0.0728(9) Uani 1 1 d . . .

H18A H 0.2598 0.3977 0.8182 0.087 Uiso 1 1 calc R . .

C19 C 0.26848(15) 0.2923(2) 0.81226(14) 0.0819(10) Uani 1 1 d . . .

H19A H 0.2506 0.2823 0.8441 0.098 Uiso 1 1 calc R . .

C20 C 0.28803(14) 0.23780(18) 0.78380(14) 0.0728(9) Uani 1 1 d . . .

H20A H 0.2845 0.1907 0.7952 0.087 Uiso 1 1 calc R . .

C21 C 0.31394(11) 0.25538(15) 0.73613(11) 0.0525(7) Uani 1 1 d . . .

C22 C 0.34421(14) 0.13766(15) 0.69936(13) 0.0677(8) Uani 1 1 d . . .

H22A H 0.3544 0.1212 0.7386 0.081 Uiso 1 1 calc R . .

H22B H 0.3759 0.1234 0.6789 0.081 Uiso 1 1 calc R . .

C23 C 0.28815(18) 0.10308(18) 0.67259(19) 0.1105(14) Uani 1 1 d . . .

H23A H 0.2929 0.0522 0.6740 0.166 Uiso 1 1 calc R . .

H23B H 0.2785 0.1181 0.6334 0.166 Uiso 1 1 calc R . .

H23C H 0.2567 0.1165 0.6930 0.166 Uiso 1 1 calc R . .

C24 C 0.24328(12) 0.38995(13) 0.37657(10) 0.0480(6) Uani 1 1 d . . .

H24A H 0.2044 0.3792 0.3551 0.058 Uiso 1 1 calc R . .

H24B H 0.2730 0.3741 0.3542 0.058 Uiso 1 1 calc R . .

C25 C 0.24885(10) 0.46721(14) 0.38613(10) 0.0439(6) Uani 1 1 d . . .

C26 C 0.24315(11) 0.56869(14) 0.42633(10) 0.0473(6) Uani 1 1 d . . .

C27 C 0.23552(13) 0.62413(14) 0.46232(12) 0.0595(7) Uani 1 1 d . . .

H27A H 0.2313 0.6161 0.5003 0.071 Uiso 1 1 calc R . .

C28 C 0.23435(15) 0.69152(16) 0.44042(14) 0.0736(9) Uani 1 1 d . . .

H28A H 0.2287 0.7301 0.4637 0.088 Uiso 1 1 calc R . .

C29 C 0.24141(15) 0.70340(18) 0.38441(15) 0.0799(10) Uani 1 1 d . . .

H29A H 0.2409 0.7500 0.3709 0.096 Uiso 1 1 calc R . .

C30 C 0.24914(14) 0.64894(17) 0.34833(13) 0.0676(8) Uani 1 1 d . . .

H30A H 0.2537 0.6572 0.3105 0.081 Uiso 1 1 calc R . .

C31 C 0.24984(12) 0.58159(15) 0.37032(11) 0.0526(7) Uani 1 1 d . . .

C32 C 0.26255(13) 0.50265(17) 0.28672(10) 0.0643(8) Uani 1 1 d . . .

H32A H 0.2416 0.5389 0.2620 0.077 Uiso 1 1 calc R . .

H32B H 0.2457 0.4566 0.2744 0.077 Uiso 1 1 calc R . .

C33 C 0.32625(17) 0.5037(3) 0.28095(14) 0.1116(15) Uani 1 1 d . . .

H33A H 0.3303 0.4951 0.2417 0.167 Uiso 1 1 calc R . .

H33B H 0.3469 0.4672 0.3048 0.167 Uiso 1 1 calc R . .

H33C H 0.3429 0.5494 0.2926 0.167 Uiso 1 1 calc R . .

C34 C 0.20811(11) 0.29410(13) 0.43295(10) 0.0472(6) Uani 1 1 d . . .

H34A H 0.2265 0.2554 0.4566 0.057 Uiso 1 1 calc R . .

H34B H 0.1952 0.2758 0.3946 0.057 Uiso 1 1 calc R . .

C35 C 0.15661(11) 0.32169(13) 0.45685(10) 0.0427(6) Uani 1 1 d . . .

C36 C 0.10400(11) 0.38618(13) 0.50442(10) 0.0451(6) Uani 1 1 d . . .

C37 C 0.08197(12) 0.43727(15) 0.53683(11) 0.0536(7) Uani 1 1 d . . .

H37A H 0.1052 0.4753 0.5525 0.064 Uiso 1 1 calc R . .

C38 C 0.02430(13) 0.42991(17) 0.54521(13) 0.0636(8) Uani 1 1 d . . .

H38A H 0.0080 0.4636 0.5670 0.076 Uiso 1 1 calc R . .

C39 C -0.01007(13) 0.37324(19) 0.52183(14) 0.0729(9) Uani 1 1 d . . .

H39A H -0.0490 0.3697 0.5287 0.087 Uiso 1 1 calc R . .

C40 C 0.01054(13) 0.32344(18) 0.48979(13) 0.0693(9) Uani 1 1 d . . .

H40A H -0.0131 0.2859 0.4738 0.083 Uiso 1 1 calc R . .

C41 C 0.06895(11) 0.33053(14) 0.48150(11) 0.0513(7) Uani 1 1 d . . .

C42 C 0.08562(15) 0.22274(17) 0.42259(13) 0.0755(10) Uani 1 1 d . . .

H42A H 0.0441 0.2251 0.4057 0.091 Uiso 1 1 calc R . .

H42B H 0.1086 0.2147 0.3920 0.091 Uiso 1 1 calc R . .

C43 C 0.0947(2) 0.16371(19) 0.46283(17) 0.1219(17) Uani 1 1 d . . .

H43A H 0.0824 0.1200 0.4432 0.183 Uiso 1 1 calc R . .

H43B H 0.0716 0.1714 0.4929 0.183 Uiso 1 1 calc R . .

H43C H 0.1359 0.1607 0.4790 0.183 Uiso 1 1 calc R . .

C44 C 0.31500(12) 0.65124(15) 0.63363(12) 0.0560(7) Uani 1 1 d . . .

C45 C 0.34004(13) 0.64323(16) 0.68974(13) 0.0647(8) Uani 1 1 d . . .

H45A H 0.3292 0.6054 0.7113 0.078 Uiso 1 1 calc R . .

C46 C 0.38163(15) 0.6924(2) 0.71372(16) 0.0835(11) Uani 1 1 d . . .

H46A H 0.3999 0.6876 0.7516 0.100 Uiso 1 1 calc R . .

C47 C 0.39567(17) 0.7479(2) 0.6813(2) 0.1010(13) Uani 1 1 d . . .

H47A H 0.4236 0.7813 0.6973 0.121 Uiso 1 1 calc R . .

C48 C 0.36929(17) 0.7552(2) 0.6256(2) 0.0917(11) Uani 1 1 d . . .

H48A H 0.3789 0.7938 0.6042 0.110 Uiso 1 1 calc R . .

C49 C 0.32953(14) 0.70706(16) 0.60168(15) 0.0698(8) Uani 1 1 d . . .

H49A H 0.3120 0.7117 0.5635 0.084 Uiso 1 1 calc R . .

C50 C 0.17481(13) 0.52543(18) 0.67349(13) 0.0656(8) Uani 1 1 d U . .

C51 C 0.15180(15) 0.4775(2) 0.70779(16) 0.0820(10) Uani 1 1 d U . .

H51A H 0.1761 0.4429 0.7276 0.098 Uiso 1 1 calc R . .

C52 C 0.09390(19) 0.4806(3) 0.7129(2) 0.1147(15) Uani 1 1 d U . .

H52A H 0.0780 0.4483 0.7362 0.138 Uiso 1 1 calc R . .

C53 C 0.0599(2) 0.5304(3) 0.6840(2) 0.1239(18) Uani 1 1 d U . .

H53A H 0.0199 0.5322 0.6876 0.149 Uiso 1 1 calc R . .

C54 C 0.08092(19) 0.5788(3) 0.64960(19) 0.1091(15) Uani 1 1 d U . .

H54A H 0.0560 0.6129 0.6299 0.131 Uiso 1 1 calc R . .

C55 C 0.14103(15) 0.5761(2) 0.64437(14) 0.0864(11) Uani 1 1 d U . .

H55A H 0.1572 0.6086 0.6214 0.104 Uiso 1 1 calc R . .

C56 C 0.39167(13) 0.42831(15) 0.12494(11) 0.0554(7) Uani 1 1 d . . .

C57 C 0.33578(13) 0.39905(17) 0.12281(12) 0.0649(8) Uani 1 1 d . . .

H57A H 0.3319 0.3497 0.1202 0.078 Uiso 1 1 calc R . .

C58 C 0.28537(14) 0.4392(2) 0.12433(13) 0.0731(9) Uani 1 1 d . . .

H58A H 0.2486 0.4170 0.1221 0.088 Uiso 1 1 calc R . .

C59 C 0.28977(16) 0.5115(2) 0.12918(14) 0.0799(10) Uani 1 1 d . . .

H59A H 0.2562 0.5393 0.1303 0.096 Uiso 1 1 calc R . .

C60 C 0.34429(17) 0.54261(18) 0.13236(14) 0.0789(9) Uani 1 1 d . . .

H60A H 0.3480 0.5919 0.1363 0.095 Uiso 1 1 calc R . .

C61 C 0.39393(14) 0.50150(16) 0.12982(12) 0.0662(8) Uani 1 1 d . . .

H61A H 0.4304 0.5241 0.1315 0.079 Uiso 1 1 calc R . .

C62 C 0.51183(12) 0.41305(14) 0.13583(11) 0.0530(7) Uani 1 1 d . . .

C63 C 0.55982(14) 0.39706(18) 0.10975(14) 0.0735(9) Uani 1 1 d . . .

H63A H 0.5535 0.3697 0.0765 0.088 Uiso 1 1 calc R . .

C64 C 0.61622(15) 0.4192(2) 0.13000(15) 0.0850(10) Uani 1 1 d . . .

H64A H 0.6471 0.4065 0.1107 0.102 Uiso 1 1 calc R . .

C65 C 0.62753(15) 0.45930(18) 0.17797(16) 0.0768(9) Uani 1 1 d . . .

H65A H 0.6657 0.4759 0.1913 0.092 Uiso 1 1 calc R . .

C66 C 0.58213(15) 0.47475(16) 0.20598(14) 0.0746(9) Uani 1 1 d . . .

H66A H 0.5893 0.5013 0.2396 0.090 Uiso 1 1 calc R . .

C67 C 0.52555(13) 0.45199(15) 0.18569(12) 0.0615(8) Uani 1 1 d . . .

H67A H 0.4953 0.4632 0.2063 0.074 Uiso 1 1 calc R . .

C68 C 0.45014(12) 0.30656(15) 0.15363(12) 0.0566(7) Uani 1 1 d . . .

C69 C 0.43409(13) 0.30550(18) 0.20758(13) 0.0693(8) Uani 1 1 d . . .

H69A H 0.4163 0.3458 0.2204 0.083 Uiso 1 1 calc R . .

C70 C 0.44344(15) 0.2470(2) 0.24285(15) 0.0838(10) Uani 1 1 d . . .

H70A H 0.4321 0.2482 0.2789 0.101 Uiso 1 1 calc R . .

C71 C 0.46948(16) 0.1867(2) 0.22493(19) 0.0898(12) Uani 1 1 d . . .

H71A H 0.4755 0.1467 0.2484 0.108 Uiso 1 1 calc R . .

C72 C 0.48594(17) 0.18674(18) 0.17300(18) 0.0889(11) Uani 1 1 d . . .

H72A H 0.5038 0.1464 0.1605 0.107 Uiso 1 1 calc R . .

C73 C 0.47683(14) 0.24497(16) 0.13838(14) 0.0715(9) Uani 1 1 d . . .

H73A H 0.4892 0.2432 0.1028 0.086 Uiso 1 1 calc R . .

C74 C 0.43436(12) 0.36186(17) 0.04645(12) 0.0620(8) Uani 1 1 d U . .

C75 C 0.39984(14) 0.30552(18) 0.02357(13) 0.0720(9) Uani 1 1 d U . .

H75A H 0.3865 0.2729 0.0483 0.086 Uiso 1 1 calc R . .

C76 C 0.38428(16) 0.2957(2) -0.03513(16) 0.0939(12) Uani 1 1 d U . .

H76A H 0.3602 0.2575 -0.0491 0.113 Uiso 1 1 calc R . .

C77 C 0.40400(19) 0.3415(3) -0.07216(16) 0.1097(15) Uani 1 1 d U . .

H77A H 0.3943 0.3343 -0.1115 0.132 Uiso 1 1 calc R . .

C78 C 0.43807(18) 0.3978(3) -0.05143(16) 0.1102(14) Uani 1 1 d U . .

H78A H 0.4519 0.4295 -0.0766 0.132 Uiso 1 1 calc R . .

C79 C 0.45243(15) 0.4082(2) 0.00737(14) 0.0836(10) Uani 1 1 d U . .

H79A H 0.4750 0.4479 0.0208 0.100 Uiso 1 1 calc R . .

C80 C 0.08565(13) 0.32963(15) 0.16168(11) 0.0578(7) Uani 1 1 d U . .

C81 C 0.11816(15) 0.30257(17) 0.12173(12) 0.0730(9) Uani 1 1 d U . .

H81A H 0.1527 0.2773 0.1348 0.088 Uiso 1 1 calc R . .

C82 C 0.1014(2) 0.3116(2) 0.06342(14) 0.1032(13) Uani 1 1 d U . .

H82A H 0.1249 0.2937 0.0379 0.124 Uiso 1 1 calc R . .

C83 C 0.0508(3) 0.3466(3) 0.04392(17) 0.1214(18) Uani 1 1 d U . .

H83A H 0.0390 0.3523 0.0047 0.146 Uiso 1 1 calc R . .

C84 C 0.0166(2) 0.3738(2) 0.08075(18) 0.1030(13) Uani 1 1 d U . .

H84A H -0.0183 0.3980 0.0668 0.124 Uiso 1 1 calc R . .

C85 C 0.03423(14) 0.36535(17) 0.13954(13) 0.0750(9) Uani 1 1 d U . .

H85A H 0.0107 0.3843 0.1645 0.090 Uiso 1 1 calc R . .

C86 C 0.17048(11) 0.28929(14) 0.24932(9) 0.0453(6) Uani 1 1 d . . .

C87 C 0.21763(12) 0.32442(15) 0.23011(11) 0.0557(7) Uani 1 1 d . . .

H87A H 0.2091 0.3624 0.2048 0.067 Uiso 1 1 calc R . .

C88 C 0.27608(13) 0.30552(18) 0.24680(13) 0.0676(9) Uani 1 1 d . . .

H88A H 0.3060 0.3299 0.2324 0.081 Uiso 1 1 calc R . .

C89 C 0.28996(13) 0.25047(19) 0.28479(13) 0.0704(9) Uani 1 1 d . . .

H89A H 0.3294 0.2373 0.2964 0.084 Uiso 1 1 calc R . .

C90 C 0.24608(13) 0.21548(16) 0.30529(11) 0.0617(8) Uani 1 1 d . . .

H90A H 0.2552 0.1783 0.3313 0.074 Uiso 1 1 calc R . .

C91 C 0.18792(12) 0.23476(14) 0.28768(10) 0.0503(7) Uani 1 1 d . . .

H91A H 0.1586 0.2097 0.3024 0.060 Uiso 1 1 calc R . .

C92 C 0.05508(11) 0.25928(14) 0.24683(10) 0.0487(6) Uani 1 1 d . . .

C93 C 0.00430(12) 0.27722(16) 0.26867(12) 0.0608(8) Uani 1 1 d . . .

H93A H -0.0035 0.3252 0.2741 0.073 Uiso 1 1 calc R . .

C94 C -0.03493(13) 0.2276(2) 0.28266(14) 0.0786(10) Uani 1 1 d . . .

H94A H -0.0685 0.2426 0.2970 0.094 Uiso 1 1 calc R . .

C95 C -0.02585(17) 0.1579(2) 0.27604(15) 0.0852(11) Uani 1 1 d . . .

H95A H -0.0516 0.1244 0.2877 0.102 Uiso 1 1 calc R . .

C96 C 0.02193(16) 0.13651(17) 0.25185(13) 0.0758(10) Uani 1 1 d . . .

H96A H 0.0279 0.0884 0.2452 0.091 Uiso 1 1 calc R . .

C97 C 0.06126(13) 0.18712(15) 0.23736(11) 0.0590(7) Uani 1 1 d . . .

H97A H 0.0932 0.1718 0.2205 0.071 Uiso 1 1 calc R . .

C98 C 0.09994(11) 0.39259(14) 0.26459(11) 0.0504(7) Uani 1 1 d . . .

C99 C 0.10826(13) 0.45745(16) 0.24107(14) 0.0674(8) Uani 1 1 d . . .

H99A H 0.1122 0.4592 0.2025 0.081 Uiso 1 1 calc R . .

C100 C 0.11114(15) 0.52041(18) 0.27119(18) 0.0815(10) Uani 1 1 d . . .

H10A H 0.1172 0.5632 0.2530 0.098 Uiso 1 1 calc R . .

C101 C 0.10518(14) 0.52033(19) 0.32679(19) 0.0829(11) Uani 1 1 d . . .

H10B H 0.1066 0.5629 0.3472 0.099 Uiso 1 1 calc R . .

C102 C 0.09702(13) 0.4571(2) 0.35291(14) 0.0753(10) Uani 1 1 d . . .

H10C H 0.0933 0.4562 0.3915 0.090 Uiso 1 1 calc R . .

C103 C 0.09430(12) 0.39455(16) 0.32191(12) 0.0614(8) Uani 1 1 d . . .

H10D H 0.0884 0.3519 0.3403 0.074 Uiso 1 1 calc R . .

C104 C 0.1886(2) 0.2664(2) 0.61044(19) 0.0982(13) Uani 1 1 d . . .

C105 C 0.1469(2) 0.2862(3) 0.6464(2) 0.1307(17) Uani 1 1 d . . .

H10H H 0.1542 0.3345 0.6591 0.157 Uiso 1 1 calc R . .

H10F H 0.1510 0.2550 0.6790 0.157 Uiso 1 1 calc R . .

H10G H 0.1074 0.2824 0.6254 0.157 Uiso 1 1 calc R . .

B1 B 0.44688(15) 0.37826(17) 0.11521(13) 0.0545(8) Uani 1 1 d . . .

B2 B 0.10256(13) 0.31734(16) 0.23082(12) 0.0479(7) Uani 1 1 d . . .

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

Fe1 0.0383(2) 0.0438(2) 0.03107(18) 0.00258(14) 0.00460(14) 0.00175(15)

Fe2 0.0360(2) 0.0436(2) 0.03072(18) -0.00093(14) 0.00296(14) -0.00201(15)

P1 0.0471(4) 0.0490(4) 0.0406(4) -0.0080(3) 0.0057(3) 0.0049(3)

O1 0.0404(9) 0.0476(10) 0.0330(8) -0.0040(7) 0.0023(7) 0.0041(7)

O2 0.0463(10) 0.0489(10) 0.0514(10) -0.0097(8) 0.0089(8) 0.0022(8)

O3 0.0465(10) 0.0604(11) 0.0460(10) -0.0153(8) 0.0042(8) 0.0019(9)

O4 0.0694(13) 0.0502(11) 0.0603(12) -0.0040(9) -0.0135(10) 0.0010(10)

O5 0.0440(11) 0.0923(14) 0.0442(10) -0.0096(10) 0.0086(8) 0.0114(10)

N1 0.0440(12) 0.0471(12) 0.0362(11) 0.0039(9) 0.0024(9) 0.0047(10)

N2 0.0403(12) 0.0551(13) 0.0439(12) -0.0008(10) 0.0068(10) 0.0042(11)

N3 0.0427(12) 0.0485(13) 0.0383(11) 0.0059(9) 0.0041(9) 0.0003(10)

N4 0.0384(11) 0.0474(12) 0.0315(10) -0.0015(9) 0.0041(9) -0.0053(9)

N5 0.0438(12) 0.0478(12) 0.0362(11) 0.0022(9) 0.0015(9) -0.0027(10)

N6 0.0392(12) 0.0481(12) 0.0370(11) -0.0022(9) 0.0042(9) -0.0067(9)

N7 0.0360(13) 0.0715(16) 0.0506(13) 0.0017(11) 0.0085(10) 0.0091(11)

N8 0.0508(14) 0.0510(13) 0.0577(14) 0.0188(11) 0.0069(11) 0.0011(11)

N9 0.0511(14) 0.0621(14) 0.0341(11) 0.0101(10) 0.0001(10) -0.0058(11)

N10 0.0541(14) 0.0593(14) 0.0421(12) -0.0067(10) 0.0084(10) -0.0210(11)

N11 0.107(3) 0.188(4) 0.108(3) 0.053(3) 0.033(2) -0.002(3)

C1 0.0436(15) 0.0449(14) 0.0332(13) -0.0015(11) 0.0061(11) 0.0010(11)

C2 0.0520(16) 0.0502(15) 0.0403(14) -0.0028(11) 0.0082(12) 0.0074(12)

C3 0.0451(15) 0.0528(15) 0.0377(13) -0.0055(11) 0.0078(11) 0.0021(12)

C4 0.0478(17) 0.0646(19) 0.0529(16) 0.0006(13) -0.0004(13) 0.0155(14)

C5 0.0399(15) 0.0555(17) 0.0393(14) 0.0001(12) 0.0031(11) 0.0067(13)

C6 0.0397(15) 0.0557(17) 0.0453(15) -0.0013(12) 0.0075(12) -0.0049(13)

C7 0.0438(16) 0.0628(19) 0.074(2) -0.0067(15) 0.0182(14) -0.0055(14)

C8 0.061(2) 0.0602(19) 0.109(3) -0.0114(18) 0.0322(19) -0.0068(16)

C9 0.059(2) 0.070(2) 0.113(3) -0.0065(19) 0.0345(19) -0.0172(17)

C10 0.0479(18) 0.076(2) 0.087(2) -0.0008(17) 0.0253(16) -0.0032(16)

C11 0.0407(16) 0.0620(18) 0.0516(16) -0.0003(13) 0.0092(12) 0.0024(13)

C12 0.0431(17) 0.087(2) 0.084(2) -0.0084(18) 0.0127(16) 0.0155(16)

C13 0.115(3) 0.174(4) 0.091(3) -0.015(3) 0.054(3) 0.033(3)

C14 0.0692(19) 0.0469(16) 0.0493(16) 0.0083(12) 0.0080(14) 0.0069(14)

C15 0.0423(15) 0.0512(16) 0.0417(14) 0.0099(12) -0.0009(11) -0.0005(12)

C16 0.0382(15) 0.0608(17) 0.0409(14) 0.0116(13) 0.0043(11) -0.0025(12)

C17 0.0560(18) 0.0657(18) 0.0491(16) 0.0077(14) 0.0126(14) -0.0019(14)

C18 0.074(2) 0.087(2) 0.064(2) 0.0099(17) 0.0305(17) -0.0001(18)

C19 0.085(3) 0.098(3) 0.073(2) 0.025(2) 0.0411(19) -0.002(2)

C20 0.069(2) 0.076(2) 0.078(2) 0.0289(18) 0.0237(18) -0.0040(18)

C21 0.0434(16) 0.0606(18) 0.0532(16) 0.0173(14) 0.0070(13) -0.0030(13)

C22 0.074(2) 0.0517(18) 0.076(2) 0.0222(15) 0.0092(17) 0.0013(16)

C23 0.114(3) 0.061(2) 0.145(4) 0.015(2) -0.014(3) -0.023(2)

C24 0.0498(16) 0.0613(17) 0.0319(13) -0.0020(12) 0.0030(11) -0.0071(13)

C25 0.0360(14) 0.0596(17) 0.0325(13) 0.0044(12) -0.0055(10) -0.0073(12)

C26 0.0460(16) 0.0499(16) 0.0434(14) 0.0091(12) -0.0005(12) -0.0009(12)

C27 0.070(2) 0.0526(17) 0.0543(17) 0.0070(14) 0.0049(15) 0.0039(15)

C28 0.089(2) 0.0518(18) 0.078(2) 0.0112(16) 0.0093(18) 0.0100(16)

C29 0.099(3) 0.058(2) 0.081(2) 0.0270(18) 0.010(2) 0.0048(18)

C30 0.075(2) 0.070(2) 0.0573(18) 0.0221(17) 0.0075(16) 0.0024(17)

C31 0.0462(16) 0.0620(19) 0.0462(15) 0.0114(13) -0.0024(12) -0.0049(13)

C32 0.076(2) 0.084(2) 0.0309(14) 0.0083(14) 0.0008(13) -0.0153(17)

C33 0.096(3) 0.195(5) 0.048(2) -0.009(2) 0.0256(19) -0.034(3)

C34 0.0512(16) 0.0496(15) 0.0408(14) -0.0078(12) 0.0073(12) -0.0100(12)

C35 0.0428(15) 0.0517(15) 0.0326(13) 0.0007(11) 0.0025(11) -0.0124(12)

C36 0.0412(15) 0.0550(16) 0.0389(14) 0.0022(12) 0.0063(11) -0.0059(12)

C37 0.0489(17) 0.0619(18) 0.0501(16) 0.0004(13) 0.0078(13) -0.0022(13)

C38 0.0494(18) 0.076(2) 0.0685(19) 0.0008(16) 0.0200(15) 0.0066(16)

C39 0.0462(18) 0.096(3) 0.080(2) 0.0006(19) 0.0199(16) -0.0091(18)

C40 0.0545(19) 0.089(2) 0.065(2) -0.0040(17) 0.0131(16) -0.0244(17)

C41 0.0448(16) 0.0627(17) 0.0466(15) 0.0008(13) 0.0078(12) -0.0114(14)

C42 0.076(2) 0.085(2) 0.070(2) -0.0282(18) 0.0266(17) -0.0393(18)

C43 0.211(5) 0.073(3) 0.095(3) -0.016(2) 0.065(3) -0.049(3)

C44 0.0516(17) 0.0495(17) 0.0653(19) -0.0172(14) 0.0043(14) 0.0077(14)

C45 0.066(2) 0.0619(19) 0.0627(19) -0.0167(15) -0.0015(15) 0.0090(15)

C46 0.067(2) 0.089(3) 0.087(3) -0.037(2) -0.0074(19) 0.015(2)

C47 0.068(3) 0.085(3) 0.147(4) -0.038(3) 0.007(3) -0.015(2)

C48 0.078(3) 0.076(2) 0.124(3) -0.007(2) 0.024(2) -0.013(2)

C49 0.067(2) 0.063(2) 0.080(2) -0.0082(17) 0.0137(17) 0.0003(17)

C50 0.0491(18) 0.091(2) 0.0563(18) -0.0348(16) 0.0064(14) 0.0113(16)

C51 0.063(2) 0.096(3) 0.092(3) -0.030(2) 0.0267(19) -0.0138(19)

C52 0.064(3) 0.141(4) 0.143(4) -0.048(3) 0.030(3) -0.018(3)

C53 0.054(3) 0.182(5) 0.133(4) -0.079(4) 0.007(3) 0.004(3)

C54 0.074(3) 0.151(4) 0.094(3) -0.059(3) -0.009(2) 0.038(3)

C55 0.072(2) 0.118(3) 0.064(2) -0.0298(19) -0.0049(17) 0.040(2)

C56 0.0594(18) 0.0655(19) 0.0422(15) 0.0091(13) 0.0105(13) -0.0013(15)

C57 0.064(2) 0.071(2) 0.0605(18) 0.0068(15) 0.0121(15) -0.0013(16)

C58 0.058(2) 0.098(3) 0.066(2) 0.0158(18) 0.0180(16) 0.0035(18)

C59 0.076(3) 0.095(3) 0.070(2) 0.0154(19) 0.0171(18) 0.025(2)

C60 0.092(3) 0.064(2) 0.082(2) 0.0118(17) 0.017(2) 0.013(2)

C61 0.070(2) 0.063(2) 0.067(2) 0.0109(15) 0.0136(16) 0.0006(16)

C62 0.0547(17) 0.0556(17) 0.0496(16) 0.0017(13) 0.0114(13) -0.0024(13)

C63 0.061(2) 0.095(2) 0.065(2) -0.0137(17) 0.0104(16) -0.0123(18)

C64 0.063(2) 0.119(3) 0.077(2) -0.005(2) 0.0212(18) -0.005(2)

C65 0.061(2) 0.075(2) 0.091(3) -0.0012(19) 0.0016(19) -0.0068(17)

C66 0.077(2) 0.064(2) 0.076(2) -0.0117(17) -0.0069(19) 0.0010(18)

C67 0.061(2) 0.0616(18) 0.0606(18) -0.0027(15) 0.0055(15) 0.0040(15)

C68 0.0494(17) 0.0598(18) 0.0582(18) -0.0031(14) 0.0014(14) -0.0098(14)

C69 0.0568(19) 0.082(2) 0.069(2) 0.0113(17) 0.0106(16) 0.0010(16)

C70 0.063(2) 0.108(3) 0.080(2) 0.034(2) 0.0082(18) -0.009(2)

C71 0.074(3) 0.072(2) 0.116(3) 0.030(2) -0.010(2) -0.013(2)

C72 0.097(3) 0.062(2) 0.101(3) -0.004(2) -0.005(2) 0.0023(19)

C73 0.079(2) 0.058(2) 0.073(2) -0.0059(17) 0.0011(17) 0.0002(17)

C74 0.0502(17) 0.081(2) 0.0541(17) -0.0072(15) 0.0068(14) -0.0001(15)

C75 0.065(2) 0.085(2) 0.0631(19) -0.0156(17) 0.0002(16) 0.0073(17)

C76 0.068(2) 0.128(3) 0.077(2) -0.035(2) -0.0148(19) 0.019(2)

C77 0.085(3) 0.191(5) 0.051(2) -0.019(3) 0.004(2) 0.031(3)

C78 0.083(3) 0.192(5) 0.055(2) 0.012(3) 0.008(2) -0.003(3)

C79 0.074(2) 0.119(3) 0.059(2) 0.0033(19) 0.0110(17) -0.012(2)

C80 0.0611(18) 0.0574(17) 0.0486(16) 0.0066(13) -0.0104(14) -0.0192(14)

C81 0.090(2) 0.084(2) 0.0433(17) -0.0024(15) 0.0041(16) -0.0226(18)

C82 0.137(4) 0.127(3) 0.0434(19) 0.001(2) 0.005(2) -0.045(3)

C83 0.163(5) 0.136(4) 0.052(2) 0.032(2) -0.023(3) -0.056(3)

C84 0.112(3) 0.095(3) 0.084(3) 0.036(2) -0.040(2) -0.027(2)

C85 0.072(2) 0.072(2) 0.070(2) 0.0184(16) -0.0219(17) -0.0194(17)

C86 0.0463(15) 0.0593(16) 0.0294(13) -0.0093(11) 0.0032(11) -0.0061(13)

C87 0.0588(19) 0.0676(18) 0.0405(15) -0.0064(13) 0.0071(13) -0.0093(15)

C88 0.0478(19) 0.102(3) 0.0556(18) -0.0190(18) 0.0163(15) -0.0130(17)

C89 0.0461(18) 0.106(3) 0.0557(18) -0.0178(18) -0.0010(15) 0.0119(18)

C90 0.064(2) 0.076(2) 0.0433(16) -0.0043(14) 0.0022(14) 0.0137(16)

C91 0.0523(17) 0.0646(18) 0.0332(13) -0.0022(12) 0.0044(12) 0.0014(14)

C92 0.0429(16) 0.0609(18) 0.0373(14) 0.0021(12) -0.0091(11) -0.0053(13)

C93 0.0465(17) 0.0702(19) 0.0619(18) 0.0073(15) -0.0035(14) -0.0075(15)

C94 0.0449(19) 0.108(3) 0.080(2) 0.021(2) 0.0025(16) -0.0176(19)

C95 0.069(2) 0.091(3) 0.088(3) 0.029(2) -0.0097(19) -0.036(2)

C96 0.089(3) 0.060(2) 0.068(2) 0.0115(16) -0.0186(19) -0.0221(19)

C97 0.0653(19) 0.0595(19) 0.0478(16) 0.0005(13) -0.0045(14) -0.0121(15)

C98 0.0385(15) 0.0556(17) 0.0533(16) -0.0008(13) -0.0045(12) -0.0039(12)

C99 0.061(2) 0.0589(19) 0.079(2) -0.0045(17) 0.0018(16) -0.0077(15)

C100 0.072(2) 0.064(2) 0.105(3) -0.003(2) 0.002(2) -0.0046(17)

C101 0.061(2) 0.062(2) 0.116(3) -0.027(2) -0.016(2) 0.0083(17)

C102 0.056(2) 0.099(3) 0.064(2) -0.023(2) -0.0132(15) 0.0201(18)

C103 0.0518(18) 0.0647(19) 0.0614(19) -0.0086(15) -0.0103(14) 0.0081(14)

C104 0.085(3) 0.122(3) 0.084(3) 0.041(3) 0.002(2) -0.019(3)

C105 0.146(4) 0.137(4) 0.117(4) -0.007(3) 0.047(3) 0.011(3)

B1 0.058(2) 0.059(2) 0.0481(18) -0.0011(15) 0.0114(15) -0.0075(16)

B2 0.0464(18) 0.0546(18) 0.0400(16) 0.0004(13) -0.0011(13) -0.0070(14)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Fe1 O1 2.0031(15) . ?

Fe1 O2 2.0506(16) . ?

Fe1 N3 2.0551(19) . ?

Fe1 N2 2.075(2) . ?

Fe1 N1 2.309(2) . ?

Fe2 O1 2.0057(16) . ?

Fe2 O3 2.0562(16) . ?

Fe2 N5 2.0668(19) . ?

Fe2 N6 2.0732(19) . ?

Fe2 N4 2.3141(18) . ?

P1 O3 1.4762(17) . ?

P1 O2 1.4784(18) . ?

P1 O5 1.5851(18) . ?

P1 O4 1.5871(19) . ?

O1 C1 1.427(3) . ?

O4 C44 1.400(3) . ?

O5 C50 1.406(3) . ?

N1 C2 1.471(3) . ?

N1 C14 1.474(3) . ?

N1 C4 1.479(3) . ?

N2 C5 1.319(3) . ?

N2 C6 1.402(3) . ?

N3 C15 1.319(3) . ?

N3 C16 1.403(3) . ?

N4 C24 1.475(3) . ?

N4 C3 1.477(3) . ?

N4 C34 1.483(3) . ?

N5 C25 1.323(3) . ?

N5 C26 1.388(3) . ?

N6 C35 1.317(3) . ?

N6 C36 1.397(3) . ?

N7 C5 1.349(3) . ?

N7 C11 1.388(3) . ?

N7 C12 1.475(3) . ?

N8 C15 1.345(3) . ?

N8 C21 1.379(3) . ?

N8 C22 1.468(3) . ?

N9 C25 1.349(3) . ?

N9 C31 1.386(3) . ?

N9 C32 1.479(3) . ?

N10 C35 1.351(3) . ?

N10 C41 1.392(3) . ?

N10 C42 1.473(3) . ?

N11 C104 1.133(5) . ?

C1 C3 1.506(3) . ?

C1 C2 1.514(3) . ?

C1 H1A 0.9900 . ?

C2 H2A 0.9800 . ?

C2 H2B 0.9800 . ?

C3 H3A 0.9800 . ?

C3 H3B 0.9800 . ?

C4 C5 1.481(4) . ?

C4 H4A 0.9800 . ?

C4 H4B 0.9800 . ?

C6 C7 1.371(4) . ?

C6 C11 1.393(3) . ?

C7 C8 1.364(4) . ?

C7 H7A 0.9400 . ?

C8 C9 1.390(4) . ?

C8 H8A 0.9400 . ?

C9 C10 1.366(4) . ?

C9 H9A 0.9400 . ?

C10 C11 1.380(4) . ?

C10 H10E 0.9400 . ?

C12 C13 1.514(5) . ?

C12 H12A 0.9800 . ?

C12 H12B 0.9800 . ?

C13 H13A 0.9700 . ?

C13 H13B 0.9700 . ?

C13 H13C 0.9700 . ?

C14 C15 1.493(4) . ?

C14 H14A 0.9800 . ?

C14 H14B 0.9800 . ?

C16 C17 1.378(4) . ?

C16 C21 1.386(4) . ?

C17 C18 1.382(4) . ?

C17 H17A 0.9400 . ?

C18 C19 1.379(4) . ?

C18 H18A 0.9400 . ?

C19 C20 1.352(4) . ?

C19 H19A 0.9400 . ?

C20 C21 1.408(4) . ?

C20 H20A 0.9400 . ?

C22 C23 1.498(4) . ?

C22 H22A 0.9800 . ?

C22 H22B 0.9800 . ?

C23 H23A 0.9700 . ?

C23 H23B 0.9700 . ?

C23 H23C 0.9700 . ?

C24 C25 1.484(3) . ?

C24 H24A 0.9800 . ?

C24 H24B 0.9800 . ?

C26 C27 1.386(4) . ?

C26 C31 1.393(4) . ?

C27 C28 1.378(4) . ?

C27 H27A 0.9400 . ?

C28 C29 1.392(4) . ?

C28 H28A 0.9400 . ?

C29 C30 1.374(4) . ?

C29 H29A 0.9400 . ?

C30 C31 1.379(4) . ?

C30 H30A 0.9400 . ?

C32 C33 1.498(4) . ?

C32 H32A 0.9800 . ?

C32 H32B 0.9800 . ?

C33 H33A 0.9700 . ?

C33 H33B 0.9700 . ?

C33 H33C 0.9700 . ?

C34 C35 1.492(3) . ?

C34 H34A 0.9800 . ?

C34 H34B 0.9800 . ?

C36 C37 1.386(3) . ?

C36 C41 1.387(3) . ?

C37 C38 1.383(4) . ?

C37 H37A 0.9400 . ?

C38 C39 1.397(4) . ?

C38 H38A 0.9400 . ?

C39 C40 1.348(4) . ?

C39 H39A 0.9400 . ?

C40 C41 1.399(4) . ?

C40 H40A 0.9400 . ?

C42 C43 1.467(5) . ?

C42 H42A 0.9800 . ?

C42 H42B 0.9800 . ?

C43 H43A 0.9700 . ?

C43 H43B 0.9700 . ?

C43 H43C 0.9700 . ?

C44 C49 1.376(4) . ?

C44 C45 1.380(4) . ?

C45 C46 1.392(4) . ?

C45 H45A 0.9400 . ?

C46 C47 1.376(5) . ?

C46 H46A 0.9400 . ?

C47 C48 1.377(6) . ?

C47 H47A 0.9400 . ?

C48 C49 1.354(5) . ?

C48 H48A 0.9400 . ?

C49 H49A 0.9400 . ?

C50 C55 1.356(4) . ?

C50 C51 1.384(5) . ?

C51 C52 1.361(5) . ?

C51 H51A 0.9400 . ?

C52 C53 1.345(7) . ?

C52 H52A 0.9400 . ?

C53 C54 1.371(7) . ?

C53 H53A 0.9400 . ?

C54 C55 1.413(5) . ?

C54 H54A 0.9400 . ?

C55 H55A 0.9400 . ?

C56 C61 1.391(4) . ?

C56 C57 1.397(4) . ?

C56 B1 1.634(4) . ?

C57 C58 1.394(4) . ?

C57 H57A 0.9400 . ?

C58 C59 1.378(5) . ?

C58 H58A 0.9400 . ?

C59 C60 1.380(5) . ?

C59 H59A 0.9400 . ?

C60 C61 1.394(4) . ?

C60 H60A 0.9400 . ?

C61 H61A 0.9400 . ?

C62 C63 1.388(4) . ?

C62 C67 1.394(4) . ?

C62 B1 1.639(4) . ?

C63 C64 1.378(4) . ?

C63 H63A 0.9400 . ?

C64 C65 1.365(5) . ?

C64 H64A 0.9400 . ?

C65 C66 1.362(4) . ?

C65 H65A 0.9400 . ?

C66 C67 1.386(4) . ?

C66 H66A 0.9400 . ?

C67 H67A 0.9400 . ?

C68 C73 1.394(4) . ?

C68 C69 1.397(4) . ?

C68 B1 1.634(4) . ?

C69 C70 1.387(4) . ?

C69 H69A 0.9400 . ?

C70 C71 1.390(5) . ?

C70 H70A 0.9400 . ?

C71 C72 1.354(5) . ?

C71 H71A 0.9400 . ?

C72 C73 1.374(5) . ?

C72 H72A 0.9400 . ?

C73 H73A 0.9400 . ?

C74 C75 1.390(4) . ?

C74 C79 1.393(4) . ?

C74 B1 1.651(4) . ?

C75 C76 1.403(4) . ?

C75 H75A 0.9400 . ?

C76 C77 1.367(6) . ?

C76 H76A 0.9400 . ?

C77 C78 1.370(6) . ?

C77 H77A 0.9400 . ?

C78 C79 1.405(5) . ?

C78 H78A 0.9400 . ?

C79 H79A 0.9400 . ?

C80 C85 1.394(4) . ?

C80 C81 1.402(4) . ?

C80 B2 1.652(4) . ?

C81 C82 1.395(4) . ?

C81 H81A 0.9400 . ?

C82 C83 1.359(6) . ?

C82 H82A 0.9400 . ?

C83 C84 1.372(6) . ?

C83 H83A 0.9400 . ?

C84 C85 1.407(5) . ?

C84 H84A 0.9400 . ?

C85 H85A 0.9400 . ?

C86 C91 1.396(3) . ?

C86 C87 1.413(3) . ?

C86 B2 1.646(4) . ?

C87 C88 1.390(4) . ?

C87 H87A 0.9400 . ?

C88 C89 1.386(4) . ?

C88 H88A 0.9400 . ?

C89 C90 1.365(4) . ?

C89 H89A 0.9400 . ?

C90 C91 1.389(4) . ?

C90 H90A 0.9400 . ?

C91 H91A 0.9400 . ?

C92 C97 1.397(4) . ?

C92 C93 1.398(4) . ?

C92 B2 1.640(4) . ?

C93 C94 1.382(4) . ?

C93 H93A 0.9400 . ?

C94 C95 1.351(5) . ?

C94 H94A 0.9400 . ?

C95 C96 1.384(5) . ?

C95 H95A 0.9400 . ?

C96 C97 1.401(4) . ?

C96 H96A 0.9400 . ?

C97 H97A 0.9400 . ?

C98 C99 1.377(4) . ?

C98 C103 1.396(4) . ?

C98 B2 1.644(4) . ?

C99 C100 1.389(4) . ?

C99 H99A 0.9400 . ?

C100 C101 1.357(5) . ?

C100 H10A 0.9400 . ?

C101 C102 1.377(5) . ?

C101 H10B 0.9400 . ?

C102 C103 1.394(4) . ?

C102 H10C 0.9400 . ?

C103 H10D 0.9400 . ?

C104 C105 1.438(6) . ?

C105 H10H 0.9700 . ?

C105 H10F 0.9700 . ?

C105 H10G 0.9700 . ?

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_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O1 Fe1 O2 98.93(7) . . ?

O1 Fe1 N3 113.47(7) . . ?

O2 Fe1 N3 104.83(8) . . ?

O1 Fe1 N2 116.39(7) . . ?

O2 Fe1 N2 100.66(8) . . ?

N3 Fe1 N2 118.52(8) . . ?

O1 Fe1 N1 81.46(6) . . ?

O2 Fe1 N1 177.89(7) . . ?

N3 Fe1 N1 76.84(7) . . ?

N2 Fe1 N1 77.34(8) . . ?

O1 Fe2 O3 98.99(6) . . ?

O1 Fe2 N5 114.51(7) . . ?

O3 Fe2 N5 105.97(8) . . ?

O1 Fe2 N6 126.76(7) . . ?

O3 Fe2 N6 100.03(7) . . ?

N5 Fe2 N6 107.06(8) . . ?

O1 Fe2 N4 80.86(6) . . ?

O3 Fe2 N4 176.30(7) . . ?

N5 Fe2 N4 77.35(7) . . ?

N6 Fe2 N4 77.26(7) . . ?

O3 P1 O2 119.47(10) . . ?

O3 P1 O5 110.00(10) . . ?

O2 P1 O5 105.89(10) . . ?

O3 P1 O4 105.61(10) . . ?

O2 P1 O4 110.50(10) . . ?

O5 P1 O4 104.43(11) . . ?

C1 O1 Fe1 113.89(13) . . ?

C1 O1 Fe2 112.93(13) . . ?

Fe1 O1 Fe2 129.19(8) . . ?

P1 O2 Fe1 133.24(10) . . ?

P1 O3 Fe2 133.92(11) . . ?

C44 O4 P1 126.66(17) . . ?

C50 O5 P1 125.46(17) . . ?

C2 N1 C14 113.2(2) . . ?

C2 N1 C4 110.94(19) . . ?

C14 N1 C4 112.8(2) . . ?

C2 N1 Fe1 100.72(14) . . ?

C14 N1 Fe1 110.03(14) . . ?

C4 N1 Fe1 108.29(15) . . ?

C5 N2 C6 105.9(2) . . ?

C5 N2 Fe1 116.62(17) . . ?

C6 N2 Fe1 135.90(17) . . ?

C15 N3 C16 105.3(2) . . ?

C15 N3 Fe1 117.77(16) . . ?

C16 N3 Fe1 136.49(17) . . ?

C24 N4 C3 110.83(18) . . ?

C24 N4 C34 113.48(18) . . ?

C3 N4 C34 112.60(19) . . ?

C24 N4 Fe2 109.53(14) . . ?

C3 N4 Fe2 102.63(13) . . ?

C34 N4 Fe2 107.10(13) . . ?

C25 N5 C26 105.8(2) . . ?

C25 N5 Fe2 117.70(16) . . ?

C26 N5 Fe2 136.53(16) . . ?

C35 N6 C36 106.0(2) . . ?

C35 N6 Fe2 116.09(16) . . ?

C36 N6 Fe2 137.85(16) . . ?

C5 N7 C11 107.3(2) . . ?

C5 N7 C12 128.1(2) . . ?

C11 N7 C12 124.6(2) . . ?

C15 N8 C21 106.9(2) . . ?

C15 N8 C22 127.2(2) . . ?

C21 N8 C22 125.8(2) . . ?

C25 N9 C31 107.1(2) . . ?

C25 N9 C32 127.3(2) . . ?

C31 N9 C32 125.6(2) . . ?

C35 N10 C41 106.7(2) . . ?

C35 N10 C42 127.8(2) . . ?

C41 N10 C42 125.2(2) . . ?

O1 C1 C3 109.88(19) . . ?

O1 C1 C2 110.15(19) . . ?

C3 C1 C2 109.66(19) . . ?

O1 C1 H1A 109.0 . . ?

C3 C1 H1A 109.0 . . ?

C2 C1 H1A 109.0 . . ?

N1 C2 C1 110.85(19) . . ?

N1 C2 H2A 109.5 . . ?

C1 C2 H2A 109.5 . . ?

N1 C2 H2B 109.5 . . ?

C1 C2 H2B 109.5 . . ?

H2A C2 H2B 108.1 . . ?

N4 C3 C1 110.91(18) . . ?

N4 C3 H3A 109.5 . . ?

C1 C3 H3A 109.5 . . ?

N4 C3 H3B 109.5 . . ?

C1 C3 H3B 109.5 . . ?

H3A C3 H3B 108.0 . . ?

N1 C4 C5 109.1(2) . . ?

N1 C4 H4A 109.9 . . ?

C5 C4 H4A 109.9 . . ?

N1 C4 H4B 109.9 . . ?

C5 C4 H4B 109.9 . . ?

H4A C4 H4B 108.3 . . ?

N2 C5 N7 112.4(2) . . ?

N2 C5 C4 121.4(2) . . ?

N7 C5 C4 126.1(2) . . ?

C7 C6 C11 120.8(2) . . ?

C7 C6 N2 130.8(2) . . ?

C11 C6 N2 108.4(2) . . ?

C8 C7 C6 117.7(3) . . ?

C8 C7 H7A 121.1 . . ?

C6 C7 H7A 121.1 . . ?

C7 C8 C9 121.1(3) . . ?

C7 C8 H8A 119.4 . . ?

C9 C8 H8A 119.4 . . ?

C10 C9 C8 122.2(3) . . ?

C10 C9 H9A 118.9 . . ?

C8 C9 H9A 118.9 . . ?

C9 C10 C11 116.3(3) . . ?

C9 C10 H10E 121.9 . . ?

C11 C10 H10E 121.9 . . ?

C10 C11 N7 132.2(3) . . ?

C10 C11 C6 121.9(3) . . ?

N7 C11 C6 106.0(2) . . ?

N7 C12 C13 111.5(3) . . ?

N7 C12 H12A 109.3 . . ?

C13 C12 H12A 109.3 . . ?

N7 C12 H12B 109.3 . . ?

C13 C12 H12B 109.3 . . ?

H12A C12 H12B 108.0 . . ?

C12 C13 H13A 109.5 . . ?

C12 C13 H13B 109.5 . . ?

H13A C13 H13B 109.5 . . ?

C12 C13 H13C 109.5 . . ?

H13A C13 H13C 109.5 . . ?

H13B C13 H13C 109.5 . . ?

N1 C14 C15 109.7(2) . . ?

N1 C14 H14A 109.7 . . ?

C15 C14 H14A 109.7 . . ?

N1 C14 H14B 109.7 . . ?

C15 C14 H14B 109.7 . . ?

H14A C14 H14B 108.2 . . ?

N3 C15 N8 112.9(2) . . ?

N3 C15 C14 122.6(2) . . ?

N8 C15 C14 124.5(2) . . ?

C17 C16 C21 121.1(2) . . ?

C17 C16 N3 130.4(2) . . ?

C21 C16 N3 108.4(2) . . ?

C16 C17 C18 117.3(3) . . ?

C16 C17 H17A 121.4 . . ?

C18 C17 H17A 121.4 . . ?

C19 C18 C17 121.2(3) . . ?

C19 C18 H18A 119.4 . . ?

C17 C18 H18A 119.4 . . ?

C20 C19 C18 122.8(3) . . ?

C20 C19 H19A 118.6 . . ?

C18 C19 H19A 118.6 . . ?

C19 C20 C21 116.4(3) . . ?

C19 C20 H20A 121.8 . . ?

C21 C20 H20A 121.8 . . ?

N8 C21 C16 106.5(2) . . ?

N8 C21 C20 132.3(3) . . ?

C16 C21 C20 121.2(3) . . ?

N8 C22 C23 112.5(3) . . ?

N8 C22 H22A 109.1 . . ?

C23 C22 H22A 109.1 . . ?

N8 C22 H22B 109.1 . . ?

C23 C22 H22B 109.1 . . ?

H22A C22 H22B 107.8 . . ?

C22 C23 H23A 109.5 . . ?

C22 C23 H23B 109.5 . . ?

H23A C23 H23B 109.5 . . ?

C22 C23 H23C 109.5 . . ?

H23A C23 H23C 109.5 . . ?

H23B C23 H23C 109.5 . . ?

N4 C24 C25 110.53(19) . . ?

N4 C24 H24A 109.5 . . ?

C25 C24 H24A 109.5 . . ?

N4 C24 H24B 109.5 . . ?

C25 C24 H24B 109.5 . . ?

H24A C24 H24B 108.1 . . ?

N5 C25 N9 112.4(2) . . ?

N5 C25 C24 122.0(2) . . ?

N9 C25 C24 125.4(2) . . ?

C27 C26 N5 130.5(2) . . ?

C27 C26 C31 120.5(2) . . ?

N5 C26 C31 108.9(2) . . ?

C28 C27 C26 117.6(3) . . ?

C28 C27 H27A 121.2 . . ?

C26 C27 H27A 121.2 . . ?

C27 C28 C29 121.1(3) . . ?

C27 C28 H28A 119.5 . . ?

C29 C28 H28A 119.5 . . ?

C30 C29 C28 121.9(3) . . ?

C30 C29 H29A 119.0 . . ?

C28 C29 H29A 119.0 . . ?

C29 C30 C31 116.8(3) . . ?

C29 C30 H30A 121.6 . . ?

C31 C30 H30A 121.6 . . ?

C30 C31 N9 132.0(3) . . ?

C30 C31 C26 122.1(3) . . ?

N9 C31 C26 105.8(2) . . ?

N9 C32 C33 111.4(2) . . ?

N9 C32 H32A 109.4 . . ?

C33 C32 H32A 109.4 . . ?

N9 C32 H32B 109.4 . . ?

C33 C32 H32B 109.4 . . ?

H32A C32 H32B 108.0 . . ?

C32 C33 H33A 109.5 . . ?

C32 C33 H33B 109.5 . . ?

H33A C33 H33B 109.5 . . ?

C32 C33 H33C 109.5 . . ?

H33A C33 H33C 109.5 . . ?

H33B C33 H33C 109.5 . . ?

N4 C34 C35 109.27(19) . . ?

N4 C34 H34A 109.8 . . ?

C35 C34 H34A 109.8 . . ?

N4 C34 H34B 109.8 . . ?

C35 C34 H34B 109.8 . . ?

H34A C34 H34B 108.3 . . ?

N6 C35 N10 112.6(2) . . ?

N6 C35 C34 122.6(2) . . ?

N10 C35 C34 124.7(2) . . ?

C37 C36 C41 120.6(2) . . ?

C37 C36 N6 130.9(2) . . ?

C41 C36 N6 108.5(2) . . ?

C38 C37 C36 117.2(3) . . ?

C38 C37 H37A 121.4 . . ?

C36 C37 H37A 121.4 . . ?

C37 C38 C39 121.1(3) . . ?

C37 C38 H38A 119.4 . . ?

C39 C38 H38A 119.4 . . ?

C40 C39 C38 122.4(3) . . ?

C40 C39 H39A 118.8 . . ?

C38 C39 H39A 118.8 . . ?

C39 C40 C41 116.6(3) . . ?

C39 C40 H40A 121.7 . . ?

C41 C40 H40A 121.7 . . ?

C36 C41 N10 106.2(2) . . ?

C36 C41 C40 122.1(3) . . ?

N10 C41 C40 131.7(3) . . ?

C43 C42 N10 111.2(3) . . ?

C43 C42 H42A 109.4 . . ?

N10 C42 H42A 109.4 . . ?

C43 C42 H42B 109.4 . . ?

N10 C42 H42B 109.4 . . ?

H42A C42 H42B 108.0 . . ?

C42 C43 H43A 109.5 . . ?

C42 C43 H43B 109.5 . . ?

H43A C43 H43B 109.5 . . ?

C42 C43 H43C 109.5 . . ?

H43A C43 H43C 109.5 . . ?

H43B C43 H43C 109.5 . . ?

C49 C44 C45 121.4(3) . . ?

C49 C44 O4 116.1(3) . . ?

C45 C44 O4 122.4(3) . . ?

C44 C45 C46 118.7(3) . . ?

C44 C45 H45A 120.7 . . ?

C46 C45 H45A 120.7 . . ?

C47 C46 C45 119.2(4) . . ?

C47 C46 H46A 120.4 . . ?

C45 C46 H46A 120.4 . . ?

C46 C47 C48 120.9(4) . . ?

C46 C47 H47A 119.6 . . ?

C48 C47 H47A 119.6 . . ?

C49 C48 C47 120.3(4) . . ?

C49 C48 H48A 119.8 . . ?

C47 C48 H48A 119.8 . . ?

C48 C49 C44 119.5(3) . . ?

C48 C49 H49A 120.3 . . ?

C44 C49 H49A 120.3 . . ?

C55 C50 C51 121.6(3) . . ?

C55 C50 O5 122.6(3) . . ?

C51 C50 O5 115.6(3) . . ?

C52 C51 C50 120.0(4) . . ?

C52 C51 H51A 120.0 . . ?

C50 C51 H51A 120.0 . . ?

C53 C52 C51 119.0(5) . . ?

C53 C52 H52A 120.5 . . ?

C51 C52 H52A 120.5 . . ?

C52 C53 C54 122.8(5) . . ?

C52 C53 H53A 118.6 . . ?

C54 C53 H53A 118.6 . . ?

C53 C54 C55 118.5(5) . . ?

C53 C54 H54A 120.8 . . ?

C55 C54 H54A 120.8 . . ?

C50 C55 C54 118.1(4) . . ?

C50 C55 H55A 120.9 . . ?

C54 C55 H55A 120.9 . . ?

C61 C56 C57 114.9(3) . . ?

C61 C56 B1 124.8(3) . . ?

C57 C56 B1 120.0(3) . . ?

C58 C57 C56 123.5(3) . . ?

C58 C57 H57A 118.3 . . ?

C56 C57 H57A 118.3 . . ?

C59 C58 C57 119.6(3) . . ?

C59 C58 H58A 120.2 . . ?

C57 C58 H58A 120.2 . . ?

C58 C59 C60 118.9(3) . . ?

C58 C59 H59A 120.5 . . ?

C60 C59 H59A 120.5 . . ?

C59 C60 C61 120.5(3) . . ?

C59 C60 H60A 119.8 . . ?

C61 C60 H60A 119.8 . . ?

C56 C61 C60 122.7(3) . . ?

C56 C61 H61A 118.6 . . ?

C60 C61 H61A 118.6 . . ?

C63 C62 C67 114.3(3) . . ?

C63 C62 B1 122.3(3) . . ?

C67 C62 B1 122.8(2) . . ?

C64 C63 C62 123.5(3) . . ?

C64 C63 H63A 118.2 . . ?

C62 C63 H63A 118.2 . . ?

C65 C64 C63 120.4(3) . . ?

C65 C64 H64A 119.8 . . ?

C63 C64 H64A 119.8 . . ?

C66 C65 C64 118.3(3) . . ?

C66 C65 H65A 120.9 . . ?

C64 C65 H65A 120.9 . . ?

C65 C66 C67 121.1(3) . . ?

C65 C66 H66A 119.5 . . ?

C67 C66 H66A 119.5 . . ?

C66 C67 C62 122.4(3) . . ?

C66 C67 H67A 118.8 . . ?

C62 C67 H67A 118.8 . . ?

C73 C68 C69 115.0(3) . . ?

C73 C68 B1 122.1(3) . . ?

C69 C68 B1 122.3(3) . . ?

C70 C69 C68 122.2(3) . . ?

C70 C69 H69A 118.9 . . ?

C68 C69 H69A 118.9 . . ?

C69 C70 C71 120.1(3) . . ?

C69 C70 H70A 119.9 . . ?

C71 C70 H70A 119.9 . . ?

C72 C71 C70 118.7(3) . . ?

C72 C71 H71A 120.7 . . ?

C70 C71 H71A 120.7 . . ?

C71 C72 C73 120.9(4) . . ?

C71 C72 H72A 119.6 . . ?

C73 C72 H72A 119.6 . . ?

C72 C73 C68 123.1(3) . . ?

C72 C73 H73A 118.5 . . ?

C68 C73 H73A 118.5 . . ?

C75 C74 C79 115.7(3) . . ?

C75 C74 B1 122.3(3) . . ?

C79 C74 B1 121.6(3) . . ?

C74 C75 C76 122.3(4) . . ?

C74 C75 H75A 118.9 . . ?

C76 C75 H75A 118.9 . . ?

C77 C76 C75 120.3(4) . . ?

C77 C76 H76A 119.9 . . ?

C75 C76 H76A 119.9 . . ?

C76 C77 C78 119.4(4) . . ?

C76 C77 H77A 120.3 . . ?

C78 C77 H77A 120.3 . . ?

C77 C78 C79 120.1(4) . . ?

C77 C78 H78A 120.0 . . ?

C79 C78 H78A 120.0 . . ?

C74 C79 C78 122.2(4) . . ?

C74 C79 H79A 118.9 . . ?

C78 C79 H79A 118.9 . . ?

C85 C80 C81 115.8(3) . . ?

C85 C80 B2 119.9(3) . . ?

C81 C80 B2 124.2(3) . . ?

C82 C81 C80 122.8(4) . . ?

C82 C81 H81A 118.6 . . ?

C80 C81 H81A 118.6 . . ?

C83 C82 C81 119.2(4) . . ?

C83 C82 H82A 120.4 . . ?

C81 C82 H82A 120.4 . . ?

C82 C83 C84 120.9(4) . . ?

C82 C83 H83A 119.5 . . ?

C84 C83 H83A 119.5 . . ?

C83 C84 C85 119.6(4) . . ?

C83 C84 H84A 120.2 . . ?

C85 C84 H84A 120.2 . . ?

C80 C85 C84 121.8(4) . . ?

C80 C85 H85A 119.1 . . ?

C84 C85 H85A 119.1 . . ?

C91 C86 C87 113.9(2) . . ?

C91 C86 B2 125.2(2) . . ?

C87 C86 B2 120.6(2) . . ?

C88 C87 C86 123.2(3) . . ?

C88 C87 H87A 118.4 . . ?

C86 C87 H87A 118.4 . . ?

C89 C88 C87 119.6(3) . . ?

C89 C88 H88A 120.2 . . ?

C87 C88 H88A 120.2 . . ?

C90 C89 C88 119.6(3) . . ?

C90 C89 H89A 120.2 . . ?

C88 C89 H89A 120.2 . . ?

C89 C90 C91 120.0(3) . . ?

C89 C90 H90A 120.0 . . ?

C91 C90 H90A 120.0 . . ?

C90 C91 C86 123.8(3) . . ?

C90 C91 H91A 118.1 . . ?

C86 C91 H91A 118.1 . . ?

C97 C92 C93 114.3(3) . . ?

C97 C92 B2 122.0(2) . . ?

C93 C92 B2 123.7(2) . . ?

C94 C93 C92 123.0(3) . . ?

C94 C93 H93A 118.5 . . ?

C92 C93 H93A 118.5 . . ?

C95 C94 C93 121.1(3) . . ?

C95 C94 H94A 119.4 . . ?

C93 C94 H94A 119.4 . . ?

C94 C95 C96 118.9(3) . . ?

C94 C95 H95A 120.5 . . ?

C96 C95 H95A 120.5 . . ?

C95 C96 C97 119.6(3) . . ?

C95 C96 H96A 120.2 . . ?

C97 C96 H96A 120.2 . . ?

C92 C97 C96 122.9(3) . . ?

C92 C97 H97A 118.6 . . ?

C96 C97 H97A 118.6 . . ?

C99 C98 C103 114.7(3) . . ?

C99 C98 B2 123.7(2) . . ?

C103 C98 B2 121.4(2) . . ?

C98 C99 C100 123.6(3) . . ?

C98 C99 H99A 118.2 . . ?

C100 C99 H99A 118.2 . . ?

C101 C100 C99 120.1(3) . . ?

C101 C100 H10A 119.9 . . ?

C99 C100 H10A 119.9 . . ?

C100 C101 C102 119.2(3) . . ?

C100 C101 H10B 120.4 . . ?

C102 C101 H10B 120.4 . . ?

C101 C102 C103 119.8(3) . . ?

C101 C102 H10C 120.1 . . ?

C103 C102 H10C 120.1 . . ?

C102 C103 C98 122.7(3) . . ?

C102 C103 H10D 118.7 . . ?

C98 C103 H10D 118.7 . . ?

N11 C104 C105 178.1(6) . . ?

C104 C105 H10H 109.5 . . ?

C104 C105 H10F 109.5 . . ?

H10H C105 H10F 109.5 . . ?

C104 C105 H10G 109.5 . . ?

H10H C105 H10G 109.5 . . ?

H10F C105 H10G 109.5 . . ?

C56 B1 C68 111.7(2) . . ?

C56 B1 C62 114.8(2) . . ?

C68 B1 C62 102.0(2) . . ?

C56 B1 C74 103.6(2) . . ?

C68 B1 C74 112.8(2) . . ?

C62 B1 C74 112.4(2) . . ?

C92 B2 C98 112.9(2) . . ?

C92 B2 C86 111.3(2) . . ?

C98 B2 C86 104.8(2) . . ?

C92 B2 C80 105.6(2) . . ?

C98 B2 C80 110.3(2) . . ?

C86 B2 C80 112.1(2) . . ?

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_geom_torsion_atom_site_label_1

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_geom_torsion_atom_site_label_4

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O2 Fe1 O1 C1 -173.02(14) . . . . ?

N3 Fe1 O1 C1 -62.49(16) . . . . ?

N2 Fe1 O1 C1 80.30(16) . . . . ?

N1 Fe1 O1 C1 9.08(14) . . . . ?

O2 Fe1 O1 Fe2 -17.39(11) . . . . ?

N3 Fe1 O1 Fe2 93.15(11) . . . . ?

N2 Fe1 O1 Fe2 -124.06(11) . . . . ?

N1 Fe1 O1 Fe2 164.71(11) . . . . ?

O3 Fe2 O1 C1 158.55(14) . . . . ?

N5 Fe2 O1 C1 -89.22(15) . . . . ?

N6 Fe2 O1 C1 48.78(16) . . . . ?

N4 Fe2 O1 C1 -17.70(14) . . . . ?

O3 Fe2 O1 Fe1 2.73(11) . . . . ?

N5 Fe2 O1 Fe1 114.96(11) . . . . ?

N6 Fe2 O1 Fe1 -107.04(11) . . . . ?

N4 Fe2 O1 Fe1 -173.53(11) . . . . ?

O3 P1 O2 Fe1 -11.14(19) . . . . ?

O5 P1 O2 Fe1 113.57(14) . . . . ?

O4 P1 O2 Fe1 -133.91(13) . . . . ?

O1 Fe1 O2 P1 25.26(15) . . . . ?

N3 Fe1 O2 P1 -92.04(15) . . . . ?

N2 Fe1 O2 P1 144.43(14) . . . . ?

N1 Fe1 O2 P1 125.9(18) . . . . ?

O2 P1 O3 Fe2 -17.4(2) . . . . ?

O5 P1 O3 Fe2 -140.11(14) . . . . ?

O4 P1 O3 Fe2 107.73(16) . . . . ?

O1 Fe2 O3 P1 19.72(16) . . . . ?

N5 Fe2 O3 P1 -99.11(16) . . . . ?

N6 Fe2 O3 P1 149.76(15) . . . . ?

N4 Fe2 O3 P1 107.2(10) . . . . ?

O3 P1 O4 C44 -164.3(2) . . . . ?

O2 P1 O4 C44 -33.7(2) . . . . ?

O5 P1 O4 C44 79.7(2) . . . . ?

O3 P1 O5 C50 -29.8(3) . . . . ?

O2 P1 O5 C50 -160.2(2) . . . . ?

O4 P1 O5 C50 83.1(2) . . . . ?

O1 Fe1 N1 C2 18.76(14) . . . . ?

O2 Fe1 N1 C2 -82.2(19) . . . . ?

N3 Fe1 N1 C2 135.43(15) . . . . ?

N2 Fe1 N1 C2 -100.86(15) . . . . ?

O1 Fe1 N1 C14 -101.01(16) . . . . ?

O2 Fe1 N1 C14 158.0(18) . . . . ?

N3 Fe1 N1 C14 15.65(16) . . . . ?

N2 Fe1 N1 C14 139.37(17) . . . . ?

O1 Fe1 N1 C4 135.23(15) . . . . ?

O2 Fe1 N1 C4 34.3(19) . . . . ?

N3 Fe1 N1 C4 -108.11(16) . . . . ?

N2 Fe1 N1 C4 15.61(15) . . . . ?

O1 Fe1 N2 C5 -74.20(18) . . . . ?

O2 Fe1 N2 C5 -179.84(17) . . . . ?

N3 Fe1 N2 C5 66.66(19) . . . . ?

N1 Fe1 N2 C5 -0.53(17) . . . . ?

O1 Fe1 N2 C6 89.2(2) . . . . ?

O2 Fe1 N2 C6 -16.4(2) . . . . ?

N3 Fe1 N2 C6 -129.9(2) . . . . ?

N1 Fe1 N2 C6 162.9(2) . . . . ?

O1 Fe1 N3 C15 62.22(19) . . . . ?

O2 Fe1 N3 C15 169.08(17) . . . . ?

N2 Fe1 N3 C15 -79.71(19) . . . . ?

N1 Fe1 N3 C15 -12.25(17) . . . . ?

O1 Fe1 N3 C16 -108.4(2) . . . . ?

O2 Fe1 N3 C16 -1.5(2) . . . . ?

N2 Fe1 N3 C16 109.7(2) . . . . ?

N1 Fe1 N3 C16 177.2(2) . . . . ?

O1 Fe2 N4 C24 -128.48(15) . . . . ?

O3 Fe2 N4 C24 143.5(10) . . . . ?

N5 Fe2 N4 C24 -10.65(15) . . . . ?

N6 Fe2 N4 C24 100.39(15) . . . . ?

O1 Fe2 N4 C3 -10.70(13) . . . . ?

O3 Fe2 N4 C3 -98.8(11) . . . . ?

N5 Fe2 N4 C3 107.13(14) . . . . ?

N6 Fe2 N4 C3 -141.83(15) . . . . ?

O1 Fe2 N4 C34 108.06(15) . . . . ?

O3 Fe2 N4 C34 20.0(11) . . . . ?

N5 Fe2 N4 C34 -134.12(16) . . . . ?

N6 Fe2 N4 C34 -23.08(15) . . . . ?

O1 Fe2 N5 C25 74.99(18) . . . . ?

O3 Fe2 N5 C25 -177.00(16) . . . . ?

N6 Fe2 N5 C25 -70.91(18) . . . . ?

N4 Fe2 N5 C25 1.32(17) . . . . ?

O1 Fe2 N5 C26 -103.5(2) . . . . ?

O3 Fe2 N5 C26 4.6(2) . . . . ?

N6 Fe2 N5 C26 110.7(2) . . . . ?

N4 Fe2 N5 C26 -177.1(2) . . . . ?

O1 Fe2 N6 C35 -54.90(19) . . . . ?

O3 Fe2 N6 C35 -164.18(17) . . . . ?

N5 Fe2 N6 C35 85.54(18) . . . . ?

N4 Fe2 N6 C35 13.25(16) . . . . ?

O1 Fe2 N6 C36 121.0(2) . . . . ?

O3 Fe2 N6 C36 11.7(2) . . . . ?

N5 Fe2 N6 C36 -98.5(2) . . . . ?

N4 Fe2 N6 C36 -170.8(2) . . . . ?

Fe1 O1 C1 C3 -156.64(15) . . . . ?

Fe2 O1 C1 C3 43.7(2) . . . . ?

Fe1 O1 C1 C2 -35.7(2) . . . . ?

Fe2 O1 C1 C2 164.58(14) . . . . ?

C14 N1 C2 C1 75.0(3) . . . . ?

C4 N1 C2 C1 -156.9(2) . . . . ?

Fe1 N1 C2 C1 -42.4(2) . . . . ?

O1 C1 C2 N1 55.1(3) . . . . ?

C3 C1 C2 N1 176.1(2) . . . . ?

C24 N4 C3 C1 152.8(2) . . . . ?

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of which blank in column 1 9

W: Number of unusual anisotropic displacement parameters 12

N: Total Potential Solvent Accessible Void Vol ..... 1097.4 Ang^3

N: Electron Count/Cell = 120 - To be included in D(calc), F000 & Mol.Wght.

PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13

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_diffrn_reflns_limit_h_max 14

_diffrn_reflns_limit_k_min -22

_diffrn_reflns_limit_k_max 22

_diffrn_reflns_limit_l_min -42

_diffrn_reflns_limit_l_max 42

_diffrn_reflns_theta_min 1.17

_diffrn_reflns_theta_max 25.09

_reflns_number_total 29541

_reflns_number_gt 14773

_reflns_threshold_expression >2sigma(I)

_computing_data_collection 'SMART, Bruker'

_computing_cell_refinement 'SAINT, Bruker'

_computing_data_reduction 'SAINT, Bruker'

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_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'SHELXTL, Bruker'
_computing_publication_material   'Bruker SHELXTL'

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

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1025P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
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_refine_ls_extinction_method none

_refine_ls_extinction_coef ?

_refine_ls_number_reflns 29541

_refine_ls_number_parameters 1879

_refine_ls_number_restraints 6

_refine_ls_R_factor_all 0.1371

_refine_ls_R_factor_gt 0.0713

_refine_ls_wR_factor_ref 0.1955

_refine_ls_wR_factor_gt 0.1768

_refine_ls_goodness_of_fit_ref 0.987

_refine_ls_restrained_S_all 0.987

_refine_ls_shift/su_max 0.000

_refine_ls_shift/su_mean 0.000

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

_atom_site_symmetry_multiplicity

_atom_site_calc_flag

_atom_site_refinement_flags

_atom_site_disorder_assembly

_atom_site_disorder_group

Fe1 Fe 0.62569(5) -0.30645(3) 0.279849(18) 0.02762(17) Uani 1 1 d . . .

Fe2 Fe 0.69138(5) -0.22703(3) 0.198908(18) 0.03090(18) Uani 1 1 d . . .

O1 O 0.5858(2) -0.27389(16) 0.23261(8) 0.0320(8) Uani 1 1 d . . .

O2 O 0.7904(2) -0.26604(18) 0.28145(9) 0.0417(9) Uani 1 1 d . . .

O3 O 0.8338(2) -0.21759(19) 0.22930(9) 0.0460(9) Uani 1 1 d . . .

O4 O 1.1589(3) -0.2491(2) 0.34885(10) 0.0566(10) Uani 1 1 d . . .

O5 O 1.3058(3) -0.17298(18) 0.30923(10) 0.0472(9) Uani 1 1 d . . .

O6 O 1.2458(3) -0.1174(3) 0.24893(13) 0.0925(16) Uani 1 1 d . . .

N1 N 0.4362(3) -0.34720(18) 0.27738(10) 0.0270(9) Uani 1 1 d . . .

N2 N 0.5317(3) -0.24002(19) 0.16206(10) 0.0312(9) Uani 1 1 d . . .

N3 N 0.5918(3) -0.27071(18) 0.33280(10) 0.0303(9) Uani 1 1 d . . .

N4 N 0.4811(3) -0.2775(2) 0.37980(10) 0.0331(9) Uani 1 1 d . . .

N5 N 0.6073(3) -0.4144(2) 0.28313(11) 0.0352(10) Uani 1 1 d . . .

N6 N 0.5033(4) -0.5263(2) 0.28067(12) 0.0431(11) Uani 1 1 d . . .

N7 N 0.7211(3) -0.2839(2) 0.14970(11) 0.0383(10) Uani 1 1 d . . .

N8 N 0.6608(4) -0.3544(2) 0.09562(12) 0.0475(12) Uani 1 1 d . . .

N9 N 0.6912(3) -0.12214(19) 0.19322(10) 0.0287(9) Uani 1 1 d . . .

N10 N 0.6285(3) -0.0413(2) 0.16495(10) 0.0344(10) Uani 1 1 d . . .

C1 C 0.4760(3) -0.3014(2) 0.21742(12) 0.0257(10) Uani 1 1 d . . .

H1A H 0.4701 -0.3506 0.2035 0.031 Uiso 1 1 calc R . .

C2 C 0.3973(3) -0.3083(2) 0.24870(12) 0.0293(11) Uani 1 1 d . . .

H2A H 0.3926 -0.2596 0.2602 0.035 Uiso 1 1 calc R . .

H2B H 0.3233 -0.3348 0.2383 0.035 Uiso 1 1 calc R . .

C3 C 0.4476(4) -0.2523(2) 0.18995(13) 0.0349(12) Uani 1 1 d . . .

H3A H 0.3752 -0.2749 0.1769 0.042 Uiso 1 1 calc R . .

H3B H 0.4433 -0.2054 0.2039 0.042 Uiso 1 1 calc R . .

C4 C 0.3961(4) -0.3289(2) 0.31504(12) 0.0310(11) Uani 1 1 d . . .

H4A H 0.3565 -0.3738 0.3242 0.037 Uiso 1 1 calc R . .

H4B H 0.3442 -0.2974 0.3129 0.037 Uiso 1 1 calc R . .

C5 C 0.4894(4) -0.2910(2) 0.34263(13) 0.0293(11) Uani 1 1 d . . .

C6 C 0.6549(4) -0.2417(2) 0.36628(14) 0.0329(11) Uani 1 1 d . . .

C7 C 0.7671(4) -0.2154(3) 0.37354(15) 0.0492(14) Uani 1 1 d . . .

H7A H 0.8155 -0.2132 0.3539 0.059 Uiso 1 1 calc R . .

C8 C 0.8057(5) -0.1925(3) 0.41055(18) 0.0650(18) Uani 1 1 d . . .

H8A H 0.8820 -0.1740 0.4162 0.078 Uiso 1 1 calc R . .

C9 C 0.7365(5) -0.1958(3) 0.43929(18) 0.0697(18) Uani 1 1 d . . .

H9A H 0.7661 -0.1794 0.4643 0.084 Uiso 1 1 calc R . .

C10 C 0.6244(5) -0.2226(3) 0.43262(15) 0.0556(15) Uani 1 1 d . . .

H10A H 0.5767 -0.2250 0.4525 0.067 Uiso 1 1 calc R . .

C11 C 0.5850(4) -0.2454(3) 0.39605(14) 0.0421(13) Uani 1 1 d . . .

C12 C 0.3815(4) -0.2922(3) 0.40038(13) 0.0412(13) Uani 1 1 d . . .

H12A H 0.3935 -0.3191 0.4214 0.049 Uiso 1 1 calc R . .

H12B H 0.3205 -0.3230 0.3835 0.049 Uiso 1 1 calc R . .

C13 C 0.3507(4) -0.2232(3) 0.41540(14) 0.0464(14) Uani 1 1 d . . .

H13A H 0.2836 -0.2347 0.4287 0.070 Uiso 1 1 calc R . .

H13B H 0.3383 -0.1967 0.3946 0.070 Uiso 1 1 calc R . .

H13C H 0.4101 -0.1933 0.4327 0.070 Uiso 1 1 calc R . .

C14 C 0.4115(4) -0.4272(2) 0.26587(13) 0.0347(12) Uani 1 1 d . . .

H14A H 0.3458 -0.4509 0.2779 0.042 Uiso 1 1 calc R . .

H14B H 0.3964 -0.4380 0.2384 0.042 Uiso 1 1 calc R . .

C15 C 0.5075(4) -0.4554(2) 0.27744(13) 0.0332(11) Uani 1 1 d . . .

C16 C 0.6742(4) -0.4605(2) 0.29137(13) 0.0338(12) Uani 1 1 d . . .

C17 C 0.7862(4) -0.4450(3) 0.30066(14) 0.0469(14) Uani 1 1 d . . .

H17A H 0.8298 -0.3972 0.3019 0.056 Uiso 1 1 calc R . .

C18 C 0.8316(5) -0.5012(3) 0.30806(15) 0.0522(15) Uani 1 1 d . . .

H18A H 0.9077 -0.4920 0.3149 0.063 Uiso 1 1 calc R . .

C19 C 0.7677(5) -0.5716(3) 0.30559(16) 0.0569(16) Uani 1 1 d . . .

H19A H 0.8018 -0.6093 0.3105 0.068 Uiso 1 1 calc R . .

C20 C 0.6566(5) -0.5882(3) 0.29628(16) 0.0556(16) Uani 1 1 d . . .

H20A H 0.6139 -0.6363 0.2945 0.067 Uiso 1 1 calc R . .

C21 C 0.6097(4) -0.5306(3) 0.28956(14) 0.0424(13) Uani 1 1 d . . .

C22 C 0.4060(5) -0.5865(3) 0.2773(2) 0.0673(19) Uani 1 1 d . . .

H22A H 0.4203 -0.6239 0.2923 0.081 Uiso 1 1 calc R . .

H22B H 0.3439 -0.5686 0.2877 0.081 Uiso 1 1 calc R . .

C23 C 0.3768(6) -0.6180(4) 0.2395(2) 0.106(3) Uani 1 1 d . . .

H23A H 0.3116 -0.6576 0.2385 0.158 Uiso 1 1 calc R . .

H23B H 0.4375 -0.6367 0.2292 0.158 Uiso 1 1 calc R . .

H23C H 0.3614 -0.5813 0.2246 0.158 Uiso 1 1 calc R . .

C24 C 0.5230(4) -0.3026(2) 0.13282(13) 0.0377(12) Uani 1 1 d . . .

H24A H 0.4870 -0.2939 0.1095 0.045 Uiso 1 1 calc R . .

H24B H 0.4783 -0.3468 0.1412 0.045 Uiso 1 1 calc R . .

C25 C 0.6357(4) -0.3124(2) 0.12582(14) 0.0356(12) Uani 1 1 d . . .

C26 C 0.8086(4) -0.3088(3) 0.13457(15) 0.0440(14) Uani 1 1 d . . .

C27 C 0.9179(5) -0.2943(3) 0.14849(17) 0.0539(16) Uani 1 1 d . . .

H27A H 0.9430 -0.2634 0.1712 0.065 Uiso 1 1 calc R . .

C28 C 0.9877(6) -0.3272(4) 0.1276(2) 0.0708(19) Uani 1 1 d . . .

H28A H 1.0628 -0.3184 0.1358 0.085 Uiso 1 1 calc R . .

C29 C 0.9487(7) -0.3730(4) 0.0948(2) 0.087(2) Uani 1 1 d . . .

H29A H 0.9982 -0.3956 0.0815 0.105 Uiso 1 1 calc R . .

C30 C 0.8407(6) -0.3873(4) 0.08039(19) 0.078(2) Uani 1 1 d . . .

H30A H 0.8160 -0.4186 0.0578 0.093 Uiso 1 1 calc R . .

C31 C 0.7708(5) -0.3534(3) 0.10093(17) 0.0575(16) Uani 1 1 d . . .

C32 C 0.5877(5) -0.3938(3) 0.06459(17) 0.0670(18) Uani 1 1 d . . .

H32A H 0.6244 -0.3874 0.0410 0.080 Uiso 1 1 calc R . .

H32B H 0.5218 -0.3738 0.0634 0.080 Uiso 1 1 calc R . .

C33 C 0.5537(6) -0.4735(3) 0.0683(2) 0.104(3) Uani 1 1 d . . .

H33A H 0.5052 -0.4987 0.0465 0.157 Uiso 1 1 calc R . .

H33B H 0.5151 -0.4800 0.0912 0.157 Uiso 1 1 calc R . .

H33C H 0.6188 -0.4934 0.0695 0.157 Uiso 1 1 calc R . .

C34 C 0.5373(4) -0.1724(2) 0.14577(13) 0.0364(12) Uani 1 1 d . . .

H34A H 0.4640 -0.1615 0.1448 0.044 Uiso 1 1 calc R . .

H34B H 0.5605 -0.1780 0.1199 0.044 Uiso 1 1 calc R . .

C35 C 0.6171(4) -0.1113(2) 0.16882(13) 0.0330(11) Uani 1 1 d . . .

C36 C 0.7580(4) -0.0540(2) 0.20592(12) 0.0302(11) Uani 1 1 d . . .

C37 C 0.8523(4) -0.0348(3) 0.22908(12) 0.0334(11) Uani 1 1 d . . .

H37A H 0.8801 -0.0698 0.2405 0.040 Uiso 1 1 calc R . .

C38 C 0.9050(4) 0.0379(3) 0.23494(13) 0.0397(12) Uani 1 1 d . . .

H38A H 0.9702 0.0532 0.2508 0.048 Uiso 1 1 calc R . .

C39 C 0.8635(4) 0.0890(3) 0.21771(14) 0.0452(14) Uani 1 1 d . . .

H39A H 0.9014 0.1384 0.2224 0.054 Uiso 1 1 calc R . .

C40 C 0.7705(4) 0.0704(2) 0.19439(14) 0.0429(13) Uani 1 1 d . . .

H40A H 0.7432 0.1054 0.1828 0.052 Uiso 1 1 calc R . .

C41 C 0.7177(4) -0.0029(3) 0.18851(13) 0.0359(12) Uani 1 1 d . . .

C42 C 0.5630(5) -0.0101(3) 0.13961(15) 0.0516(15) Uani 1 1 d . . .

H42A H 0.5293 -0.0474 0.1185 0.062 Uiso 1 1 calc R . .

H42B H 0.6114 0.0302 0.1292 0.062 Uiso 1 1 calc R . .

C43 C 0.4744(6) 0.0174(4) 0.1594(2) 0.098(3) Uani 1 1 d . . .

H43A H 0.4335 0.0386 0.1418 0.148 Uiso 1 1 calc R . .

H43B H 0.5074 0.0542 0.1803 0.148 Uiso 1 1 calc R . .

H43C H 0.4246 -0.0228 0.1689 0.148 Uiso 1 1 calc R . .

C44 C 0.8593(4) -0.2350(2) 0.26087(14) 0.0315(11) Uani 1 1 d . . .

C45 C 0.9778(4) -0.2171(2) 0.27376(13) 0.0315(11) Uani 1 1 d . . .

C46 C 1.0091(4) -0.2413(2) 0.30661(13) 0.0347(12) Uani 1 1 d . . .

H46A H 0.9557 -0.2673 0.3210 0.042 Uiso 1 1 calc R . .

C47 C 1.1188(4) -0.2267(3) 0.31790(14) 0.0378(12) Uani 1 1 d . . .

C48 C 1.1968(4) -0.1857(3) 0.29782(14) 0.0341(12) Uani 1 1 d . . .

C49 C 1.1646(4) -0.1596(3) 0.26610(15) 0.0523(15) Uani 1 1 d . . .

C50 C 1.0541(4) -0.1765(3) 0.25361(14) 0.0471(14) Uani 1 1 d . . .

H50A H 1.0317 -0.1601 0.2314 0.056 Uiso 1 1 calc R . .

C51 C 1.0809(5) -0.2852(4) 0.37196(18) 0.083(2) Uani 1 1 d . . .

H51A H 1.1190 -0.2980 0.3934 0.125 Uiso 1 1 calc R . .

H51B H 1.0359 -0.3292 0.3575 0.125 Uiso 1 1 calc R . .

H51C H 1.0339 -0.2532 0.3809 0.125 Uiso 1 1 calc R . .

C52 C 1.3442(4) -0.1066(3) 0.33396(15) 0.0570(16) Uani 1 1 d . . .

H52A H 1.4220 -0.1004 0.3411 0.085 Uiso 1 1 calc R . .

H52B H 1.3027 -0.1082 0.3564 0.085 Uiso 1 1 calc R . .

H52C H 1.3340 -0.0659 0.3212 0.085 Uiso 1 1 calc R . .

C53 C 1.2114(6) -0.0819(6) 0.2193(2) 0.163(5) Uani 1 1 d . . .

H53A H 1.2756 -0.0518 0.2098 0.245 Uiso 1 1 calc R . .

H53B H 1.1628 -0.0516 0.2289 0.245 Uiso 1 1 calc R . .

H53C H 1.1721 -0.1183 0.1990 0.245 Uiso 1 1 calc R . .

Fe3 Fe 0.75925(5) 0.20900(3) 0.296125(18) 0.02713(17) Uani 1 1 d . . .

Fe4 Fe 0.82066(5) 0.29133(3) 0.214886(17) 0.02578(17) Uani 1 1 d . . .

O11 O 0.8624(2) 0.25832(15) 0.26199(8) 0.0266(7) Uani 1 1 d . . .

O12 O 0.6157(3) 0.20014(18) 0.26585(9) 0.0435(9) Uani 1 1 d . . .

O13 O 0.6576(3) 0.24813(18) 0.21318(9) 0.0418(9) Uani 1 1 d . . .

O14 O 0.1991(3) 0.1261(2) 0.25514(10) 0.0617(11) Uani 1 1 d . . .

O15 O 0.1408(2) 0.17093(18) 0.19241(9) 0.0428(9) Uani 1 1 d . . .

O16 O 0.2877(3) 0.2367(2) 0.14889(10) 0.0516(10) Uani 1 1 d . . .

N11 N 0.9208(3) 0.22492(18) 0.33156(10) 0.0274(9) Uani 1 1 d . . .

N12 N 1.0081(3) 0.33588(18) 0.21655(10) 0.0270(9) Uani 1 1 d . . .

N13 N 0.7598(3) 0.10526(18) 0.30462(10) 0.0273(9) Uani 1 1 d . . .

N14 N 0.8266(3) 0.02501(19) 0.33192(10) 0.0301(9) Uani 1 1 d . . .

N15 N 0.7287(3) 0.26366(19) 0.34575(10) 0.0293(9) Uani 1 1 d . . .

N16 N 0.7915(3) 0.3414(2) 0.39724(11) 0.0367(10) Uani 1 1 d . . .

N17 N 0.8347(3) 0.39960(19) 0.21204(10) 0.0316(9) Uani 1 1 d . . .

N18 N 0.9332(3) 0.51212(19) 0.21490(11) 0.0375(10) Uani 1 1 d . . .

N19 N 0.8547(3) 0.25244(19) 0.16220(10) 0.0291(9) Uani 1 1 d . . .

N20 N 0.9677(3) 0.2554(2) 0.11591(11) 0.0438(11) Uani 1 1 d . . .

C61 C 0.9719(4) 0.2875(2) 0.27715(12) 0.0298(11) Uani 1 1 d . . .

H61A H 0.9758 0.3361 0.2915 0.036 Uiso 1 1 calc R . .

C62 C 1.0038(3) 0.2388(2) 0.30378(12) 0.0263(10) Uani 1 1 d . . .

H62A H 1.0094 0.1925 0.2895 0.032 Uiso 1 1 calc R . .

H62B H 1.0761 0.2623 0.3167 0.032 Uiso 1 1 calc R . .

C63 C 1.0491(3) 0.2967(2) 0.24561(12) 0.0257(10) Uani 1 1 d . . .

H63A H 1.1227 0.3243 0.2560 0.031 Uiso 1 1 calc R . .

H63B H 1.0557 0.2486 0.2339 0.031 Uiso 1 1 calc R . .

C64 C 0.9224(4) 0.1570(2) 0.34824(12) 0.0292(11) Uani 1 1 d . . .

H64A H 0.9958 0.1466 0.3467 0.035 Uiso 1 1 calc R . .

H64B H 0.9064 0.1632 0.3750 0.035 Uiso 1 1 calc R . .

C65 C 0.8382(3) 0.0956(2) 0.32731(12) 0.0264(10) Uani 1 1 d . . .

C66 C 0.6915(4) 0.0365(2) 0.29396(12) 0.0276(11) Uani 1 1 d . . .

C67 C 0.5936(4) 0.0163(3) 0.27139(13) 0.0367(12) Uani 1 1 d . . .

H67A H 0.5649 0.0506 0.2596 0.044 Uiso 1 1 calc R . .

C68 C 0.5406(4) -0.0562(3) 0.26702(14) 0.0419(13) Uani 1 1 d . . .

H68A H 0.4732 -0.0720 0.2523 0.050 Uiso 1 1 calc R . .

C69 C 0.5847(4) -0.1067(3) 0.28387(14) 0.0426(13) Uani 1 1 d . . .

H69A H 0.5472 -0.1562 0.2798 0.051 Uiso 1 1 calc R . .

C70 C 0.6811(4) -0.0867(2) 0.30630(13) 0.0357(12) Uani 1 1 d . . .

H70A H 0.7099 -0.1210 0.3179 0.043 Uiso 1 1 calc R . .

C71 C 0.7336(4) -0.0138(2) 0.31098(12) 0.0289(11) Uani 1 1 d . . .

C72 C 0.8970(4) -0.0059(2) 0.35656(13) 0.0360(12) Uani 1 1 d . . .

H72A H 0.8501 -0.0409 0.3707 0.043 Uiso 1 1 calc R . .

H72B H 0.9418 0.0333 0.3748 0.043 Uiso 1 1 calc R . .

C73 C 0.9715(4) -0.0435(3) 0.33385(15) 0.0556(16) Uani 1 1 d . . .

H73A H 1.0174 -0.0628 0.3507 0.083 Uiso 1 1 calc R . .

H73B H 1.0182 -0.0089 0.3199 0.083 Uiso 1 1 calc R . .

H73C H 0.9272 -0.0833 0.3163 0.083 Uiso 1 1 calc R . .

C74 C 0.9298(4) 0.2872(2) 0.36097(12) 0.0305(11) Uani 1 1 d . . .

H74A H 0.9743 0.3315 0.3526 0.037 Uiso 1 1 calc R . .

H74B H 0.9663 0.2783 0.3842 0.037 Uiso 1 1 calc R . .

C75 C 0.8163(4) 0.2971(2) 0.36845(13) 0.0323(11) Uani 1 1 d . . .

C76 C 0.6404(4) 0.2862(2) 0.36179(14) 0.0364(12) Uani 1 1 d . . .

C77 C 0.5300(4) 0.2671(3) 0.35050(15) 0.0419(13) Uani 1 1 d . . .

H77A H 0.5029 0.2331 0.3290 0.050 Uiso 1 1 calc R . .

C78 C 0.4610(5) 0.2994(3) 0.37171(17) 0.0562(16) Uani 1 1 d . . .

H78A H 0.3847 0.2869 0.3649 0.067 Uiso 1 1 calc R . .

C79 C 0.5016(5) 0.3500(3) 0.40295(17) 0.0568(16) Uani 1 1 d . . .

H79A H 0.4523 0.3722 0.4167 0.068 Uiso 1 1 calc R . .

C80 C 0.6108(5) 0.3686(3) 0.41439(15) 0.0523(15) Uani 1 1 d . . .

H80A H 0.6379 0.4026 0.4359 0.063 Uiso 1 1 calc R . .

C81 C 0.6802(4) 0.3355(3) 0.39315(14) 0.0366(12) Uani 1 1 d . . .

C82 C 0.8687(4) 0.3888(3) 0.42633(14) 0.0465(14) Uani 1 1 d . . .

H82A H 0.9383 0.3729 0.4269 0.056 Uiso 1 1 calc R . .

H82B H 0.8381 0.3844 0.4511 0.056 Uiso 1 1 calc R . .

C83 C 0.8917(5) 0.4677(3) 0.41943(18) 0.0712(19) Uani 1 1 d . . .

H83A H 0.9441 0.4973 0.4391 0.107 Uiso 1 1 calc R . .

H83B H 0.8234 0.4841 0.4197 0.107 Uiso 1 1 calc R . .

H83C H 0.9224 0.4723 0.3950 0.107 Uiso 1 1 calc R . .

C84 C 1.0315(4) 0.4153(2) 0.22925(13) 0.0343(12) Uani 1 1 d . . .

H84A H 1.0967 0.4405 0.2175 0.041 Uiso 1 1 calc R . .

H84B H 1.0464 0.4247 0.2568 0.041 Uiso 1 1 calc R . .

C85 C 0.9335(4) 0.4429(2) 0.21819(12) 0.0310(11) Uani 1 1 d . . .

C86 C 0.7640(4) 0.4435(3) 0.20441(14) 0.0392(13) Uani 1 1 d . . .

C87 C 0.6531(4) 0.4263(3) 0.19494(14) 0.0427(13) Uani 1 1 d . . .

H87A H 0.6111 0.3780 0.1933 0.051 Uiso 1 1 calc R . .

C88 C 0.6054(4) 0.4821(3) 0.18784(14) 0.0497(15) Uani 1 1 d . . .

H88A H 0.5291 0.4719 0.1812 0.060 Uiso 1 1 calc R . .

C89 C 0.6670(5) 0.5530(3) 0.19030(16) 0.0564(16) Uani 1 1 d . . .

H89A H 0.6313 0.5900 0.1853 0.068 Uiso 1 1 calc R . .

C90 C 0.7759(5) 0.5709(3) 0.19956(15) 0.0528(15) Uani 1 1 d . . .

H90A H 0.8167 0.6196 0.2015 0.063 Uiso 1 1 calc R . .

C91 C 0.8261(4) 0.5146(3) 0.20617(14) 0.0392(12) Uani 1 1 d . . .

C92 C 1.0294(5) 0.5743(3) 0.21847(17) 0.0555(16) Uani 1 1 d . . .

H92A H 1.0102 0.6137 0.2061 0.067 Uiso 1 1 calc R . .

H92B H 1.0899 0.5593 0.2053 0.067 Uiso 1 1 calc R . .

C93 C 1.0678(5) 0.6024(3) 0.25811(18) 0.075(2) Uani 1 1 d . . .

H93A H 1.1305 0.6438 0.2589 0.112 Uiso 1 1 calc R . .

H93B H 1.0897 0.5643 0.2703 0.112 Uiso 1 1 calc R . .

H93C H 1.0085 0.6177 0.2713 0.112 Uiso 1 1 calc R . .

C94 C 1.0476(4) 0.3189(3) 0.17920(12) 0.0340(12) Uani 1 1 d . . .

H94A H 1.1057 0.2921 0.1815 0.041 Uiso 1 1 calc R . .

H94B H 1.0795 0.3644 0.1691 0.041 Uiso 1 1 calc R . .

C95 C 0.9558(4) 0.2741(2) 0.15254(12) 0.0286(11) Uani 1 1 d . . .

C96 C 0.7958(4) 0.2176(2) 0.12943(13) 0.0361(12) Uani 1 1 d . . .

C97 C 0.6837(4) 0.1864(3) 0.12269(15) 0.0450(13) Uani 1 1 d . . .

H97A H 0.6353 0.1859 0.1423 0.054 Uiso 1 1 calc R . .

C98 C 0.6459(5) 0.1565(3) 0.08660(17) 0.0619(17) Uani 1 1 d . . .

H98A H 0.5704 0.1343 0.0815 0.074 Uiso 1 1 calc R . .

C99 C 0.7155(5) 0.1581(3) 0.05760(17) 0.0667(18) Uani 1 1 d . . .

H99A H 0.6861 0.1370 0.0331 0.080 Uiso 1 1 calc R . .

C100 C 0.8247(5) 0.1890(3) 0.06310(15) 0.0626(17) Uani 1 1 d . . .

H10B H 0.8719 0.1905 0.0431 0.075 Uiso 1 1 calc R . .

C101 C 0.8641(4) 0.2188(3) 0.10018(14) 0.0402(13) Uani 1 1 d . . .

C102 C 1.0653(4) 0.2741(3) 0.09467(15) 0.0552(16) Uani 1 1 d . . .

H10C H 1.1256 0.3066 0.1111 0.066 Uiso 1 1 calc R . .

H10D H 1.0491 0.2999 0.0737 0.066 Uiso 1 1 calc R . .

C103 C 1.0996(5) 0.2061(4) 0.07961(18) 0.081(2) Uani 1 1 d . . .

H10E H 1.1649 0.2188 0.0655 0.122 Uiso 1 1 calc R . .

H10F H 1.0400 0.1745 0.0630 0.122 Uiso 1 1 calc R . .

H10G H 1.1160 0.1809 0.1005 0.122 Uiso 1 1 calc R . .

C104 C 0.5915(4) 0.2181(2) 0.23513(14) 0.0315(11) Uani 1 1 d . . .

C105 C 0.4715(4) 0.2035(2) 0.22350(13) 0.0312(11) Uani 1 1 d . . .

C106 C 0.3937(4) 0.1694(3) 0.24617(14) 0.0410(13) Uani 1 1 d . . .

H10H H 0.4158 0.1544 0.2688 0.049 Uiso 1 1 calc R . .

C107 C 0.2830(4) 0.1578(3) 0.23505(14) 0.0392(12) Uani 1 1 d . . .

C108 C 0.2504(4) 0.1799(2) 0.20247(13) 0.0317(11) Uani 1 1 d . . .

C109 C 0.3275(4) 0.2149(2) 0.17968(13) 0.0335(12) Uani 1 1 d . . .

C110 C 0.4387(4) 0.2253(2) 0.19027(13) 0.0340(12) Uani 1 1 d . . .

H11A H 0.4921 0.2473 0.1747 0.041 Uiso 1 1 calc R . .

C111 C 0.2315(5) 0.1079(4) 0.29060(18) 0.094(3) Uani 1 1 d . . .

H11B H 0.1663 0.0856 0.3028 0.141 Uiso 1 1 calc R . .

H11C H 0.2714 0.1518 0.3064 0.141 Uiso 1 1 calc R . .

H11D H 0.2788 0.0738 0.2868 0.141 Uiso 1 1 calc R . .

C112 C 0.0975(4) 0.1069(3) 0.16740(14) 0.0527(15) Uani 1 1 d . . .

H11E H 0.0196 0.1030 0.1613 0.079 Uiso 1 1 calc R . .

H11F H 0.1062 0.0648 0.1792 0.079 Uiso 1 1 calc R . .

H11G H 0.1367 0.1085 0.1444 0.079 Uiso 1 1 calc R . .

C113 C 0.3653(5) 0.2748(4) 0.12577(16) 0.0695(19) Uani 1 1 d . . .

H11H H 0.3263 0.2879 0.1046 0.104 Uiso 1 1 calc R . .

H11I H 0.4132 0.2437 0.1164 0.104 Uiso 1 1 calc R . .

H11J H 0.4095 0.3187 0.1405 0.104 Uiso 1 1 calc R . .

B1 B 0.8424(5) 0.1617(3) 0.47701(15) 0.0359(14) Uani 1 1 d . . .

C121 C 0.8420(5) 0.1188(2) 0.51428(14) 0.0462(14) Uani 1 1 d . . .

C122 C 0.9338(5) 0.1041(3) 0.53173(16) 0.0661(18) Uani 1 1 d . . .

H12C H 1.0029 0.1167 0.5214 0.079 Uiso 1 1 calc R . .

C123 C 0.9246(6) 0.0703(3) 0.56486(17) 0.0683(19) Uani 1 1 d . . .

H12D H 0.9878 0.0611 0.5768 0.082 Uiso 1 1 calc R . .

C124 C 0.8263(6) 0.0512(3) 0.57960(17) 0.0643(18) Uani 1 1 d . . .

H12E H 0.8215 0.0288 0.6018 0.077 Uiso 1 1 calc R . .

C125 C 0.7353(6) 0.0633(3) 0.56324(16) 0.0672(18) Uani 1 1 d . . .

H12F H 0.6665 0.0493 0.5736 0.081 Uiso 1 1 calc R . .

C126 C 0.7437(5) 0.0964(3) 0.53119(15) 0.0564(16) Uani 1 1 d . . .

H12G H 0.6789 0.1044 0.5199 0.068 Uiso 1 1 calc R . .

C127 C 0.9615(4) 0.1773(3) 0.45922(13) 0.0406(13) Uani 1 1 d . . .

C128 C 1.0073(5) 0.1196(3) 0.44655(16) 0.0557(16) Uani 1 1 d . . .

H12H H 0.9699 0.0721 0.4501 0.067 Uiso 1 1 calc R . .

C129 C 1.1045(5) 0.1283(3) 0.42907(18) 0.0676(18) Uani 1 1 d . . .

H12I H 1.1334 0.0877 0.4214 0.081 Uiso 1 1 calc R . .

C130 C 1.1595(5) 0.1971(4) 0.42286(17) 0.0693(18) Uani 1 1 d . . .

H13D H 1.2255 0.2031 0.4104 0.083 Uiso 1 1 calc R . .

C131 C 1.1196(5) 0.2566(3) 0.43456(16) 0.0597(16) Uani 1 1 d . . .

H13E H 1.1574 0.3037 0.4306 0.072 Uiso 1 1 calc R . .

C132 C 1.0208(4) 0.2453(3) 0.45272(14) 0.0490(14) Uani 1 1 d . . .

H13F H 0.9930 0.2863 0.4610 0.059 Uiso 1 1 calc R . .

C133 C 0.7542(4) 0.1116(2) 0.44445(13) 0.0359(12) Uani 1 1 d . . .

C134 C 0.7173(4) 0.0358(2) 0.44290(15) 0.0471(14) Uani 1 1 d . . .

H13G H 0.7418 0.0125 0.4623 0.056 Uiso 1 1 calc R . .

C135 C 0.6477(5) -0.0048(3) 0.41447(16) 0.0545(16) Uani 1 1 d . . .

H13H H 0.6259 -0.0557 0.4142 0.065 Uiso 1 1 calc R . .

C136 C 0.6082(4) 0.0273(3) 0.38583(15) 0.0499(14) Uani 1 1 d . . .

H13I H 0.5578 -0.0010 0.3666 0.060 Uiso 1 1 calc R . .

C137 C 0.6434(4) 0.1006(3) 0.38595(14) 0.0411(13) Uani 1 1 d . . .

H13J H 0.6184 0.1232 0.3664 0.049 Uiso 1 1 calc R . .

C138 C 0.7141(4) 0.1409(3) 0.41417(13) 0.0385(12) Uani 1 1 d . . .

H13K H 0.7376 0.1915 0.4134 0.046 Uiso 1 1 calc R . .

C139 C 0.8071(4) 0.2376(3) 0.49372(13) 0.0388(12) Uani 1 1 d . . .

C140 C 0.8793(5) 0.2891(3) 0.51904(14) 0.0471(14) Uani 1 1 d . . .

H14C H 0.9484 0.2801 0.5257 0.057 Uiso 1 1 calc R . .

C141 C 0.8545(6) 0.3534(3) 0.53502(16) 0.0588(17) Uani 1 1 d . . .

H14D H 0.9062 0.3873 0.5519 0.071 Uiso 1 1 calc R . .

C142 C 0.7545(6) 0.3667(3) 0.52591(17) 0.0636(18) Uani 1 1 d . . .

H14E H 0.7378 0.4107 0.5360 0.076 Uiso 1 1 calc R . .

C143 C 0.6784(5) 0.3166(3) 0.50223(15) 0.0540(15) Uani 1 1 d . . .

H14F H 0.6078 0.3246 0.4970 0.065 Uiso 1 1 calc R . .

C144 C 0.7065(4) 0.2534(3) 0.48590(13) 0.0415(13) Uani 1 1 d . . .

H14G H 0.6546 0.2201 0.4688 0.050 Uiso 1 1 calc R . .

B2 B 0.6977(6) -0.1477(3) 0.01918(17) 0.0496(17) Uani 1 1 d . . .

C151 C 0.5706(3) -0.1405(3) 0.02861(12) 0.073(2) Uani 1 1 d G . .

C152 C 0.4993(6) -0.1977(3) 0.04159(13) 0.109(3) Uani 1 1 d G . .

H15A H 0.5194 -0.2425 0.0423 0.131 Uiso 1 1 calc R . .

C153 C 0.3986(5) -0.1895(4) 0.05358(13) 0.170(6) Uani 1 1 d G . .

H15B H 0.3498 -0.2286 0.0624 0.203 Uiso 1 1 calc R . .

C154 C 0.3692(3) -0.1239(5) 0.05260(13) 0.182(7) Uani 1 1 d G . .

H15C H 0.3004 -0.1183 0.0608 0.218 Uiso 1 1 calc R . .

C155 C 0.4406(5) -0.0667(3) 0.03963(15) 0.138(4) Uani 1 1 d G . .

H15D H 0.4205 -0.0219 0.0390 0.166 Uiso 1 1 calc R . .

C156 C 0.5413(4) -0.0750(3) 0.02763(13) 0.096(3) Uani 1 1 d G . .

H15E H 0.5900 -0.0358 0.0188 0.116 Uiso 1 1 calc R . .

C157 C 0.7690(3) -0.11110(18) 0.05963(8) 0.0443(13) Uani 1 1 d G . .

C158 C 0.8026(3) -0.03620(17) 0.06654(9) 0.0586(16) Uani 1 1 d G . .

H15F H 0.7865 -0.0075 0.0483 0.070 Uiso 1 1 calc R . .

C159 C 0.8596(3) -0.00333(14) 0.10017(10) 0.0684(19) Uani 1 1 d G . .

H15G H 0.8826 0.0479 0.1049 0.082 Uiso 1 1 calc R . .

C160 C 0.8831(3) -0.0454(2) 0.12690(8) 0.0550(15) Uani 1 1 d G . .

H16A H 0.9221 -0.0229 0.1499 0.066 Uiso 1 1 calc R . .

C161 C 0.8495(3) -0.12026(19) 0.11999(8) 0.0505(14) Uani 1 1 d G . .

H16B H 0.8655 -0.1490 0.1383 0.061 Uiso 1 1 calc R . .

C162 C 0.7924(3) -0.15313(13) 0.08636(9) 0.0482(14) Uani 1 1 d G . .

H16C H 0.7694 -0.2043 0.0816 0.058 Uiso 1 1 calc R . .

C163 C 0.7407(4) -0.1033(2) -0.01671(9) 0.0530(15) Uani 1 1 d G . .

C164 C 0.6675(3) -0.1097(3) -0.04746(13) 0.090(3) Uani 1 1 d G . .

H16D H 0.5947 -0.1375 -0.0473 0.108 Uiso 1 1 calc R . .

C165 C 0.7008(5) -0.0754(3) -0.07839(10) 0.120(4) Uani 1 1 d G . .

H16E H 0.6508 -0.0798 -0.0994 0.143 Uiso 1 1 calc R . .

C166 C 0.8074(6) -0.0347(3) -0.07857(13) 0.127(4) Uani 1 1 d G . .

H16F H 0.8302 -0.0113 -0.0997 0.152 Uiso 1 1 calc R . .

C167 C 0.8806(4) -0.0283(3) -0.04782(17) 0.141(4) Uani 1 1 d G . .

H16G H 0.9534 -0.0005 -0.0479 0.169 Uiso 1 1 calc R . .

C168 C 0.8473(4) -0.0626(3) -0.01689(13) 0.101(3) Uani 1 1 d G . .

H16H H 0.8973 -0.0582 0.0041 0.121 Uiso 1 1 calc R . .

C169 C 0.7073(5) -0.23187(19) 0.00434(12) 0.078(2) Uani 1 1 d G . .

C170 C 0.6238(4) -0.2774(3) -0.01928(13) 0.129(4) Uani 1 1 d G . .

H17B H 0.5577 -0.2630 -0.0242 0.155 Uiso 1 1 calc R . .

C171 C 0.6369(6) -0.3440(3) -0.03574(13) 0.207(8) Uani 1 1 d G . .

H17C H 0.5798 -0.3751 -0.0519 0.248 Uiso 1 1 calc R . .

C172 C 0.7336(7) -0.3651(2) -0.02858(16) 0.252(11) Uani 1 1 d G . .

H17D H 0.7426 -0.4106 -0.0398 0.303 Uiso 1 1 calc R . .

C173 C 0.8171(6) -0.3196(3) -0.00496(17) 0.224(8) Uani 1 1 d G . .

H17E H 0.8832 -0.3340 -0.0001 0.269 Uiso 1 1 calc R . .

C174 C 0.8040(5) -0.2530(3) 0.01150(13) 0.126(4) Uani 1 1 d G . .

H17F H 0.8611 -0.2219 0.0276 0.151 Uiso 1 1 calc R . .

S1 S 0.15690(12) 0.48846(8) 0.34219(4) 0.0536(4) Uani 1 1 d . A 2

F1 F 0.3312(5) 0.4827(4) 0.3792(2) 0.232(4) Uani 1 1 d . A 2

F2 F 0.1842(7) 0.4514(4) 0.40688(15) 0.210(4) Uani 1 1 d . A 2

F3 F 0.2250(4) 0.3817(3) 0.36385(16) 0.142(2) Uani 1 1 d . A 2

O21 O 0.1734(5) 0.5628(2) 0.3579(2) 0.152(3) Uani 1 1 d . A 2

O22 O 0.2078(5) 0.4820(4) 0.30950(15) 0.141(3) Uani 1 1 d . A 2

O23 O 0.0496(3) 0.4481(2) 0.34044(13) 0.0781(14) Uani 1 1 d . A 2

C181 C 0.2299(7) 0.4540(5) 0.3755(3) 0.097(3) Uani 1 1 d . A 2

S2 S 1.28792(12) -0.49817(9) 0.15350(4) 0.0581(4) Uani 1 1 d . B 2

F11 F 1.1082(5) -0.4885(4) 0.1217(2) 0.206(4) Uani 1 1 d . B 2

F12 F 1.2411(8) -0.4748(5) 0.08758(15) 0.268(6) Uani 1 1 d . B 2

F13 F 1.2293(5) -0.3914(3) 0.1290(2) 0.177(3) Uani 1 1 d . B 2

O31 O 1.2619(5) -0.5746(2) 0.1405(2) 0.145(3) Uani 1 1 d . B 2

O32 O 1.2448(5) -0.4844(4) 0.18733(15) 0.143(2) Uani 1 1 d . B 2

O33 O 1.3970(3) -0.4629(2) 0.15131(14) 0.0874(15) Uani 1 1 d . B 2

C191 C 1.2152(8) -0.4628(5) 0.1193(3) 0.107(3) Uani 1 1 d . B 2

N21 N 0.3352(5) 0.0833(3) 0.36723(15) 0.0877(19) Uani 1 1 d D C 2

C201 C 0.4197(6) 0.1274(4) 0.43528(16) 0.100(3) Uani 1 1 d D C 2

H20B H 0.4647 0.1768 0.4372 0.150 Uiso 1 1 calc R C 2

H20C H 0.4649 0.0950 0.4423 0.150 Uiso 1 1 calc R C 2

H20D H 0.3600 0.1261 0.4521 0.150 Uiso 1 1 calc R C 2

C202 C 0.3737(5) 0.1038(3) 0.39660(15) 0.0697(19) Uani 1 1 d D C 2

N31 N 1.2156(13) -0.1615(10) 0.1342(3) 0.265(8) Uani 1 1 d D D 2

C301 C 1.0763(9) -0.1740(7) 0.0771(4) 0.185(6) Uani 1 1 d D D 2

H30B H 1.0128 -0.1567 0.0858 0.278 Uiso 1 1 calc R D 2

H30C H 1.0528 -0.2249 0.0663 0.278 Uiso 1 1 calc R D 2

H30D H 1.1098 -0.1452 0.0580 0.278 Uiso 1 1 calc R D 2

C302 C 1.1566(11) -0.1669(9) 0.1088(4) 0.236(12) Uani 1 1 d D D 2

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

Fe1 0.0252(4) 0.0227(4) 0.0349(4) 0.0091(3) 0.0021(3) 0.0027(3)

Fe2 0.0274(4) 0.0307(4) 0.0349(4) 0.0117(3) 0.0022(3) 0.0034(3)

O1 0.0276(19) 0.0348(19) 0.0342(19) 0.0151(15) 0.0016(14) 0.0031(15)

O2 0.0087(16) 0.054(2) 0.060(2) 0.0250(19) 0.0011(15) -0.0070(15)

O3 0.029(2) 0.063(2) 0.045(2) 0.0210(19) -0.0014(16) 0.0004(17)

O4 0.039(2) 0.068(3) 0.064(3) 0.026(2) -0.0118(19) 0.008(2)

O5 0.027(2) 0.047(2) 0.061(2) -0.0088(19) -0.0058(17) 0.0040(17)

O6 0.034(2) 0.156(5) 0.080(3) 0.055(3) 0.006(2) -0.015(3)

N1 0.031(2) 0.0185(19) 0.031(2) 0.0044(16) 0.0032(17) 0.0049(17)

N2 0.030(2) 0.024(2) 0.038(2) 0.0040(18) -0.0020(18) 0.0016(17)

N3 0.036(2) 0.020(2) 0.034(2) 0.0063(17) -0.0028(19) 0.0027(18)

N4 0.032(2) 0.034(2) 0.029(2) -0.0006(18) 0.0015(19) 0.0025(19)

N5 0.030(2) 0.030(2) 0.048(3) 0.012(2) 0.005(2) 0.0098(19)

N6 0.053(3) 0.021(2) 0.058(3) 0.012(2) 0.012(2) 0.011(2)

N7 0.035(3) 0.038(2) 0.046(3) 0.019(2) 0.008(2) 0.006(2)

N8 0.068(3) 0.029(2) 0.049(3) 0.000(2) 0.010(2) 0.018(2)

N9 0.028(2) 0.025(2) 0.029(2) 0.0025(17) -0.0003(18) -0.0016(18)

N10 0.039(2) 0.028(2) 0.035(2) 0.0082(19) -0.0027(19) 0.0024(19)

C1 0.020(2) 0.022(2) 0.033(3) 0.005(2) -0.007(2) 0.0012(19)

C2 0.024(3) 0.026(3) 0.039(3) 0.004(2) 0.000(2) 0.007(2)

C3 0.038(3) 0.031(3) 0.036(3) 0.009(2) -0.003(2) 0.005(2)

C4 0.032(3) 0.029(3) 0.028(3) 0.003(2) 0.006(2) 0.000(2)

C5 0.030(3) 0.015(2) 0.042(3) 0.009(2) 0.007(2) 0.001(2)

C6 0.030(3) 0.022(3) 0.045(3) 0.008(2) -0.001(2) 0.001(2)

C7 0.041(3) 0.051(4) 0.053(4) 0.005(3) -0.007(3) 0.007(3)

C8 0.055(4) 0.061(4) 0.065(4) 0.003(3) -0.018(3) -0.008(3)

C9 0.062(5) 0.077(5) 0.059(4) -0.003(4) -0.014(4) 0.003(4)

C10 0.061(4) 0.056(4) 0.043(4) 0.005(3) -0.003(3) 0.002(3)

C11 0.055(4) 0.034(3) 0.036(3) 0.001(2) -0.002(3) 0.008(3)

C12 0.040(3) 0.047(3) 0.032(3) 0.005(2) 0.007(2) 0.001(3)

C13 0.046(3) 0.048(3) 0.043(3) -0.003(3) 0.002(3) 0.011(3)

C14 0.028(3) 0.029(3) 0.046(3) 0.005(2) 0.003(2) 0.004(2)

C15 0.038(3) 0.026(3) 0.038(3) 0.007(2) 0.014(2) 0.008(2)

C16 0.042(3) 0.028(3) 0.040(3) 0.014(2) 0.009(2) 0.018(2)

C17 0.047(4) 0.044(3) 0.059(4) 0.018(3) 0.007(3) 0.021(3)

C18 0.055(4) 0.057(4) 0.057(4) 0.025(3) 0.011(3) 0.029(3)

C19 0.063(4) 0.053(4) 0.073(4) 0.033(3) 0.012(3) 0.038(3)

C20 0.068(4) 0.037(3) 0.074(4) 0.028(3) 0.025(3) 0.022(3)

C21 0.053(4) 0.031(3) 0.052(3) 0.019(3) 0.018(3) 0.019(3)

C22 0.051(4) 0.030(3) 0.117(6) 0.008(4) 0.014(4) 0.002(3)

C23 0.080(6) 0.078(5) 0.136(7) -0.030(5) 0.048(5) -0.012(4)

C24 0.045(3) 0.027(3) 0.038(3) 0.004(2) -0.001(2) 0.002(2)

C25 0.049(3) 0.021(3) 0.038(3) 0.011(2) 0.005(3) 0.007(2)

C26 0.047(4) 0.037(3) 0.055(4) 0.024(3) 0.019(3) 0.012(3)

C27 0.050(4) 0.055(4) 0.071(4) 0.034(3) 0.025(3) 0.024(3)

C28 0.068(5) 0.071(5) 0.089(5) 0.028(4) 0.023(4) 0.036(4)

C29 0.091(6) 0.065(5) 0.124(7) 0.021(5) 0.035(5) 0.050(5)

C30 0.098(6) 0.069(5) 0.077(5) 0.001(4) 0.027(4) 0.042(4)

C31 0.075(5) 0.043(4) 0.061(4) 0.007(3) 0.017(3) 0.024(3)

C32 0.086(5) 0.045(4) 0.061(4) -0.013(3) 0.008(4) 0.006(3)

C33 0.122(7) 0.039(4) 0.134(7) -0.020(4) 0.013(5) -0.004(4)

C34 0.039(3) 0.026(3) 0.043(3) 0.012(2) -0.006(2) 0.002(2)

C35 0.043(3) 0.024(3) 0.030(3) 0.003(2) 0.006(2) 0.005(2)

C36 0.031(3) 0.032(3) 0.025(3) 0.004(2) 0.005(2) 0.003(2)

C37 0.032(3) 0.035(3) 0.027(3) 0.002(2) 0.004(2) -0.002(2)

C38 0.038(3) 0.038(3) 0.038(3) -0.002(2) 0.004(2) 0.001(3)

C39 0.046(3) 0.038(3) 0.041(3) 0.002(3) 0.008(3) -0.011(3)

C40 0.050(4) 0.022(3) 0.054(3) 0.006(2) 0.010(3) 0.002(3)

C41 0.037(3) 0.042(3) 0.028(3) 0.005(2) 0.009(2) 0.008(3)

C42 0.065(4) 0.032(3) 0.053(4) 0.018(3) -0.018(3) -0.001(3)

C43 0.084(6) 0.113(6) 0.120(7) 0.030(5) -0.006(5) 0.060(5)

C44 0.023(3) 0.026(3) 0.046(3) 0.004(2) -0.001(2) 0.007(2)

C45 0.019(3) 0.028(3) 0.046(3) 0.004(2) 0.005(2) 0.003(2)

C46 0.023(3) 0.038(3) 0.044(3) 0.011(2) 0.003(2) 0.007(2)

C47 0.033(3) 0.031(3) 0.050(3) 0.001(2) -0.001(3) 0.010(2)

C48 0.021(3) 0.036(3) 0.042(3) -0.009(2) -0.002(2) 0.007(2)

C49 0.025(3) 0.079(4) 0.045(3) 0.008(3) 0.003(3) -0.007(3)

C50 0.026(3) 0.073(4) 0.039(3) 0.020(3) 0.000(2) -0.001(3)

C51 0.057(4) 0.111(6) 0.085(5) 0.062(5) -0.009(4) 0.005(4)

C52 0.042(3) 0.061(4) 0.054(4) -0.009(3) -0.006(3) -0.007(3)

C53 0.062(5) 0.291(14) 0.125(8) 0.139(9) 0.000(5) -0.038(7)

Fe3 0.0261(4) 0.0234(4) 0.0310(4) 0.0074(3) 0.0011(3) 0.0020(3)

Fe4 0.0231(4) 0.0221(4) 0.0317(4) 0.0069(3) 0.0017(3) 0.0024(3)

O11 0.0171(16) 0.0269(17) 0.0334(18) 0.0058(14) -0.0002(13) -0.0001(13)

O12 0.033(2) 0.046(2) 0.050(2) 0.0175(18) -0.0020(17) 0.0004(16)

O13 0.038(2) 0.050(2) 0.037(2) 0.0145(17) -0.0014(16) 0.0058(17)

O14 0.028(2) 0.097(3) 0.054(2) 0.035(2) -0.0020(18) -0.010(2)

O15 0.0266(19) 0.046(2) 0.050(2) -0.0079(17) -0.0069(16) 0.0048(16)

O16 0.036(2) 0.072(3) 0.052(2) 0.028(2) -0.0049(18) 0.0131(19)

N11 0.034(2) 0.0156(19) 0.030(2) 0.0042(16) 0.0065(17) -0.0016(17)

N12 0.027(2) 0.024(2) 0.029(2) 0.0043(17) 0.0000(17) 0.0042(17)

N13 0.031(2) 0.021(2) 0.026(2) -0.0010(17) 0.0006(17) 0.0022(17)

N14 0.035(2) 0.020(2) 0.035(2) 0.0039(17) 0.0033(18) 0.0041(18)

N15 0.032(2) 0.023(2) 0.034(2) 0.0067(17) 0.0030(19) 0.0059(18)

N16 0.052(3) 0.023(2) 0.034(2) 0.0005(19) 0.006(2) 0.008(2)

N17 0.034(2) 0.023(2) 0.039(2) 0.0069(18) 0.0043(19) 0.0083(19)

N18 0.039(3) 0.015(2) 0.058(3) 0.0136(19) 0.007(2) 0.0013(19)

N19 0.027(2) 0.025(2) 0.034(2) 0.0046(18) 0.0019(18) 0.0023(17)

N20 0.041(3) 0.051(3) 0.039(3) 0.006(2) 0.013(2) 0.009(2)

C61 0.031(3) 0.025(3) 0.031(3) 0.002(2) 0.000(2) 0.001(2)

C62 0.018(2) 0.023(2) 0.038(3) 0.004(2) 0.003(2) 0.0056(19)

C63 0.020(2) 0.023(2) 0.033(3) 0.004(2) -0.002(2) 0.0045(19)

C64 0.034(3) 0.021(2) 0.031(3) 0.003(2) -0.004(2) 0.006(2)

C65 0.026(3) 0.023(3) 0.031(3) 0.007(2) 0.001(2) 0.005(2)

C66 0.031(3) 0.024(3) 0.027(3) 0.004(2) 0.006(2) 0.003(2)

C67 0.034(3) 0.032(3) 0.040(3) -0.001(2) 0.001(2) 0.003(2)

C68 0.033(3) 0.032(3) 0.048(3) -0.008(2) 0.002(2) -0.011(2)

C69 0.045(3) 0.023(3) 0.055(4) 0.000(2) 0.008(3) -0.001(2)

C70 0.048(3) 0.021(3) 0.036(3) 0.006(2) 0.002(2) 0.003(2)

C71 0.032(3) 0.025(3) 0.025(3) 0.000(2) 0.002(2) -0.002(2)

C72 0.048(3) 0.025(3) 0.037(3) 0.011(2) -0.006(2) 0.009(2)

C73 0.063(4) 0.064(4) 0.051(4) 0.012(3) -0.001(3) 0.037(3)

C74 0.040(3) 0.021(2) 0.028(3) 0.002(2) 0.000(2) 0.001(2)

C75 0.046(3) 0.023(3) 0.028(3) 0.009(2) 0.008(2) 0.006(2)

C76 0.047(3) 0.025(3) 0.043(3) 0.013(2) 0.010(3) 0.013(2)

C77 0.037(3) 0.038(3) 0.052(3) 0.013(3) 0.005(3) 0.007(3)

C78 0.045(4) 0.057(4) 0.076(4) 0.018(3) 0.013(3) 0.023(3)

C79 0.054(4) 0.062(4) 0.065(4) 0.014(3) 0.022(3) 0.031(3)

C80 0.076(5) 0.040(3) 0.048(3) 0.007(3) 0.009(3) 0.024(3)

C81 0.044(3) 0.028(3) 0.042(3) 0.010(2) 0.013(3) 0.013(2)

C82 0.059(4) 0.031(3) 0.044(3) -0.003(2) 0.001(3) 0.004(3)

C83 0.087(5) 0.033(3) 0.083(5) 0.003(3) 0.001(4) -0.004(3)

C84 0.040(3) 0.016(2) 0.045(3) 0.010(2) 0.004(2) 0.001(2)

C85 0.041(3) 0.018(2) 0.034(3) 0.010(2) 0.007(2) 0.005(2)

C86 0.047(3) 0.033(3) 0.044(3) 0.009(2) 0.016(3) 0.016(3)

C87 0.036(3) 0.039(3) 0.056(3) 0.009(3) 0.008(3) 0.012(3)

C88 0.048(4) 0.057(4) 0.056(4) 0.022(3) 0.013(3) 0.028(3)

C89 0.057(4) 0.052(4) 0.076(4) 0.035(3) 0.019(3) 0.031(3)

C90 0.070(4) 0.033(3) 0.063(4) 0.023(3) 0.023(3) 0.018(3)

C91 0.042(3) 0.034(3) 0.045(3) 0.010(2) 0.014(2) 0.011(3)

C92 0.056(4) 0.026(3) 0.088(5) 0.025(3) 0.013(3) 0.005(3)

C93 0.066(4) 0.056(4) 0.083(5) -0.008(4) 0.018(4) -0.019(3)

C94 0.030(3) 0.038(3) 0.036(3) 0.012(2) 0.003(2) 0.008(2)

C95 0.032(3) 0.027(3) 0.028(3) 0.003(2) 0.002(2) 0.011(2)

C96 0.043(3) 0.029(3) 0.036(3) 0.007(2) -0.001(3) 0.008(2)

C97 0.044(3) 0.044(3) 0.046(3) 0.010(3) -0.002(3) 0.009(3)

C98 0.065(4) 0.054(4) 0.058(4) 0.007(3) -0.018(3) -0.002(3)

C99 0.054(4) 0.083(5) 0.049(4) -0.003(3) -0.010(3) -0.004(4)

C100 0.070(5) 0.079(5) 0.032(3) -0.005(3) 0.000(3) 0.008(4)

C101 0.038(3) 0.037(3) 0.040(3) 0.000(2) 0.003(3) 0.000(2)

C102 0.054(4) 0.065(4) 0.041(3) -0.010(3) 0.014(3) 0.011(3)

C103 0.082(5) 0.095(5) 0.066(5) 0.000(4) 0.002(4) 0.026(4)

C104 0.027(3) 0.024(3) 0.043(3) 0.000(2) -0.006(2) 0.008(2)

C105 0.036(3) 0.024(3) 0.032(3) 0.002(2) 0.000(2) 0.005(2)

C106 0.034(3) 0.041(3) 0.047(3) 0.009(3) -0.002(3) 0.007(2)

C107 0.027(3) 0.045(3) 0.041(3) 0.007(3) 0.003(2) -0.003(2)

C108 0.029(3) 0.031(3) 0.034(3) -0.002(2) -0.001(2) 0.008(2)

C109 0.039(3) 0.029(3) 0.033(3) 0.000(2) -0.005(2) 0.011(2)

C110 0.032(3) 0.027(3) 0.042(3) 0.004(2) 0.000(2) 0.005(2)

C111 0.054(4) 0.141(7) 0.080(5) 0.060(5) 0.011(4) -0.017(4)

C112 0.038(3) 0.060(4) 0.047(3) -0.009(3) -0.004(3) -0.007(3)

C113 0.057(4) 0.108(5) 0.053(4) 0.048(4) 0.005(3) 0.021(4)

B1 0.054(4) 0.023(3) 0.032(3) 0.008(2) 0.002(3) 0.011(3)

C121 0.072(4) 0.019(3) 0.044(3) -0.003(2) -0.004(3) 0.008(3)

C122 0.070(4) 0.051(4) 0.066(4) 0.022(3) -0.021(3) -0.012(3)

C123 0.074(5) 0.060(4) 0.061(4) 0.026(3) -0.025(4) -0.010(3)

C124 0.093(5) 0.039(3) 0.058(4) 0.015(3) 0.001(4) 0.006(4)

C125 0.109(6) 0.053(4) 0.049(4) 0.016(3) 0.021(4) 0.033(4)

C126 0.073(5) 0.059(4) 0.044(4) 0.013(3) 0.014(3) 0.024(3)

C127 0.042(3) 0.045(3) 0.036(3) 0.008(2) -0.007(2) 0.012(3)

C128 0.045(4) 0.047(4) 0.074(4) -0.008(3) -0.004(3) 0.017(3)

C129 0.056(4) 0.056(4) 0.092(5) 0.001(4) 0.004(4) 0.020(3)

C130 0.054(4) 0.093(5) 0.070(5) 0.015(4) 0.010(3) 0.033(4)

C131 0.056(4) 0.061(4) 0.064(4) 0.020(3) -0.001(3) 0.014(3)

C132 0.052(4) 0.050(4) 0.053(4) 0.021(3) 0.009(3) 0.023(3)

C133 0.042(3) 0.025(3) 0.039(3) 0.000(2) 0.012(2) 0.005(2)

C134 0.061(4) 0.021(3) 0.052(3) -0.002(2) 0.000(3) 0.000(3)

C135 0.071(4) 0.025(3) 0.059(4) 0.000(3) 0.021(3) -0.005(3)

C136 0.047(3) 0.046(4) 0.047(3) -0.008(3) 0.009(3) -0.003(3)

C137 0.033(3) 0.044(3) 0.039(3) 0.000(3) 0.008(2) -0.003(3)

C138 0.040(3) 0.036(3) 0.036(3) 0.004(2) 0.008(2) 0.000(2)

C139 0.051(3) 0.029(3) 0.032(3) 0.006(2) 0.006(2) 0.001(3)

C140 0.056(4) 0.034(3) 0.046(3) 0.006(3) 0.003(3) -0.003(3)

C141 0.087(5) 0.026(3) 0.051(4) -0.002(3) 0.014(3) -0.011(3)

C142 0.106(6) 0.030(3) 0.059(4) 0.010(3) 0.033(4) 0.018(4)

C143 0.072(4) 0.053(4) 0.048(4) 0.014(3) 0.023(3) 0.028(3)

C144 0.054(4) 0.040(3) 0.033(3) 0.009(2) 0.006(2) 0.013(3)

B2 0.067(5) 0.045(4) 0.036(4) 0.007(3) 0.013(3) 0.009(3)

C151 0.092(6) 0.088(5) 0.029(3) -0.003(3) -0.003(3) 0.006(5)

C152 0.079(6) 0.179(9) 0.048(4) 0.024(5) -0.003(4) -0.017(6)

C153 0.091(9) 0.34(2) 0.060(6) 0.043(8) -0.005(6) 0.016(9)

C154 0.049(6) 0.42(2) 0.050(6) 0.016(9) 0.000(4) 0.013(9)

C155 0.111(8) 0.250(13) 0.068(6) -0.034(7) 0.007(5) 0.100(9)

C156 0.082(6) 0.130(7) 0.073(5) -0.015(5) 0.011(4) 0.029(5)

C157 0.053(4) 0.041(3) 0.040(3) 0.007(3) 0.018(3) 0.011(3)

C158 0.090(5) 0.039(3) 0.046(4) 0.008(3) 0.011(3) 0.010(3)

C159 0.098(5) 0.038(3) 0.055(4) -0.001(3) 0.015(4) -0.010(3)

C160 0.055(4) 0.062(4) 0.040(3) -0.001(3) 0.011(3) -0.002(3)

C161 0.050(4) 0.058(4) 0.040(3) 0.007(3) 0.008(3) 0.004(3)

C162 0.053(4) 0.042(3) 0.049(4) 0.007(3) 0.012(3) 0.009(3)

C163 0.067(4) 0.044(3) 0.052(4) -0.002(3) 0.008(3) 0.024(3)

C164 0.107(6) 0.151(7) 0.038(4) 0.026(4) 0.009(4) 0.074(6)

C165 0.184(10) 0.148(9) 0.075(6) 0.051(6) 0.037(6) 0.116(8)

C166 0.274(14) 0.070(6) 0.055(5) 0.012(4) 0.065(7) 0.069(8)

C167 0.192(11) 0.115(8) 0.105(7) 0.024(6) 0.078(8) 0.000(7)

C168 0.094(6) 0.130(7) 0.066(5) 0.026(5) 0.025(4) -0.007(5)

C169 0.156(7) 0.038(4) 0.036(4) 0.007(3) 0.027(4) 0.006(4)

C170 0.247(11) 0.053(5) 0.043(4) -0.002(4) 0.020(6) -0.056(6)

C171 0.46(2) 0.046(5) 0.064(6) -0.010(5) 0.075(9) -0.048(10)

C172 0.63(3) 0.059(6) 0.115(10) 0.037(6) 0.219(15) 0.123(12)

C173 0.52(3) 0.113(9) 0.107(9) 0.054(7) 0.168(12) 0.172(13)

C174 0.269(12) 0.085(6) 0.063(5) 0.024(4) 0.069(6) 0.103(7)

S1 0.0418(9) 0.0581(10) 0.0582(10) 0.0189(8) 0.0058(7) -0.0003(7)

F1 0.121(5) 0.178(6) 0.360(11) 0.059(6) -0.165(6) -0.023(4)

F2 0.359(11) 0.262(8) 0.057(3) 0.027(4) -0.011(5) 0.174(8)

F3 0.146(5) 0.100(4) 0.205(6) 0.054(4) 0.006(4) 0.066(4)

O21 0.172(6) 0.022(3) 0.236(7) -0.024(3) -0.056(5) 0.004(3)

O22 0.142(5) 0.225(7) 0.110(4) 0.097(5) 0.075(4) 0.108(5)

O23 0.034(2) 0.046(2) 0.148(4) 0.028(3) -0.013(2) -0.0097(19)

C181 0.094(7) 0.094(6) 0.091(6) 0.018(5) -0.043(5) -0.001(5)

S2 0.0367(9) 0.0706(11) 0.0611(10) 0.0172(8) 0.0035(7) -0.0045(8)

F11 0.102(4) 0.221(7) 0.275(9) -0.061(6) -0.118(5) 0.065(5)

F12 0.479(15) 0.367(12) 0.041(3) 0.012(5) -0.013(5) 0.284(11)

F13 0.159(5) 0.086(4) 0.302(8) 0.037(4) -0.042(5) 0.066(4)

O31 0.129(5) 0.031(3) 0.253(8) -0.004(4) -0.025(5) -0.013(3)

O32 0.115(5) 0.243(8) 0.090(4) 0.021(5) 0.032(4) 0.075(5)

O33 0.052(3) 0.051(3) 0.164(5) 0.039(3) 0.011(3) 0.007(2)

C191 0.104(7) 0.117(8) 0.104(7) -0.010(6) -0.035(6) 0.053(6)

N21 0.088(5) 0.094(5) 0.081(5) 0.023(4) 0.002(4) 0.017(4)

C201 0.071(5) 0.117(7) 0.102(6) -0.016(5) 0.001(4) 0.018(5)

C202 0.051(4) 0.063(5) 0.099(6) 0.019(4) 0.020(4) 0.016(4)

N31 0.275(17) 0.300(19) 0.149(13) -0.031(12) 0.102(11) -0.064(14)

C301 0.116(10) 0.126(10) 0.30(2) -0.008(11) 0.074(10) 0.007(8)

C302 0.25(2) 0.178(13) 0.20(2) -0.080(16) 0.166(16) -0.095(16)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Fe1 O1 1.967(3) . ?

Fe1 O2 2.036(3) . ?

Fe1 N3 2.045(4) . ?

Fe1 N5 2.046(4) . ?

Fe1 N1 2.328(4) . ?

Fe2 O1 1.970(3) . ?

Fe2 O3 2.025(3) . ?

Fe2 N9 2.044(4) . ?

Fe2 N7 2.063(4) . ?

Fe2 N2 2.314(4) . ?

O1 C1 1.425(5) . ?

O2 C44 1.254(5) . ?

O3 C44 1.273(5) . ?

O4 C47 1.361(6) . ?

O4 C51 1.423(6) . ?

O5 C48 1.375(5) . ?

O5 C52 1.438(6) . ?

O6 C49 1.367(6) . ?

O6 C53 1.436(8) . ?

N1 C2 1.474(5) . ?

N1 C4 1.497(5) . ?

N1 C14 1.497(5) . ?

N2 C34 1.473(5) . ?

N2 C24 1.481(5) . ?

N2 C3 1.486(6) . ?

N3 C5 1.332(5) . ?

N3 C6 1.403(6) . ?

N4 C5 1.347(5) . ?

N4 C11 1.386(6) . ?

N4 C12 1.469(6) . ?

N5 C15 1.316(5) . ?

N5 C16 1.398(5) . ?

N6 C15 1.366(5) . ?

N6 C21 1.386(6) . ?

N6 C22 1.469(6) . ?

N7 C25 1.321(6) . ?

N7 C26 1.399(6) . ?

N8 C25 1.366(6) . ?

N8 C31 1.385(7) . ?

N8 C32 1.441(7) . ?

N9 C35 1.324(6) . ?

N9 C36 1.397(5) . ?

N10 C35 1.342(5) . ?

N10 C41 1.388(6) . ?

N10 C42 1.472(6) . ?

C1 C2 1.526(6) . ?

C1 C3 1.529(6) . ?

C1 H1A 1.0000 . ?

C2 H2A 0.9900 . ?

C2 H2B 0.9900 . ?

C3 H3A 0.9900 . ?

C3 H3B 0.9900 . ?

C4 C5 1.500(6) . ?

C4 H4A 0.9900 . ?

C4 H4B 0.9900 . ?

C6 C7 1.390(6) . ?

C6 C11 1.411(7) . ?

C7 C8 1.388(7) . ?

C7 H7A 0.9500 . ?

C8 C9 1.376(8) . ?

C8 H8A 0.9500 . ?

C9 C10 1.389(7) . ?

C9 H9A 0.9500 . ?

C10 C11 1.376(7) . ?

C10 H10A 0.9500 . ?

C12 C13 1.507(6) . ?

C12 H12A 0.9900 . ?

C12 H12B 0.9900 . ?

C13 H13A 0.9800 . ?

C13 H13B 0.9800 . ?

C13 H13C 0.9800 . ?

C14 C15 1.495(6) . ?

C14 H14A 0.9900 . ?

C14 H14B 0.9900 . ?

C16 C17 1.391(6) . ?

C16 C21 1.395(6) . ?

C17 C18 1.376(7) . ?

C17 H17A 0.9500 . ?

C18 C19 1.395(8) . ?

C18 H18A 0.9500 . ?

C19 C20 1.380(7) . ?

C19 H19A 0.9500 . ?

C20 C21 1.403(7) . ?

C20 H20A 0.9500 . ?

C22 C23 1.425(9) . ?

C22 H22A 0.9900 . ?

C22 H22B 0.9900 . ?

C23 H23A 0.9800 . ?

C23 H23B 0.9800 . ?

C23 H23C 0.9800 . ?

C24 C25 1.498(6) . ?

C24 H24A 0.9900 . ?

C24 H24B 0.9900 . ?

C26 C31 1.399(7) . ?

C26 C27 1.400(7) . ?

C27 C28 1.388(8) . ?

C27 H27A 0.9500 . ?

C28 C29 1.387(9) . ?

C28 H28A 0.9500 . ?

C29 C30 1.390(9) . ?

C29 H29A 0.9500 . ?

C30 C31 1.392(8) . ?

C30 H30A 0.9500 . ?

C32 C33 1.512(8) . ?

C32 H32A 0.9900 . ?

C32 H32B 0.9900 . ?

C33 H33A 0.9800 . ?

C33 H33B 0.9800 . ?

C33 H33C 0.9800 . ?

C34 C35 1.497(6) . ?

C34 H34A 0.9900 . ?

C34 H34B 0.9900 . ?

C36 C37 1.377(6) . ?

C36 C41 1.398(6) . ?

C37 C38 1.387(6) . ?

C37 H37A 0.9500 . ?

C38 C39 1.404(7) . ?

C38 H38A 0.9500 . ?

C39 C40 1.367(7) . ?

C39 H39A 0.9500 . ?

C40 C41 1.398(6) . ?

C40 H40A 0.9500 . ?

C42 C43 1.504(8) . ?

C42 H42A 0.9900 . ?

C42 H42B 0.9900 . ?

C43 H43A 0.9800 . ?

C43 H43B 0.9800 . ?

C43 H43C 0.9800 . ?

C44 C45 1.494(6) . ?

C45 C50 1.378(6) . ?

C45 C46 1.396(6) . ?

C46 C47 1.380(6) . ?

C46 H46A 0.9500 . ?

C47 C48 1.393(7) . ?

C48 C49 1.384(7) . ?

C49 C50 1.398(6) . ?

C50 H50A 0.9500 . ?

C51 H51A 0.9800 . ?

C51 H51B 0.9800 . ?

C51 H51C 0.9800 . ?

C52 H52A 0.9800 . ?

C52 H52B 0.9800 . ?

C52 H52C 0.9800 . ?

C53 H53A 0.9800 . ?

C53 H53B 0.9800 . ?

C53 H53C 0.9800 . ?

Fe3 O11 1.982(3) . ?

Fe3 O12 2.037(3) . ?

Fe3 N13 2.047(4) . ?

Fe3 N15 2.059(4) . ?

Fe3 N11 2.299(4) . ?

Fe4 O11 1.974(3) . ?

Fe4 O13 2.026(3) . ?

Fe4 N19 2.054(4) . ?

Fe4 N17 2.056(4) . ?

Fe4 N12 2.314(4) . ?

O11 C61 1.424(5) . ?

O12 C104 1.245(5) . ?

O13 C104 1.259(5) . ?

O14 C107 1.369(5) . ?

O14 C111 1.432(6) . ?

O15 C108 1.379(5) . ?

O15 C112 1.420(5) . ?

O16 C109 1.349(5) . ?

O16 C113 1.436(6) . ?

N11 C62 1.476(5) . ?

N11 C74 1.481(5) . ?

N11 C64 1.499(5) . ?

N12 C94 1.478(5) . ?

N12 C84 1.495(5) . ?

N12 C63 1.498(5) . ?

N13 C65 1.316(5) . ?

N13 C66 1.401(5) . ?

N14 C65 1.358(5) . ?

N14 C71 1.377(5) . ?

N14 C72 1.492(5) . ?

N15 C75 1.335(6) . ?

N15 C76 1.400(6) . ?

N16 C75 1.353(5) . ?

N16 C81 1.380(6) . ?

N16 C82 1.473(6) . ?

N17 C85 1.322(5) . ?

N17 C86 1.396(6) . ?

N18 C85 1.346(5) . ?

N18 C91 1.384(6) . ?

N18 C92 1.483(6) . ?

N19 C95 1.318(5) . ?

N19 C96 1.384(6) . ?

N20 C95 1.350(5) . ?

N20 C101 1.396(6) . ?

N20 C102 1.469(6) . ?

C61 C62 1.518(6) . ?

C61 C63 1.523(6) . ?

C61 H61A 1.0000 . ?

C62 H62A 0.9900 . ?

C62 H62B 0.9900 . ?

C63 H63A 0.9900 . ?

C63 H63B 0.9900 . ?

C64 C65 1.497(6) . ?

C64 H64A 0.9900 . ?

C64 H64B 0.9900 . ?

C66 C71 1.391(6) . ?

C66 C67 1.401(6) . ?

C67 C68 1.385(6) . ?

C67 H67A 0.9500 . ?

C68 C69 1.403(7) . ?

C68 H68A 0.9500 . ?

C69 C70 1.383(6) . ?

C69 H69A 0.9500 . ?

C70 C71 1.390(6) . ?

C70 H70A 0.9500 . ?

C72 C73 1.514(6) . ?

C72 H72A 0.9900 . ?

C72 H72B 0.9900 . ?

C73 H73A 0.9800 . ?

C73 H73B 0.9800 . ?

C73 H73C 0.9800 . ?

C74 C75 1.513(6) . ?

C74 H74A 0.9900 . ?

C74 H74B 0.9900 . ?

C76 C81 1.383(6) . ?

C76 C77 1.386(6) . ?

C77 C78 1.379(7) . ?

C77 H77A 0.9500 . ?

C78 C79 1.395(8) . ?

C78 H78A 0.9500 . ?

C79 C80 1.374(7) . ?

C79 H79A 0.9500 . ?

C80 C81 1.391(7) . ?

C80 H80A 0.9500 . ?

C82 C83 1.524(7) . ?

C82 H82A 0.9900 . ?

C82 H82B 0.9900 . ?

C83 H83A 0.9800 . ?

C83 H83B 0.9800 . ?

C83 H83C 0.9800 . ?

C84 C85 1.505(6) . ?

C84 H84A 0.9900 . ?

C84 H84B 0.9900 . ?

C86 C87 1.378(7) . ?

C86 C91 1.400(7) . ?

C87 C88 1.383(6) . ?

C87 H87A 0.9500 . ?

C88 C89 1.393(7) . ?

C88 H88A 0.9500 . ?

C89 C90 1.353(7) . ?

C89 H89A 0.9500 . ?

C90 C91 1.407(7) . ?

C90 H90A 0.9500 . ?

C92 C93 1.489(7) . ?

C92 H92A 0.9900 . ?

C92 H92B 0.9900 . ?

C93 H93A 0.9800 . ?

C93 H93B 0.9800 . ?

C93 H93C 0.9800 . ?

C94 C95 1.506(6) . ?

C94 H94A 0.9900 . ?

C94 H94B 0.9900 . ?

C96 C101 1.384(6) . ?

C96 C97 1.400(6) . ?

C97 C98 1.379(7) . ?

C97 H97A 0.9500 . ?

C98 C99 1.387(8) . ?

C98 H98A 0.9500 . ?

C99 C100 1.364(7) . ?

C99 H99A 0.9500 . ?

C100 C101 1.415(7) . ?

C100 H10B 0.9500 . ?

C102 C103 1.512(8) . ?

C102 H10C 0.9900 . ?

C102 H10D 0.9900 . ?

C103 H10E 0.9800 . ?

C103 H10F 0.9800 . ?

C103 H10G 0.9800 . ?

C104 C105 1.505(6) . ?

C105 C110 1.392(6) . ?

C105 C106 1.395(6) . ?

C106 C107 1.395(6) . ?

C106 H10H 0.9500 . ?

C107 C108 1.374(6) . ?

C108 C109 1.399(6) . ?

C109 C110 1.399(6) . ?

C110 H11A 0.9500 . ?

C111 H11B 0.9800 . ?

C111 H11C 0.9800 . ?

C111 H11D 0.9800 . ?

C112 H11E 0.9800 . ?

C112 H11F 0.9800 . ?

C112 H11G 0.9800 . ?

C113 H11H 0.9800 . ?

C113 H11I 0.9800 . ?

C113 H11J 0.9800 . ?

B1 C127 1.630(8) . ?

B1 C133 1.639(7) . ?

B1 C121 1.654(7) . ?

B1 C139 1.668(7) . ?

C121 C122 1.394(7) . ?

C121 C126 1.400(7) . ?

C122 C123 1.420(7) . ?

C122 H12C 0.9500 . ?

C123 C124 1.354(8) . ?

C123 H12D 0.9500 . ?

C124 C125 1.347(8) . ?

C124 H12E 0.9500 . ?

C125 C126 1.378(7) . ?

C125 H12F 0.9500 . ?

C126 H12G 0.9500 . ?

C127 C128 1.398(7) . ?

C127 C132 1.398(7) . ?

C128 C129 1.381(8) . ?

C128 H12H 0.9500 . ?

C129 C130 1.390(8) . ?

C129 H12I 0.9500 . ?

C130 C131 1.374(8) . ?

C130 H13D 0.9500 . ?

C131 C132 1.412(7) . ?

C131 H13E 0.9500 . ?

C132 H13F 0.9500 . ?

C133 C138 1.411(6) . ?

C133 C134 1.414(6) . ?

C134 C135 1.363(7) . ?

C134 H13G 0.9500 . ?

C135 C136 1.393(7) . ?

C135 H13H 0.9500 . ?

C136 C137 1.371(7) . ?

C136 H13I 0.9500 . ?

C137 C138 1.364(6) . ?

C137 H13J 0.9500 . ?

C138 H13K 0.9500 . ?

C139 C144 1.392(7) . ?

C139 C140 1.396(7) . ?

C140 C141 1.403(7) . ?

C140 H14C 0.9500 . ?

C141 C142 1.374(8) . ?

C141 H14D 0.9500 . ?

C142 C143 1.377(8) . ?

C142 H14E 0.9500 . ?

C143 C144 1.406(7) . ?

C143 H14F 0.9500 . ?

C144 H14G 0.9500 . ?

B2 C169 1.670(7) . ?

B2 C163 1.671(7) . ?

B2 C157 1.673(7) . ?

B2 C151 1.679(8) . ?

C151 C152 1.3900 . ?

C151 C156 1.3900 . ?

C152 C153 1.3900 . ?

C152 H15A 0.9500 . ?

C153 C154 1.3900 . ?

C153 H15B 0.9500 . ?

C154 C155 1.3900 . ?

C154 H15C 0.9500 . ?

C155 C156 1.3900 . ?

C155 H15D 0.9500 . ?

C156 H15E 0.9500 . ?

C157 C158 1.3900 . ?

C157 C162 1.3900 . ?

C158 C159 1.3900 . ?

C158 H15F 0.9500 . ?

C159 C160 1.3900 . ?

C159 H15G 0.9500 . ?

C160 C161 1.3900 . ?

C160 H16A 0.9500 . ?

C161 C162 1.3900 . ?

C161 H16B 0.9500 . ?

C162 H16C 0.9500 . ?

C163 C164 1.3900 . ?

C163 C168 1.3900 . ?

C164 C165 1.3900 . ?

C164 H16D 0.9500 . ?

C165 C166 1.3900 . ?

C165 H16E 0.9500 . ?

C166 C167 1.3900 . ?

C166 H16F 0.9500 . ?

C167 C168 1.3900 . ?

C167 H16G 0.9500 . ?

C168 H16H 0.9500 . ?

C169 C170 1.3900 . ?

C169 C174 1.3900 . ?

C170 C171 1.3900 . ?

C170 H17B 0.9500 . ?

C171 C172 1.3900 . ?

C171 H17C 0.9500 . ?

C172 C173 1.3900 . ?

C172 H17D 0.9500 . ?

C173 C174 1.3900 . ?

C173 H17E 0.9500 . ?

C174 H17F 0.9500 . ?

S1 O22 1.368(5) . ?

S1 O23 1.390(4) . ?

S1 O21 1.435(4) . ?

S1 C181 1.759(8) . ?

F1 C181 1.262(9) . ?

F2 C181 1.291(10) . ?

F3 C181 1.386(9) . ?

S2 O32 1.375(5) . ?

S2 O33 1.394(4) . ?

S2 O31 1.442(5) . ?

S2 C191 1.791(8) . ?

F11 C191 1.334(11) . ?

F12 C191 1.212(10) . ?

F13 C191 1.340(9) . ?

N21 C202 1.1353(19) . ?

C201 C202 1.4681(19) . ?

C201 H20B 0.9800 . ?

C201 H20C 0.9800 . ?

C201 H20D 0.9800 . ?

N31 C302 1.136(2) . ?

C301 C302 1.470(2) . ?

C301 H30B 0.9800 . ?

C301 H30C 0.9800 . ?

C301 H30D 0.9800 . ?

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_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

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_geom_angle_site_symmetry_3

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O1 Fe1 O2 98.27(13) . . ?

O1 Fe1 N3 127.81(13) . . ?

O2 Fe1 N3 101.29(14) . . ?

O1 Fe1 N5 120.01(14) . . ?

O2 Fe1 N5 104.83(14) . . ?

N3 Fe1 N5 100.79(14) . . ?

O1 Fe1 N1 79.87(12) . . ?

O2 Fe1 N1 177.21(13) . . ?

N3 Fe1 N1 78.39(14) . . ?

N5 Fe1 N1 77.94(13) . . ?

O1 Fe2 O3 100.51(13) . . ?

O1 Fe2 N9 115.97(13) . . ?

O3 Fe2 N9 102.87(14) . . ?

O1 Fe2 N7 120.49(14) . . ?

O3 Fe2 N7 100.53(15) . . ?

N9 Fe2 N7 112.33(14) . . ?

O1 Fe2 N2 81.01(13) . . ?

O3 Fe2 N2 177.60(14) . . ?

N9 Fe2 N2 78.00(13) . . ?

N7 Fe2 N2 77.07(15) . . ?

C1 O1 Fe1 116.9(2) . . ?

C1 O1 Fe2 116.5(2) . . ?

Fe1 O1 Fe2 124.73(15) . . ?

C44 O2 Fe1 138.1(3) . . ?

C44 O3 Fe2 134.7(3) . . ?

C47 O4 C51 116.8(4) . . ?

C48 O5 C52 113.2(4) . . ?

C49 O6 C53 116.4(5) . . ?

C2 N1 C4 112.4(3) . . ?

C2 N1 C14 112.6(3) . . ?

C4 N1 C14 111.6(3) . . ?

C2 N1 Fe1 103.7(2) . . ?

C4 N1 Fe1 109.4(2) . . ?

C14 N1 Fe1 106.7(2) . . ?

C34 N2 C24 111.8(4) . . ?

C34 N2 C3 112.9(4) . . ?

C24 N2 C3 113.6(4) . . ?

C34 N2 Fe2 108.0(3) . . ?

C24 N2 Fe2 108.1(3) . . ?

C3 N2 Fe2 101.7(3) . . ?

C5 N3 C6 105.5(4) . . ?

C5 N3 Fe1 118.0(3) . . ?

C6 N3 Fe1 134.7(3) . . ?

C5 N4 C11 107.7(4) . . ?

C5 N4 C12 127.5(4) . . ?

C11 N4 C12 124.7(4) . . ?

C15 N5 C16 105.7(4) . . ?

C15 N5 Fe1 117.1(3) . . ?

C16 N5 Fe1 137.2(3) . . ?

C15 N6 C21 106.5(4) . . ?

C15 N6 C22 127.6(4) . . ?

C21 N6 C22 125.8(4) . . ?

C25 N7 C26 105.7(4) . . ?

C25 N7 Fe2 116.6(3) . . ?

C26 N7 Fe2 137.3(4) . . ?

C25 N8 C31 106.6(5) . . ?

C25 N8 C32 127.4(5) . . ?

C31 N8 C32 126.1(5) . . ?

C35 N9 C36 106.1(4) . . ?

C35 N9 Fe2 117.0(3) . . ?

C36 N9 Fe2 136.6(3) . . ?

C35 N10 C41 107.0(4) . . ?

C35 N10 C42 127.3(4) . . ?

C41 N10 C42 125.7(4) . . ?

O1 C1 C2 110.4(3) . . ?

O1 C1 C3 109.6(3) . . ?

C2 C1 C3 111.3(4) . . ?

O1 C1 H1A 108.5 . . ?

C2 C1 H1A 108.5 . . ?

C3 C1 H1A 108.5 . . ?

N1 C2 C1 109.7(3) . . ?

N1 C2 H2A 109.7 . . ?

C1 C2 H2A 109.7 . . ?

N1 C2 H2B 109.7 . . ?

C1 C2 H2B 109.7 . . ?

H2A C2 H2B 108.2 . . ?

N2 C3 C1 110.5(4) . . ?

N2 C3 H3A 109.5 . . ?

C1 C3 H3A 109.5 . . ?

N2 C3 H3B 109.5 . . ?

C1 C3 H3B 109.5 . . ?

H3A C3 H3B 108.1 . . ?

N1 C4 C5 111.0(4) . . ?

N1 C4 H4A 109.4 . . ?

C5 C4 H4A 109.4 . . ?

N1 C4 H4B 109.4 . . ?

C5 C4 H4B 109.4 . . ?

H4A C4 H4B 108.0 . . ?

N3 C5 N4 112.7(4) . . ?

N3 C5 C4 122.6(4) . . ?

N4 C5 C4 124.6(4) . . ?

C7 C6 N3 131.3(5) . . ?

C7 C6 C11 120.0(5) . . ?

N3 C6 C11 108.5(4) . . ?

C8 C7 C6 117.6(5) . . ?

C8 C7 H7A 121.2 . . ?

C6 C7 H7A 121.2 . . ?

C9 C8 C7 121.8(6) . . ?

C9 C8 H8A 119.1 . . ?

C7 C8 H8A 119.1 . . ?

C8 C9 C10 121.4(6) . . ?

C8 C9 H9A 119.3 . . ?

C10 C9 H9A 119.3 . . ?

C11 C10 C9 117.3(5) . . ?

C11 C10 H10A 121.3 . . ?

C9 C10 H10A 121.3 . . ?

C10 C11 N4 132.5(5) . . ?

C10 C11 C6 121.8(5) . . ?

N4 C11 C6 105.6(4) . . ?

N4 C12 C13 111.3(4) . . ?

N4 C12 H12A 109.4 . . ?

C13 C12 H12A 109.4 . . ?

N4 C12 H12B 109.4 . . ?

C13 C12 H12B 109.4 . . ?

H12A C12 H12B 108.0 . . ?

C12 C13 H13A 109.5 . . ?

C12 C13 H13B 109.5 . . ?

H13A C13 H13B 109.5 . . ?

C12 C13 H13C 109.5 . . ?

H13A C13 H13C 109.5 . . ?

H13B C13 H13C 109.5 . . ?

C15 C14 N1 109.1(4) . . ?

C15 C14 H14A 109.9 . . ?

N1 C14 H14A 109.9 . . ?

C15 C14 H14B 109.9 . . ?

N1 C14 H14B 109.9 . . ?

H14A C14 H14B 108.3 . . ?

N5 C15 N6 112.8(4) . . ?

N5 C15 C14 122.7(4) . . ?

N6 C15 C14 124.4(4) . . ?

C17 C16 C21 121.4(4) . . ?

C17 C16 N5 129.8(4) . . ?

C21 C16 N5 108.8(4) . . ?

C18 C17 C16 117.8(5) . . ?

C18 C17 H17A 121.1 . . ?

C16 C17 H17A 121.1 . . ?

C17 C18 C19 121.0(5) . . ?

C17 C18 H18A 119.5 . . ?

C19 C18 H18A 119.5 . . ?

C20 C19 C18 122.2(5) . . ?

C20 C19 H19A 118.9 . . ?

C18 C19 H19A 118.9 . . ?

C19 C20 C21 116.9(5) . . ?

C19 C20 H20A 121.5 . . ?

C21 C20 H20A 121.5 . . ?

N6 C21 C16 106.2(4) . . ?

N6 C21 C20 133.0(5) . . ?

C16 C21 C20 120.8(5) . . ?

C23 C22 N6 112.1(5) . . ?

C23 C22 H22A 109.2 . . ?

N6 C22 H22A 109.2 . . ?

C23 C22 H22B 109.2 . . ?

N6 C22 H22B 109.2 . . ?

H22A C22 H22B 107.9 . . ?

C22 C23 H23A 109.5 . . ?

C22 C23 H23B 109.5 . . ?

H23A C23 H23B 109.5 . . ?

C22 C23 H23C 109.5 . . ?

H23A C23 H23C 109.5 . . ?

H23B C23 H23C 109.5 . . ?

N2 C24 C25 108.7(4) . . ?

N2 C24 H24A 109.9 . . ?

C25 C24 H24A 109.9 . . ?

N2 C24 H24B 109.9 . . ?

C25 C24 H24B 109.9 . . ?

H24A C24 H24B 108.3 . . ?

N7 C25 N8 112.7(5) . . ?

N7 C25 C24 122.7(4) . . ?

N8 C25 C24 124.5(5) . . ?

N7 C26 C31 108.7(5) . . ?

N7 C26 C27 129.3(5) . . ?

C31 C26 C27 122.1(5) . . ?

C28 C27 C26 116.9(6) . . ?

C28 C27 H27A 121.5 . . ?

C26 C27 H27A 121.5 . . ?

C29 C28 C27 120.4(7) . . ?

C29 C28 H28A 119.8 . . ?

C27 C28 H28A 119.8 . . ?

C28 C29 C30 123.4(6) . . ?

C28 C29 H29A 118.3 . . ?

C30 C29 H29A 118.3 . . ?

C29 C30 C31 116.4(7) . . ?

C29 C30 H30A 121.8 . . ?

C31 C30 H30A 121.8 . . ?

N8 C31 C30 132.8(6) . . ?

N8 C31 C26 106.4(5) . . ?

C30 C31 C26 120.8(6) . . ?

N8 C32 C33 111.6(5) . . ?

N8 C32 H32A 109.3 . . ?

C33 C32 H32A 109.3 . . ?

N8 C32 H32B 109.3 . . ?

C33 C32 H32B 109.3 . . ?

H32A C32 H32B 108.0 . . ?

C32 C33 H33A 109.5 . . ?

C32 C33 H33B 109.5 . . ?

H33A C33 H33B 109.5 . . ?

C32 C33 H33C 109.5 . . ?

H33A C33 H33C 109.5 . . ?

H33B C33 H33C 109.5 . . ?

N2 C34 C35 110.1(4) . . ?

N2 C34 H34A 109.6 . . ?

C35 C34 H34A 109.6 . . ?

N2 C34 H34B 109.6 . . ?

C35 C34 H34B 109.6 . . ?

H34A C34 H34B 108.2 . . ?

N9 C35 N10 112.7(4) . . ?

N9 C35 C34 122.4(4) . . ?

N10 C35 C34 124.7(4) . . ?

C37 C36 N9 130.3(4) . . ?

C37 C36 C41 121.7(4) . . ?

N9 C36 C41 107.9(4) . . ?

C36 C37 C38 117.1(5) . . ?

C36 C37 H37A 121.5 . . ?

C38 C37 H37A 121.5 . . ?

C37 C38 C39 120.9(5) . . ?

C37 C38 H38A 119.5 . . ?

C39 C38 H38A 119.5 . . ?

C40 C39 C38 122.4(5) . . ?

C40 C39 H39A 118.8 . . ?

C38 C39 H39A 118.8 . . ?

C39 C40 C41 116.5(5) . . ?

C39 C40 H40A 121.8 . . ?

C41 C40 H40A 121.8 . . ?

N10 C41 C36 106.4(4) . . ?

N10 C41 C40 132.0(5) . . ?

C36 C41 C40 121.4(5) . . ?

N10 C42 C43 111.7(5) . . ?

N10 C42 H42A 109.3 . . ?

C43 C42 H42A 109.3 . . ?

N10 C42 H42B 109.3 . . ?

C43 C42 H42B 109.3 . . ?

H42A C42 H42B 107.9 . . ?

C42 C43 H43A 109.5 . . ?

C42 C43 H43B 109.5 . . ?

H43A C43 H43B 109.5 . . ?

C42 C43 H43C 109.5 . . ?

H43A C43 H43C 109.5 . . ?

H43B C43 H43C 109.5 . . ?

O2 C44 O3 123.4(4) . . ?

O2 C44 C45 118.9(4) . . ?

O3 C44 C45 117.7(4) . . ?

C50 C45 C46 121.0(4) . . ?

C50 C45 C44 120.1(4) . . ?

C46 C45 C44 118.9(4) . . ?

C47 C46 C45 119.0(4) . . ?

C47 C46 H46A 120.5 . . ?

C45 C46 H46A 120.5 . . ?

O4 C47 C46 124.1(5) . . ?

O4 C47 C48 115.3(4) . . ?

C46 C47 C48 120.6(5) . . ?

O5 C48 C49 120.4(4) . . ?

O5 C48 C47 119.6(4) . . ?

C49 C48 C47 120.0(4) . . ?

O6 C49 C48 116.2(5) . . ?

O6 C49 C50 124.0(5) . . ?

C48 C49 C50 119.8(5) . . ?

C45 C50 C49 119.6(5) . . ?

C45 C50 H50A 120.2 . . ?

C49 C50 H50A 120.2 . . ?

O4 C51 H51A 109.5 . . ?

O4 C51 H51B 109.5 . . ?

H51A C51 H51B 109.5 . . ?

O4 C51 H51C 109.5 . . ?

H51A C51 H51C 109.5 . . ?

H51B C51 H51C 109.5 . . ?

O5 C52 H52A 109.5 . . ?

O5 C52 H52B 109.5 . . ?

H52A C52 H52B 109.5 . . ?

O5 C52 H52C 109.5 . . ?

H52A C52 H52C 109.5 . . ?

H52B C52 H52C 109.5 . . ?

O6 C53 H53A 109.5 . . ?

O6 C53 H53B 109.5 . . ?

H53A C53 H53B 109.5 . . ?

O6 C53 H53C 109.5 . . ?

H53A C53 H53C 109.5 . . ?

H53B C53 H53C 109.5 . . ?

O11 Fe3 O12 99.36(13) . . ?

O11 Fe3 N13 119.49(13) . . ?

O12 Fe3 N13 104.60(14) . . ?

O11 Fe3 N15 120.79(13) . . ?

O12 Fe3 N15 100.27(14) . . ?

N13 Fe3 N15 108.35(14) . . ?

O11 Fe3 N11 80.38(12) . . ?

O12 Fe3 N11 177.04(13) . . ?

N13 Fe3 N11 78.01(13) . . ?

N15 Fe3 N11 77.44(14) . . ?

O11 Fe4 O13 98.08(12) . . ?

O11 Fe4 N19 125.65(13) . . ?

O13 Fe4 N19 100.32(14) . . ?

O11 Fe4 N17 120.25(13) . . ?

O13 Fe4 N17 104.99(14) . . ?

N19 Fe4 N17 103.38(14) . . ?

O11 Fe4 N12 80.93(12) . . ?

O13 Fe4 N12 177.63(13) . . ?

N19 Fe4 N12 78.63(13) . . ?

N17 Fe4 N12 77.34(14) . . ?

C61 O11 Fe4 116.6(2) . . ?

C61 O11 Fe3 116.0(2) . . ?

Fe4 O11 Fe3 125.48(14) . . ?

C104 O12 Fe3 134.1(3) . . ?

C104 O13 Fe4 136.1(3) . . ?

C107 O14 C111 115.4(4) . . ?

C108 O15 C112 112.9(4) . . ?

C109 O16 C113 117.4(4) . . ?

C62 N11 C74 112.8(3) . . ?

C62 N11 C64 111.6(3) . . ?

C74 N11 C64 111.4(3) . . ?

C62 N11 Fe3 102.8(2) . . ?

C74 N11 Fe3 108.6(3) . . ?

C64 N11 Fe3 109.2(2) . . ?

C94 N12 C84 112.6(3) . . ?

C94 N12 C63 112.9(3) . . ?

C84 N12 C63 111.0(3) . . ?

C94 N12 Fe4 109.5(3) . . ?

C84 N12 Fe4 107.7(3) . . ?

C63 N12 Fe4 102.4(2) . . ?

C65 N13 C66 105.8(4) . . ?

C65 N13 Fe3 117.8(3) . . ?

C66 N13 Fe3 136.3(3) . . ?

C65 N14 C71 107.6(4) . . ?

C65 N14 C72 127.2(4) . . ?

C71 N14 C72 125.2(4) . . ?

C75 N15 C76 105.3(4) . . ?

C75 N15 Fe3 116.1(3) . . ?

C76 N15 Fe3 137.8(3) . . ?

C75 N16 C81 106.5(4) . . ?

C75 N16 C82 126.8(4) . . ?

C81 N16 C82 126.7(4) . . ?

C85 N17 C86 106.2(4) . . ?

C85 N17 Fe4 117.6(3) . . ?

C86 N17 Fe4 136.3(3) . . ?

C85 N18 C91 107.3(4) . . ?

C85 N18 C92 126.9(4) . . ?

C91 N18 C92 125.8(4) . . ?

C95 N19 C96 104.9(4) . . ?

C95 N19 Fe4 117.0(3) . . ?

C96 N19 Fe4 137.0(3) . . ?

C95 N20 C101 106.3(4) . . ?

C95 N20 C102 128.8(4) . . ?

C101 N20 C102 124.7(4) . . ?

O11 C61 C62 109.9(3) . . ?

O11 C61 C63 109.9(3) . . ?

C62 C61 C63 111.3(4) . . ?

O11 C61 H61A 108.6 . . ?

C62 C61 H61A 108.6 . . ?

C63 C61 H61A 108.6 . . ?

N11 C62 C61 109.7(3) . . ?

N11 C62 H62A 109.7 . . ?

C61 C62 H62A 109.7 . . ?

N11 C62 H62B 109.7 . . ?

C61 C62 H62B 109.7 . . ?

H62A C62 H62B 108.2 . . ?

N12 C63 C61 111.0(3) . . ?

N12 C63 H63A 109.4 . . ?

C61 C63 H63A 109.4 . . ?

N12 C63 H63B 109.4 . . ?

C61 C63 H63B 109.4 . . ?

H63A C63 H63B 108.0 . . ?

C65 C64 N11 109.3(3) . . ?

C65 C64 H64A 109.8 . . ?

N11 C64 H64A 109.8 . . ?

C65 C64 H64B 109.8 . . ?

N11 C64 H64B 109.8 . . ?

H64A C64 H64B 108.3 . . ?

N13 C65 N14 112.0(4) . . ?

N13 C65 C64 122.8(4) . . ?

N14 C65 C64 124.9(4) . . ?

C71 C66 C67 121.6(4) . . ?

C71 C66 N13 108.7(4) . . ?

C67 C66 N13 129.7(4) . . ?

C68 C67 C66 116.8(5) . . ?

C68 C67 H67A 121.6 . . ?

C66 C67 H67A 121.6 . . ?

C67 C68 C69 121.2(5) . . ?

C67 C68 H68A 119.4 . . ?

C69 C68 H68A 119.4 . . ?

C70 C69 C68 122.0(4) . . ?

C70 C69 H69A 119.0 . . ?

C68 C69 H69A 119.0 . . ?

C69 C70 C71 116.7(4) . . ?

C69 C70 H70A 121.6 . . ?

C71 C70 H70A 121.6 . . ?

N14 C71 C66 105.9(4) . . ?

N14 C71 C70 132.4(4) . . ?

C66 C71 C70 121.7(4) . . ?

N14 C72 C73 111.1(4) . . ?

N14 C72 H72A 109.4 . . ?

C73 C72 H72A 109.4 . . ?

N14 C72 H72B 109.4 . . ?

C73 C72 H72B 109.4 . . ?

H72A C72 H72B 108.0 . . ?

C72 C73 H73A 109.5 . . ?

C72 C73 H73B 109.5 . . ?

H73A C73 H73B 109.5 . . ?

C72 C73 H73C 109.5 . . ?

H73A C73 H73C 109.5 . . ?

H73B C73 H73C 109.5 . . ?

N11 C74 C75 108.9(4) . . ?

N11 C74 H74A 109.9 . . ?

C75 C74 H74A 109.9 . . ?

N11 C74 H74B 109.9 . . ?

C75 C74 H74B 109.9 . . ?

H74A C74 H74B 108.3 . . ?

N15 C75 N16 112.5(4) . . ?

N15 C75 C74 122.2(4) . . ?

N16 C75 C74 125.3(4) . . ?

C81 C76 C77 121.5(5) . . ?

C81 C76 N15 108.4(4) . . ?

C77 C76 N15 130.1(5) . . ?

C78 C77 C76 117.4(5) . . ?

C78 C77 H77A 121.3 . . ?

C76 C77 H77A 121.3 . . ?

C77 C78 C79 121.0(5) . . ?

C77 C78 H78A 119.5 . . ?

C79 C78 H78A 119.5 . . ?

C80 C79 C78 121.7(5) . . ?

C80 C79 H79A 119.1 . . ?

C78 C79 H79A 119.1 . . ?

C79 C80 C81 117.2(5) . . ?

C79 C80 H80A 121.4 . . ?

C81 C80 H80A 121.4 . . ?

N16 C81 C76 107.2(4) . . ?

N16 C81 C80 131.5(5) . . ?

C76 C81 C80 121.2(5) . . ?

N16 C82 C83 111.9(4) . . ?

N16 C82 H82A 109.2 . . ?

C83 C82 H82A 109.2 . . ?

N16 C82 H82B 109.2 . . ?

C83 C82 H82B 109.2 . . ?

H82A C82 H82B 107.9 . . ?

C82 C83 H83A 109.5 . . ?

C82 C83 H83B 109.5 . . ?

H83A C83 H83B 109.5 . . ?

C82 C83 H83C 109.5 . . ?

H83A C83 H83C 109.5 . . ?

H83B C83 H83C 109.5 . . ?

N12 C84 C85 108.6(4) . . ?

N12 C84 H84A 110.0 . . ?

C85 C84 H84A 110.0 . . ?

N12 C84 H84B 110.0 . . ?

C85 C84 H84B 110.0 . . ?

H84A C84 H84B 108.4 . . ?

N17 C85 N18 112.4(4) . . ?

N17 C85 C84 121.7(4) . . ?

N18 C85 C84 125.9(4) . . ?

C87 C86 N17 130.7(5) . . ?

C87 C86 C91 121.2(5) . . ?

N17 C86 C91 108.0(4) . . ?

C86 C87 C88 117.4(5) . . ?

C86 C87 H87A 121.3 . . ?

C88 C87 H87A 121.3 . . ?

C87 C88 C89 121.3(5) . . ?

C87 C88 H88A 119.4 . . ?

C89 C88 H88A 119.4 . . ?

C90 C89 C88 122.2(5) . . ?

C90 C89 H89A 118.9 . . ?

C88 C89 H89A 118.9 . . ?

C89 C90 C91 117.3(5) . . ?

C89 C90 H90A 121.3 . . ?

C91 C90 H90A 121.3 . . ?

N18 C91 C86 106.1(4) . . ?

N18 C91 C90 133.3(5) . . ?

C86 C91 C90 120.6(5) . . ?

N18 C92 C93 112.8(4) . . ?

N18 C92 H92A 109.0 . . ?

C93 C92 H92A 109.0 . . ?

N18 C92 H92B 109.0 . . ?

C93 C92 H92B 109.0 . . ?

H92A C92 H92B 107.8 . . ?

C92 C93 H93A 109.5 . . ?

C92 C93 H93B 109.5 . . ?

H93A C93 H93B 109.5 . . ?

C92 C93 H93C 109.5 . . ?

H93A C93 H93C 109.5 . . ?

H93B C93 H93C 109.5 . . ?

N12 C94 C95 111.0(4) . . ?

N12 C94 H94A 109.4 . . ?

C95 C94 H94A 109.4 . . ?

N12 C94 H94B 109.4 . . ?

C95 C94 H94B 109.4 . . ?

H94A C94 H94B 108.0 . . ?

N19 C95 N20 113.4(4) . . ?

N19 C95 C94 123.3(4) . . ?

N20 C95 C94 123.2(4) . . ?

C101 C96 N19 110.1(4) . . ?

C101 C96 C97 119.9(5) . . ?

N19 C96 C97 130.0(5) . . ?

C98 C97 C96 117.8(5) . . ?

C98 C97 H97A 121.1 . . ?

C96 C97 H97A 121.1 . . ?

C97 C98 C99 121.6(6) . . ?

C97 C98 H98A 119.2 . . ?

C99 C98 H98A 119.2 . . ?

C100 C99 C98 122.1(6) . . ?

C100 C99 H99A 119.0 . . ?

C98 C99 H99A 119.0 . . ?

C99 C100 C101 116.5(5) . . ?

C99 C100 H10B 121.8 . . ?

C101 C100 H10B 121.8 . . ?

C96 C101 N20 105.4(4) . . ?

C96 C101 C100 122.1(5) . . ?

N20 C101 C100 132.4(5) . . ?

N20 C102 C103 109.6(5) . . ?

N20 C102 H10C 109.7 . . ?

C103 C102 H10C 109.7 . . ?

N20 C102 H10D 109.7 . . ?

C103 C102 H10D 109.7 . . ?

H10C C102 H10D 108.2 . . ?

C102 C103 H10E 109.5 . . ?

C102 C103 H10F 109.5 . . ?

H10E C103 H10F 109.5 . . ?

C102 C103 H10G 109.5 . . ?

H10E C103 H10G 109.5 . . ?

H10F C103 H10G 109.5 . . ?

O12 C104 O13 126.3(4) . . ?

O12 C104 C105 116.6(4) . . ?

O13 C104 C105 117.1(4) . . ?

C110 C105 C106 120.2(4) . . ?

C110 C105 C104 119.5(4) . . ?

C106 C105 C104 120.2(4) . . ?

C107 C106 C105 119.0(5) . . ?

C107 C106 H10H 120.5 . . ?

C105 C106 H10H 120.5 . . ?

O14 C107 C108 114.7(4) . . ?

O14 C107 C106 124.5(5) . . ?

C108 C107 C106 120.8(4) . . ?

C107 C108 O15 120.5(4) . . ?

C107 C108 C109 120.8(4) . . ?

O15 C108 C109 118.6(4) . . ?

O16 C109 C108 116.5(4) . . ?

O16 C109 C110 124.8(4) . . ?

C108 C109 C110 118.6(4) . . ?

C105 C110 C109 120.5(4) . . ?

C105 C110 H11A 119.8 . . ?

C109 C110 H11A 119.8 . . ?

O14 C111 H11B 109.5 . . ?

O14 C111 H11C 109.5 . . ?

H11B C111 H11C 109.5 . . ?

O14 C111 H11D 109.5 . . ?

H11B C111 H11D 109.5 . . ?

H11C C111 H11D 109.5 . . ?

O15 C112 H11E 109.5 . . ?

O15 C112 H11F 109.5 . . ?

H11E C112 H11F 109.5 . . ?

O15 C112 H11G 109.5 . . ?

H11E C112 H11G 109.5 . . ?

H11F C112 H11G 109.5 . . ?

O16 C113 H11H 109.5 . . ?

O16 C113 H11I 109.5 . . ?

H11H C113 H11I 109.5 . . ?

O16 C113 H11J 109.5 . . ?

H11H C113 H11J 109.5 . . ?

H11I C113 H11J 109.5 . . ?

C127 B1 C133 107.1(4) . . ?

C127 B1 C121 112.2(4) . . ?

C133 B1 C121 109.3(4) . . ?

C127 B1 C139 112.4(4) . . ?

C133 B1 C139 112.9(4) . . ?

C121 B1 C139 102.8(4) . . ?

C122 C121 C126 115.3(5) . . ?

C122 C121 B1 125.3(5) . . ?

C126 C121 B1 119.4(5) . . ?

C121 C122 C123 120.4(6) . . ?

C121 C122 H12C 119.8 . . ?

C123 C122 H12C 119.8 . . ?

C124 C123 C122 120.4(6) . . ?

C124 C123 H12D 119.8 . . ?

C122 C123 H12D 119.8 . . ?

C125 C124 C123 121.1(6) . . ?

C125 C124 H12E 119.5 . . ?

C123 C124 H12E 119.5 . . ?

C124 C125 C126 118.8(7) . . ?

C124 C125 H12F 120.6 . . ?

C126 C125 H12F 120.6 . . ?

C125 C126 C121 124.0(6) . . ?

C125 C126 H12G 118.0 . . ?

C121 C126 H12G 118.0 . . ?

C128 C127 C132 115.2(5) . . ?

C128 C127 B1 119.9(5) . . ?

C132 C127 B1 124.8(5) . . ?

C129 C128 C127 123.0(6) . . ?

C129 C128 H12H 118.5 . . ?

C127 C128 H12H 118.5 . . ?

C128 C129 C130 119.5(6) . . ?

C128 C129 H12I 120.3 . . ?

C130 C129 H12I 120.3 . . ?

C131 C130 C129 120.9(6) . . ?

C131 C130 H13D 119.6 . . ?

C129 C130 H13D 119.6 . . ?

C130 C131 C132 117.8(6) . . ?

C130 C131 H13E 121.1 . . ?

C132 C131 H13E 121.1 . . ?

C127 C132 C131 123.6(5) . . ?

C127 C132 H13F 118.2 . . ?

C131 C132 H13F 118.2 . . ?

C138 C133 C134 114.6(5) . . ?

C138 C133 B1 121.9(4) . . ?

C134 C133 B1 123.5(4) . . ?

C135 C134 C133 122.1(5) . . ?

C135 C134 H13G 119.0 . . ?

C133 C134 H13G 119.0 . . ?

C134 C135 C136 120.9(5) . . ?

C134 C135 H13H 119.5 . . ?

C136 C135 H13H 119.5 . . ?

C137 C136 C135 118.9(5) . . ?

C137 C136 H13I 120.6 . . ?

C135 C136 H13I 120.6 . . ?

C138 C137 C136 120.1(5) . . ?

C138 C137 H13J 120.0 . . ?

C136 C137 H13J 120.0 . . ?

C137 C138 C133 123.5(5) . . ?

C137 C138 H13K 118.3 . . ?

C133 C138 H13K 118.3 . . ?

C144 C139 C140 115.5(5) . . ?

C144 C139 B1 125.0(4) . . ?

C140 C139 B1 119.5(5) . . ?

C139 C140 C141 122.9(6) . . ?

C139 C140 H14C 118.5 . . ?

C141 C140 H14C 118.5 . . ?

C142 C141 C140 119.2(6) . . ?

C142 C141 H14D 120.4 . . ?

C140 C141 H14D 120.4 . . ?

C141 C142 C143 120.5(6) . . ?

C141 C142 H14E 119.8 . . ?

C143 C142 H14E 119.8 . . ?

C142 C143 C144 119.1(6) . . ?

C142 C143 H14F 120.5 . . ?

C144 C143 H14F 120.5 . . ?

C139 C144 C143 122.9(5) . . ?

C139 C144 H14G 118.6 . . ?

C143 C144 H14G 118.6 . . ?

C169 B2 C163 102.7(4) . . ?

C169 B2 C157 114.6(4) . . ?

C163 B2 C157 113.0(4) . . ?

C169 B2 C151 114.1(5) . . ?

C163 B2 C151 110.7(4) . . ?

C157 B2 C151 102.1(4) . . ?

C152 C151 C156 120.0 . . ?

C152 C151 B2 119.5(5) . . ?

C156 C151 B2 120.1(5) . . ?

C151 C152 C153 120.0 . . ?

C151 C152 H15A 120.0 . . ?

C153 C152 H15A 120.0 . . ?

C154 C153 C152 120.0 . . ?

C154 C153 H15B 120.0 . . ?

C152 C153 H15B 120.0 . . ?

C155 C154 C153 120.0 . . ?

C155 C154 H15C 120.0 . . ?

C153 C154 H15C 120.0 . . ?

C154 C155 C156 120.0 . . ?

C154 C155 H15D 120.0 . . ?

C156 C155 H15D 120.0 . . ?

C155 C156 C151 120.0 . . ?

C155 C156 H15E 120.0 . . ?

C151 C156 H15E 120.0 . . ?

C158 C157 C162 120.0 . . ?

C158 C157 B2 118.0(3) . . ?

C162 C157 B2 122.0(3) . . ?

C157 C158 C159 120.0 . . ?

C157 C158 H15F 120.0 . . ?

C159 C158 H15F 120.0 . . ?

C160 C159 C158 120.0 . . ?

C160 C159 H15G 120.0 . . ?

C158 C159 H15G 120.0 . . ?

C159 C160 C161 120.0 . . ?

C159 C160 H16A 120.0 . . ?

C161 C160 H16A 120.0 . . ?

C162 C161 C160 120.0 . . ?

C162 C161 H16B 120.0 . . ?

C160 C161 H16B 120.0 . . ?

C161 C162 C157 120.0 . . ?

C161 C162 H16C 120.0 . . ?

C157 C162 H16C 120.0 . . ?

C164 C163 C168 120.0 . . ?

C164 C163 B2 118.1(4) . . ?

C168 C163 B2 121.9(4) . . ?

C163 C164 C165 120.0 . . ?

C163 C164 H16D 120.0 . . ?

C165 C164 H16D 120.0 . . ?

C166 C165 C164 120.0 . . ?

C166 C165 H16E 120.0 . . ?

C164 C165 H16E 120.0 . . ?

C165 C166 C167 120.0 . . ?

C165 C166 H16F 120.0 . . ?

C167 C166 H16F 120.0 . . ?

C168 C167 C166 120.0 . . ?

C168 C167 H16G 120.0 . . ?

C166 C167 H16G 120.0 . . ?

C167 C168 C163 120.0 . . ?

C167 C168 H16H 120.0 . . ?

C163 C168 H16H 120.0 . . ?

C170 C169 C174 120.0 . . ?

C170 C169 B2 119.4(4) . . ?

C174 C169 B2 120.0(4) . . ?

C171 C170 C169 120.0 . . ?

C171 C170 H17B 120.0 . . ?

C169 C170 H17B 120.0 . . ?

C172 C171 C170 120.0 . . ?

C172 C171 H17C 120.0 . . ?

C170 C171 H17C 120.0 . . ?

C173 C172 C171 120.0 . . ?

C173 C172 H17D 120.0 . . ?

C171 C172 H17D 120.0 . . ?

C172 C173 C174 120.0 . . ?

C172 C173 H17E 120.0 . . ?

C174 C173 H17E 120.0 . . ?

C173 C174 C169 120.0 . . ?

C173 C174 H17F 120.0 . . ?

C169 C174 H17F 120.0 . . ?

O22 S1 O23 114.4(4) . . ?

O22 S1 O21 111.2(4) . . ?

O23 S1 O21 115.3(3) . . ?

O22 S1 C181 106.5(4) . . ?

O23 S1 C181 106.1(4) . . ?

O21 S1 C181 101.9(4) . . ?

F1 C181 F2 113.2(8) . . ?

F1 C181 F3 103.9(8) . . ?

F2 C181 F3 102.1(8) . . ?

F1 C181 S1 114.4(7) . . ?

F2 C181 S1 112.5(7) . . ?

F3 C181 S1 109.5(5) . . ?

O32 S2 O33 115.3(4) . . ?

O32 S2 O31 111.1(4) . . ?

O33 S2 O31 115.0(3) . . ?

O32 S2 C191 107.3(4) . . ?

O33 S2 C191 104.0(4) . . ?

O31 S2 C191 102.8(4) . . ?

F12 C191 F11 111.0(9) . . ?

F12 C191 F13 109.8(10) . . ?

F11 C191 F13 103.6(7) . . ?

F12 C191 S2 114.3(7) . . ?

F11 C191 S2 108.5(8) . . ?

F13 C191 S2 109.0(6) . . ?

C202 C201 H20B 109.5 . . ?

C202 C201 H20C 109.5 . . ?

H20B C201 H20C 109.5 . . ?

C202 C201 H20D 109.5 . . ?

H20B C201 H20D 109.5 . . ?

H20C C201 H20D 109.5 . . ?

N21 C202 C201 177.1(8) . . ?

C302 C301 H30B 109.5 . . ?

C302 C301 H30C 109.5 . . ?

H30B C301 H30C 109.5 . . ?

C302 C301 H30D 109.5 . . ?

H30B C301 H30D 109.5 . . ?

H30C C301 H30D 109.5 . . ?

N31 C302 C301 177.4(19) . . ?

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

O2 Fe1 O1 C1 170.1(3) . . . . ?

N3 Fe1 O1 C1 -78.6(3) . . . . ?

N5 Fe1 O1 C1 57.6(3) . . . . ?

N1 Fe1 O1 C1 -12.0(3) . . . . ?

O2 Fe1 O1 Fe2 6.0(2) . . . . ?

N3 Fe1 O1 Fe2 117.3(2) . . . . ?

N5 Fe1 O1 Fe2 -106.4(2) . . . . ?

N1 Fe1 O1 Fe2 -176.1(2) . . . . ?

O3 Fe2 O1 C1 -168.8(3) . . . . ?

N9 Fe2 O1 C1 81.1(3) . . . . ?

N7 Fe2 O1 C1 -59.9(3) . . . . ?

N2 Fe2 O1 C1 9.3(3) . . . . ?

O3 Fe2 O1 Fe1 -4.7(2) . . . . ?

N9 Fe2 O1 Fe1 -114.73(19) . . . . ?

N7 Fe2 O1 Fe1 104.3(2) . . . . ?

N2 Fe2 O1 Fe1 173.4(2) . . . . ?

O1 Fe1 O2 C44 -5.7(5) . . . . ?

N3 Fe1 O2 C44 -137.1(5) . . . . ?

N5 Fe1 O2 C44 118.4(5) . . . . ?

N1 Fe1 O2 C44 -54(3) . . . . ?

O1 Fe2 O3 C44 0.6(5) . . . . ?

N9 Fe2 O3 C44 120.6(4) . . . . ?

N7 Fe2 O3 C44 -123.4(4) . . . . ?

N2 Fe2 O3 C44 -129(3) . . . . ?

O1 Fe1 N1 C2 -15.0(2) . . . . ?

O2 Fe1 N1 C2 33(3) . . . . ?

N3 Fe1 N1 C2 117.3(3) . . . . ?

N5 Fe1 N1 C2 -138.9(3) . . . . ?

O1 Fe1 N1 C4 -135.1(3) . . . . ?

O2 Fe1 N1 C4 -87(3) . . . . ?

N3 Fe1 N1 C4 -2.9(3) . . . . ?

N5 Fe1 N1 C4 101.0(3) . . . . ?

O1 Fe1 N1 C14 104.1(3) . . . . ?

O2 Fe1 N1 C14 152(3) . . . . ?

N3 Fe1 N1 C14 -123.7(3) . . . . ?

N5 Fe1 N1 C14 -19.8(3) . . . . ?

O1 Fe2 N2 C34 136.7(3) . . . . ?

O3 Fe2 N2 C34 -94(3) . . . . ?

N9 Fe2 N2 C34 17.6(3) . . . . ?

N7 Fe2 N2 C34 -99.0(3) . . . . ?

O1 Fe2 N2 C24 -102.1(3) . . . . ?

O3 Fe2 N2 C24 27(3) . . . . ?

N9 Fe2 N2 C24 138.8(3) . . . . ?

N7 Fe2 N2 C24 22.2(3) . . . . ?

O1 Fe2 N2 C3 17.8(3) . . . . ?

O3 Fe2 N2 C3 147(3) . . . . ?

N9 Fe2 N2 C3 -101.4(3) . . . . ?

N7 Fe2 N2 C3 142.1(3) . . . . ?

O1 Fe1 N3 C5 73.7(3) . . . . ?

O2 Fe1 N3 C5 -176.4(3) . . . . ?

N5 Fe1 N3 C5 -68.7(3) . . . . ?

N1 Fe1 N3 C5 6.5(3) . . . . ?

O1 Fe1 N3 C6 -124.2(4) . . . . ?

O2 Fe1 N3 C6 -14.3(4) . . . . ?

N5 Fe1 N3 C6 93.4(4) . . . . ?

N1 Fe1 N3 C6 168.6(4) . . . . ?

O1 Fe1 N5 C15 -61.9(4) . . . . ?

O2 Fe1 N5 C15 -170.8(3) . . . . ?

N3 Fe1 N5 C15 84.3(3) . . . . ?

N1 Fe1 N5 C15 8.8(3) . . . . ?

O1 Fe1 N5 C16 120.8(4) . . . . ?

O2 Fe1 N5 C16 11.8(5) . . . . ?

N3 Fe1 N5 C16 -93.0(5) . . . . ?

N1 Fe1 N5 C16 -168.5(5) . . . . ?

O1 Fe2 N7 C25 57.7(4) . . . . ?

O3 Fe2 N7 C25 166.7(3) . . . . ?

N9 Fe2 N7 C25 -84.6(3) . . . . ?

N2 Fe2 N7 C25 -13.5(3) . . . . ?

O1 Fe2 N7 C26 -114.0(4) . . . . ?

O3 Fe2 N7 C26 -5.1(5) . . . . ?

N9 Fe2 N7 C26 103.7(4) . . . . ?

N2 Fe2 N7 C26 174.7(5) . . . . ?

O1 Fe2 N9 C35 -83.1(3) . . . . ?

O3 Fe2 N9 C35 168.3(3) . . . . ?

N7 Fe2 N9 C35 61.0(4) . . . . ?

N2 Fe2 N9 C35 -9.4(3) . . . . ?

O1 Fe2 N9 C36 105.2(4) . . . . ?

O3 Fe2 N9 C36 -3.5(4) . . . . ?

N7 Fe2 N9 C36 -110.7(4) . . . . ?

N2 Fe2 N9 C36 178.8(4) . . . . ?

Fe1 O1 C1 C2 36.9(4) . . . . ?

Fe2 O1 C1 C2 -157.7(3) . . . . ?

Fe1 O1 C1 C3 159.9(3) . . . . ?

Fe2 O1 C1 C3 -34.7(4) . . . . ?

C4 N1 C2 C1 155.0(3) . . . . ?

C14 N1 C2 C1 -78.0(4) . . . . ?

Fe1 N1 C2 C1 36.9(4) . . . . ?

O1 C1 C2 N1 -50.0(4) . . . . ?

C3 C1 C2 N1 -172.0(3) . . . . ?

C34 N2 C3 C1 -155.6(4) . . . . ?

C24 N2 C3 C1 75.8(5) . . . . ?

Fe2 N2 C3 C1 -40.1(4) . . . . ?

O1 C1 C3 N2 51.6(5) . . . . ?

C2 C1 C3 N2 174.0(4) . . . . ?

C2 N1 C4 C5 -115.2(4) . . . . ?

C14 N1 C4 C5 117.2(4) . . . . ?

Fe1 N1 C4 C5 -0.6(4) . . . . ?

C6 N3 C5 N4 0.0(5) . . . . ?

Fe1 N3 C5 N4 166.8(3) . . . . ?

C6 N3 C5 C4 -176.5(4) . . . . ?

Fe1 N3 C5 C4 -9.6(5) . . . . ?

C11 N4 C5 N3 0.5(5) . . . . ?

C12 N4 C5 N3 179.5(4) . . . . ?

C11 N4 C5 C4 176.8(4) . . . . ?

C12 N4 C5 C4 -4.1(7) . . . . ?

N1 C4 C5 N3 6.4(6) . . . . ?

N1 C4 C5 N4 -169.6(4) . . . . ?

C5 N3 C6 C7 176.4(5) . . . . ?

Fe1 N3 C6 C7 12.8(7) . . . . ?

C5 N3 C6 C11 -0.4(5) . . . . ?

Fe1 N3 C6 C11 -164.0(3) . . . . ?

N3 C6 C7 C8 -177.5(5) . . . . ?

C11 C6 C7 C8 -1.0(7) . . . . ?

C6 C7 C8 C9 0.4(9) . . . . ?

C7 C8 C9 C10 0.3(10) . . . . ?

C8 C9 C10 C11 -0.3(9) . . . . ?

C9 C10 C11 N4 176.4(5) . . . . ?

C9 C10 C11 C6 -0.3(8) . . . . ?

C5 N4 C11 C10 -177.9(5) . . . . ?

C12 N4 C11 C10 3.1(8) . . . . ?

C5 N4 C11 C6 -0.7(5) . . . . ?

C12 N4 C11 C6 -179.8(4) . . . . ?

C7 C6 C11 C10 1.0(7) . . . . ?

N3 C6 C11 C10 178.2(4) . . . . ?

C7 C6 C11 N4 -176.5(4) . . . . ?

N3 C6 C11 N4 0.7(5) . . . . ?

C5 N4 C12 C13 -109.8(5) . . . . ?

C11 N4 C12 C13 69.0(6) . . . . ?

C2 N1 C14 C15 139.4(4) . . . . ?

C4 N1 C14 C15 -93.1(4) . . . . ?

Fe1 N1 C14 C15 26.3(4) . . . . ?

C16 N5 C15 N6 -1.1(5) . . . . ?

Fe1 N5 C15 N6 -179.2(3) . . . . ?

C16 N5 C15 C14 -176.8(4) . . . . ?

Fe1 N5 C15 C14 5.1(6) . . . . ?

C21 N6 C15 N5 0.6(5) . . . . ?

C22 N6 C15 N5 177.9(5) . . . . ?

C21 N6 C15 C14 176.2(4) . . . . ?

C22 N6 C15 C14 -6.4(8) . . . . ?

N1 C14 C15 N5 -23.3(6) . . . . ?

N1 C14 C15 N6 161.5(4) . . . . ?

C15 N5 C16 C17 -178.0(5) . . . . ?

Fe1 N5 C16 C17 -0.4(8) . . . . ?

C15 N5 C16 C21 1.1(5) . . . . ?

Fe1 N5 C16 C21 178.7(4) . . . . ?

C21 C16 C17 C18 0.0(7) . . . . ?

N5 C16 C17 C18 179.0(5) . . . . ?

C16 C17 C18 C19 1.2(8) . . . . ?

C17 C18 C19 C20 -1.0(9) . . . . ?

C18 C19 C20 C21 -0.4(8) . . . . ?

C15 N6 C21 C16 0.1(5) . . . . ?

C22 N6 C21 C16 -177.3(5) . . . . ?

C15 N6 C21 C20 -180.0(6) . . . . ?

C22 N6 C21 C20 2.7(9) . . . . ?

C17 C16 C21 N6 178.4(4) . . . . ?

N5 C16 C21 N6 -0.8(5) . . . . ?

C17 C16 C21 C20 -1.5(8) . . . . ?

N5 C16 C21 C20 179.3(4) . . . . ?

C19 C20 C21 N6 -178.3(5) . . . . ?

C19 C20 C21 C16 1.6(8) . . . . ?

C15 N6 C22 C23 86.0(7) . . . . ?

C21 N6 C22 C23 -97.1(7) . . . . ?

C34 N2 C24 C25 92.6(4) . . . . ?

C3 N2 C24 C25 -138.2(4) . . . . ?

Fe2 N2 C24 C25 -26.2(4) . . . . ?

C26 N7 C25 N8 -0.3(5) . . . . ?

Fe2 N7 C25 N8 -174.5(3) . . . . ?

C26 N7 C25 C24 176.3(4) . . . . ?

Fe2 N7 C25 C24 2.1(6) . . . . ?

C31 N8 C25 N7 0.9(5) . . . . ?

C32 N8 C25 N7 179.4(5) . . . . ?

C31 N8 C25 C24 -175.6(4) . . . . ?

C32 N8 C25 C24 2.9(8) . . . . ?

N2 C24 C25 N7 18.3(6) . . . . ?

N2 C24 C25 N8 -165.5(4) . . . . ?

C25 N7 C26 C31 -0.4(5) . . . . ?

Fe2 N7 C26 C31 172.0(4) . . . . ?

C25 N7 C26 C27 179.4(5) . . . . ?

Fe2 N7 C26 C27 -8.2(8) . . . . ?

N7 C26 C27 C28 179.4(5) . . . . ?

C31 C26 C27 C28 -0.8(8) . . . . ?

C26 C27 C28 C29 -1.0(9) . . . . ?

C27 C28 C29 C30 1.7(11) . . . . ?

C28 C29 C30 C31 -0.5(10) . . . . ?

C25 N8 C31 C30 177.9(6) . . . . ?

C32 N8 C31 C30 -0.7(10) . . . . ?

C25 N8 C31 C26 -1.1(6) . . . . ?

C32 N8 C31 C26 -179.7(5) . . . . ?

C29 C30 C31 N8 179.9(6) . . . . ?

C29 C30 C31 C26 -1.3(9) . . . . ?

N7 C26 C31 N8 1.0(6) . . . . ?

C27 C26 C31 N8 -178.9(5) . . . . ?

N7 C26 C31 C30 -178.2(5) . . . . ?

C27 C26 C31 C30 2.0(8) . . . . ?

C25 N8 C32 C33 -101.9(6) . . . . ?

C31 N8 C32 C33 76.3(7) . . . . ?

C24 N2 C34 C35 -140.8(4) . . . . ?

C3 N2 C34 C35 89.7(5) . . . . ?

Fe2 N2 C34 C35 -21.9(4) . . . . ?

C36 N9 C35 N10 -1.2(5) . . . . ?

Fe2 N9 C35 N10 -175.3(3) . . . . ?

C36 N9 C35 C34 173.2(4) . . . . ?

Fe2 N9 C35 C34 -0.9(6) . . . . ?

C41 N10 C35 N9 0.4(5) . . . . ?

C42 N10 C35 N9 178.1(4) . . . . ?

C41 N10 C35 C34 -173.8(4) . . . . ?

C42 N10 C35 C34 3.8(8) . . . . ?

N2 C34 C35 N9 17.1(6) . . . . ?

N2 C34 C35 N10 -169.2(4) . . . . ?

C35 N9 C36 C37 -174.1(5) . . . . ?

Fe2 N9 C36 C37 -1.8(8) . . . . ?

C35 N9 C36 C41 1.5(5) . . . . ?

Fe2 N9 C36 C41 173.8(3) . . . . ?

N9 C36 C37 C38 176.1(4) . . . . ?

C41 C36 C37 C38 1.0(7) . . . . ?

C36 C37 C38 C39 -0.3(7) . . . . ?

C37 C38 C39 C40 -0.3(8) . . . . ?

C38 C39 C40 C41 0.2(7) . . . . ?

C35 N10 C41 C36 0.5(5) . . . . ?

C42 N10 C41 C36 -177.2(4) . . . . ?

C35 N10 C41 C40 175.9(5) . . . . ?

C42 N10 C41 C40 -1.8(8) . . . . ?

C37 C36 C41 N10 174.8(4) . . . . ?

N9 C36 C41 N10 -1.2(5) . . . . ?

C37 C36 C41 C40 -1.2(7) . . . . ?

N9 C36 C41 C40 -177.2(4) . . . . ?

C39 C40 C41 N10 -174.3(5) . . . . ?

C39 C40 C41 C36 0.5(7) . . . . ?

C35 N10 C42 C43 97.7(6) . . . . ?

C41 N10 C42 C43 -85.0(6) . . . . ?

Fe1 O2 C44 O3 2.7(8) . . . . ?

Fe1 O2 C44 C45 -177.5(3) . . . . ?

Fe2 O3 C44 O2 0.6(7) . . . . ?

Fe2 O3 C44 C45 -179.3(3) . . . . ?

O2 C44 C45 C50 -173.3(5) . . . . ?

O3 C44 C45 C50 6.6(7) . . . . ?

O2 C44 C45 C46 5.8(6) . . . . ?

O3 C44 C45 C46 -174.3(4) . . . . ?

C50 C45 C46 C47 -3.0(7) . . . . ?

C44 C45 C46 C47 177.9(4) . . . . ?

C51 O4 C47 C46 -4.6(7) . . . . ?

C51 O4 C47 C48 174.2(5) . . . . ?

C45 C46 C47 O4 -178.3(4) . . . . ?

C45 C46 C47 C48 3.0(7) . . . . ?

C52 O5 C48 C49 88.8(6) . . . . ?

C52 O5 C48 C47 -92.7(5) . . . . ?

O4 C47 C48 O5 2.3(6) . . . . ?

C46 C47 C48 O5 -178.9(4) . . . . ?

O4 C47 C48 C49 -179.3(5) . . . . ?

C46 C47 C48 C49 -0.5(7) . . . . ?

C53 O6 C49 C48 -171.5(7) . . . . ?

C53 O6 C49 C50 8.1(10) . . . . ?

O5 C48 C49 O6 -4.1(8) . . . . ?

C47 C48 C49 O6 177.5(5) . . . . ?

O5 C48 C49 C50 176.3(5) . . . . ?

C47 C48 C49 C50 -2.1(8) . . . . ?

C46 C45 C50 C49 0.4(8) . . . . ?

C44 C45 C50 C49 179.5(5) . . . . ?

O6 C49 C50 C45 -177.4(5) . . . . ?

C48 C49 C50 C45 2.2(8) . . . . ?

O13 Fe4 O11 C61 -170.2(3) . . . . ?

N19 Fe4 O11 C61 80.9(3) . . . . ?

N17 Fe4 O11 C61 -57.6(3) . . . . ?

N12 Fe4 O11 C61 12.0(3) . . . . ?

O13 Fe4 O11 Fe3 -6.4(2) . . . . ?

N19 Fe4 O11 Fe3 -115.38(19) . . . . ?

N17 Fe4 O11 Fe3 106.21(19) . . . . ?

N12 Fe4 O11 Fe3 175.73(19) . . . . ?

O12 Fe3 O11 C61 167.5(3) . . . . ?

N13 Fe3 O11 C61 -79.7(3) . . . . ?

N15 Fe3 O11 C61 59.6(3) . . . . ?

N11 Fe3 O11 C61 -9.5(3) . . . . ?

O12 Fe3 O11 Fe4 3.7(2) . . . . ?

N13 Fe3 O11 Fe4 116.44(18) . . . . ?

N15 Fe3 O11 Fe4 -104.27(19) . . . . ?

N11 Fe3 O11 Fe4 -173.31(19) . . . . ?

O11 Fe3 O12 C104 0.3(5) . . . . ?

N13 Fe3 O12 C104 -123.7(4) . . . . ?

N15 Fe3 O12 C104 124.1(4) . . . . ?

N11 Fe3 O12 C104 85(3) . . . . ?

O11 Fe4 O13 C104 9.4(5) . . . . ?

N19 Fe4 O13 C104 138.0(4) . . . . ?

N17 Fe4 O13 C104 -115.0(4) . . . . ?

N12 Fe4 O13 C104 74(3) . . . . ?

O11 Fe3 N11 C62 -18.0(2) . . . . ?

O12 Fe3 N11 C62 -103(3) . . . . ?

N13 Fe3 N11 C62 105.1(3) . . . . ?

N15 Fe3 N11 C62 -142.7(3) . . . . ?

O11 Fe3 N11 C74 101.7(3) . . . . ?

O12 Fe3 N11 C74 17(3) . . . . ?

N13 Fe3 N11 C74 -135.2(3) . . . . ?

N15 Fe3 N11 C74 -23.1(3) . . . . ?

O11 Fe3 N11 C64 -136.7(3) . . . . ?

O12 Fe3 N11 C64 138(2) . . . . ?

N13 Fe3 N11 C64 -13.5(3) . . . . ?

N15 Fe3 N11 C64 98.6(3) . . . . ?

O11 Fe4 N12 C94 134.6(3) . . . . ?

O13 Fe4 N12 C94 69(3) . . . . ?

N19 Fe4 N12 C94 5.2(3) . . . . ?

N17 Fe4 N12 C94 -101.5(3) . . . . ?

O11 Fe4 N12 C84 -102.6(3) . . . . ?

O13 Fe4 N12 C84 -168(3) . . . . ?

N19 Fe4 N12 C84 128.0(3) . . . . ?

N17 Fe4 N12 C84 21.3(3) . . . . ?

O11 Fe4 N12 C63 14.5(2) . . . . ?

O13 Fe4 N12 C63 -51(3) . . . . ?

N19 Fe4 N12 C63 -114.8(3) . . . . ?

N17 Fe4 N12 C63 138.5(3) . . . . ?

O11 Fe3 N13 C65 77.7(3) . . . . ?

O12 Fe3 N13 C65 -172.4(3) . . . . ?

N15 Fe3 N13 C65 -66.1(3) . . . . ?

N11 Fe3 N13 C65 6.2(3) . . . . ?

O11 Fe3 N13 C66 -107.3(4) . . . . ?

O12 Fe3 N13 C66 2.6(4) . . . . ?

N15 Fe3 N13 C66 108.9(4) . . . . ?

N11 Fe3 N13 C66 -178.8(4) . . . . ?

O11 Fe3 N15 C75 -53.6(3) . . . . ?

O12 Fe3 N15 C75 -161.1(3) . . . . ?

N13 Fe3 N15 C75 89.7(3) . . . . ?

N11 Fe3 N15 C75 17.0(3) . . . . ?

O11 Fe3 N15 C76 114.4(4) . . . . ?

O12 Fe3 N15 C76 6.9(4) . . . . ?

N13 Fe3 N15 C76 -102.3(4) . . . . ?

N11 Fe3 N15 C76 -175.0(4) . . . . ?

O11 Fe4 N17 C85 61.3(4) . . . . ?

O13 Fe4 N17 C85 170.2(3) . . . . ?

N19 Fe4 N17 C85 -85.1(3) . . . . ?

N12 Fe4 N17 C85 -10.2(3) . . . . ?

O11 Fe4 N17 C86 -119.8(4) . . . . ?

O13 Fe4 N17 C86 -10.8(5) . . . . ?

N19 Fe4 N17 C86 93.9(4) . . . . ?

N12 Fe4 N17 C86 168.8(5) . . . . ?

O11 Fe4 N19 C95 -76.1(3) . . . . ?

O13 Fe4 N19 C95 176.0(3) . . . . ?

N17 Fe4 N19 C95 67.8(3) . . . . ?

N12 Fe4 N19 C95 -6.1(3) . . . . ?

O11 Fe4 N19 C96 118.4(4) . . . . ?

O13 Fe4 N19 C96 10.5(4) . . . . ?

N17 Fe4 N19 C96 -97.7(4) . . . . ?

N12 Fe4 N19 C96 -171.6(4) . . . . ?

Fe4 O11 C61 C62 -159.3(3) . . . . ?

Fe3 O11 C61 C62 35.4(4) . . . . ?

Fe4 O11 C61 C63 -36.5(4) . . . . ?

Fe3 O11 C61 C63 158.2(3) . . . . ?

C74 N11 C62 C61 -76.2(4) . . . . ?

C64 N11 C62 C61 157.5(3) . . . . ?

Fe3 N11 C62 C61 40.6(4) . . . . ?

O11 C61 C62 N11 -52.1(5) . . . . ?

C63 C61 C62 N11 -174.1(3) . . . . ?

C94 N12 C63 C61 -154.5(4) . . . . ?

C84 N12 C63 C61 77.9(4) . . . . ?

Fe4 N12 C63 C61 -36.8(4) . . . . ?

O11 C61 C63 N12 49.9(5) . . . . ?

C62 C61 C63 N12 171.9(3) . . . . ?

C62 N11 C64 C65 -95.2(4) . . . . ?

C74 N11 C64 C65 137.8(4) . . . . ?

Fe3 N11 C64 C65 17.7(4) . . . . ?

C66 N13 C65 N14 0.8(5) . . . . ?

Fe3 N13 C65 N14 177.2(3) . . . . ?

C66 N13 C65 C64 -173.4(4) . . . . ?

Fe3 N13 C65 C64 3.0(6) . . . . ?

C71 N14 C65 N13 -0.5(5) . . . . ?

C72 N14 C65 N13 -177.6(4) . . . . ?

C71 N14 C65 C64 173.5(4) . . . . ?

C72 N14 C65 C64 -3.5(7) . . . . ?

N11 C64 C65 N13 -15.1(6) . . . . ?

N11 C64 C65 N14 171.5(4) . . . . ?

C65 N13 C66 C71 -0.7(5) . . . . ?

Fe3 N13 C66 C71 -176.1(3) . . . . ?

C65 N13 C66 C67 177.0(5) . . . . ?

Fe3 N13 C66 C67 1.7(7) . . . . ?

C71 C66 C67 C68 0.3(7) . . . . ?

N13 C66 C67 C68 -177.2(4) . . . . ?

C66 C67 C68 C69 -1.3(7) . . . . ?

C67 C68 C69 C70 1.7(8) . . . . ?

C68 C69 C70 C71 -1.0(7) . . . . ?

C65 N14 C71 C66 0.1(5) . . . . ?

C72 N14 C71 C66 177.2(4) . . . . ?

C65 N14 C71 C70 -177.5(5) . . . . ?

C72 N14 C71 C70 -0.4(8) . . . . ?

C67 C66 C71 N14 -177.6(4) . . . . ?

N13 C66 C71 N14 0.4(5) . . . . ?

C67 C66 C71 C70 0.3(7) . . . . ?

N13 C66 C71 C70 178.3(4) . . . . ?

C69 C70 C71 N14 177.2(5) . . . . ?

C69 C70 C71 C66 0.0(7) . . . . ?

C65 N14 C72 C73 -104.8(5) . . . . ?

C71 N14 C72 C73 78.7(6) . . . . ?

C62 N11 C74 C75 137.6(4) . . . . ?

C64 N11 C74 C75 -95.9(4) . . . . ?

Fe3 N11 C74 C75 24.4(4) . . . . ?

C76 N15 C75 N16 -2.0(5) . . . . ?

Fe3 N15 C75 N16 169.6(3) . . . . ?

C76 N15 C75 C74 -179.9(4) . . . . ?

Fe3 N15 C75 C74 -8.2(5) . . . . ?

C81 N16 C75 N15 0.7(5) . . . . ?

C82 N16 C75 N15 -176.9(4) . . . . ?

C81 N16 C75 C74 178.5(4) . . . . ?

C82 N16 C75 C74 0.9(7) . . . . ?

N11 C74 C75 N15 -12.9(6) . . . . ?

N11 C74 C75 N16 169.5(4) . . . . ?

C75 N15 C76 C81 2.6(5) . . . . ?

Fe3 N15 C76 C81 -166.3(3) . . . . ?

C75 N15 C76 C77 -178.3(5) . . . . ?

Fe3 N15 C76 C77 12.8(8) . . . . ?

C81 C76 C77 C78 0.2(7) . . . . ?

N15 C76 C77 C78 -178.9(5) . . . . ?

C76 C77 C78 C79 0.9(8) . . . . ?

C77 C78 C79 C80 -1.5(9) . . . . ?

C78 C79 C80 C81 0.9(8) . . . . ?

C75 N16 C81 C76 0.9(5) . . . . ?

C82 N16 C81 C76 178.6(4) . . . . ?

C75 N16 C81 C80 -179.8(5) . . . . ?

C82 N16 C81 C80 -2.1(8) . . . . ?

C77 C76 C81 N16 178.6(4) . . . . ?

N15 C76 C81 N16 -2.2(5) . . . . ?

C77 C76 C81 C80 -0.7(7) . . . . ?

N15 C76 C81 C80 178.5(4) . . . . ?

C79 C80 C81 N16 -179.0(5) . . . . ?

C79 C80 C81 C76 0.2(7) . . . . ?

C75 N16 C82 C83 103.2(6) . . . . ?

C81 N16 C82 C83 -74.0(6) . . . . ?

C94 N12 C84 C85 93.2(4) . . . . ?

C63 N12 C84 C85 -139.0(4) . . . . ?

Fe4 N12 C84 C85 -27.7(4) . . . . ?

C86 N17 C85 N18 -0.5(5) . . . . ?

Fe4 N17 C85 N18 178.8(3) . . . . ?

C86 N17 C85 C84 177.0(4) . . . . ?

Fe4 N17 C85 C84 -3.7(6) . . . . ?

C91 N18 C85 N17 0.4(5) . . . . ?

C92 N18 C85 N17 -177.5(4) . . . . ?

C91 N18 C85 C84 -176.9(4) . . . . ?

C92 N18 C85 C84 5.2(8) . . . . ?

N12 C84 C85 N17 23.1(6) . . . . ?

N12 C84 C85 N18 -159.8(4) . . . . ?

C85 N17 C86 C87 177.7(5) . . . . ?

Fe4 N17 C86 C87 -1.4(8) . . . . ?

C85 N17 C86 C91 0.3(5) . . . . ?

Fe4 N17 C86 C91 -178.7(3) . . . . ?

N17 C86 C87 C88 -178.1(5) . . . . ?

C91 C86 C87 C88 -1.0(7) . . . . ?

C86 C87 C88 C89 -0.2(8) . . . . ?

C87 C88 C89 C90 0.2(9) . . . . ?

C88 C89 C90 C91 1.0(8) . . . . ?

C85 N18 C91 C86 -0.2(5) . . . . ?

C92 N18 C91 C86 177.7(5) . . . . ?

C85 N18 C91 C90 179.8(5) . . . . ?

C92 N18 C91 C90 -2.3(9) . . . . ?

C87 C86 C91 N18 -177.8(4) . . . . ?

N17 C86 C91 N18 -0.1(5) . . . . ?

C87 C86 C91 C90 2.2(7) . . . . ?

N17 C86 C91 C90 179.9(4) . . . . ?

C89 C90 C91 N18 177.8(5) . . . . ?

C89 C90 C91 C86 -2.2(8) . . . . ?

C85 N18 C92 C93 -79.0(7) . . . . ?

C91 N18 C92 C93 103.5(6) . . . . ?

C84 N12 C94 C95 -123.5(4) . . . . ?

C63 N12 C94 C95 109.8(4) . . . . ?

Fe4 N12 C94 C95 -3.7(4) . . . . ?

C96 N19 C95 N20 -0.6(5) . . . . ?

Fe4 N19 C95 N20 -170.5(3) . . . . ?

C96 N19 C95 C94 176.2(4) . . . . ?

Fe4 N19 C95 C94 6.3(5) . . . . ?

C101 N20 C95 N19 0.9(5) . . . . ?

C102 N20 C95 N19 175.4(5) . . . . ?

C101 N20 C95 C94 -175.9(4) . . . . ?

C102 N20 C95 C94 -1.4(7) . . . . ?

N12 C94 C95 N19 -1.2(6) . . . . ?

N12 C94 C95 N20 175.3(4) . . . . ?

C95 N19 C96 C101 0.2(5) . . . . ?

Fe4 N19 C96 C101 166.8(3) . . . . ?

C95 N19 C96 C97 -177.0(5) . . . . ?

Fe4 N19 C96 C97 -10.4(8) . . . . ?

C101 C96 C97 C98 1.3(7) . . . . ?

N19 C96 C97 C98 178.2(5) . . . . ?

C96 C97 C98 C99 -1.2(8) . . . . ?

C97 C98 C99 C100 0.1(10) . . . . ?

C98 C99 C100 C101 0.8(9) . . . . ?

N19 C96 C101 N20 0.3(5) . . . . ?

C97 C96 C101 N20 177.8(4) . . . . ?

N19 C96 C101 C100 -177.9(5) . . . . ?

C97 C96 C101 C100 -0.4(8) . . . . ?

C95 N20 C101 C96 -0.7(5) . . . . ?

C102 N20 C101 C96 -175.5(5) . . . . ?

C95 N20 C101 C100 177.3(6) . . . . ?

C102 N20 C101 C100 2.5(9) . . . . ?

C99 C100 C101 C96 -0.6(8) . . . . ?

C99 C100 C101 N20 -178.3(6) . . . . ?

C95 N20 C102 C103 117.8(6) . . . . ?

C101 N20 C102 C103 -68.6(7) . . . . ?

Fe3 O12 C104 O13 1.2(8) . . . . ?

Fe3 O12 C104 C105 -177.7(3) . . . . ?

Fe4 O13 C104 O12 -7.5(8) . . . . ?

Fe4 O13 C104 C105 171.4(3) . . . . ?

O12 C104 C105 C110 177.1(4) . . . . ?

O13 C104 C105 C110 -1.9(6) . . . . ?

O12 C104 C105 C106 -1.9(6) . . . . ?

O13 C104 C105 C106 179.1(4) . . . . ?

C110 C105 C106 C107 -0.2(7) . . . . ?

C104 C105 C106 C107 178.8(4) . . . . ?

C111 O14 C107 C108 -175.2(5) . . . . ?

C111 O14 C107 C106 3.2(8) . . . . ?

C105 C106 C107 O14 -178.9(5) . . . . ?

C105 C106 C107 C108 -0.6(7) . . . . ?

O14 C107 C108 O15 1.1(7) . . . . ?

C106 C107 C108 O15 -177.3(4) . . . . ?

O14 C107 C108 C109 178.4(4) . . . . ?

C106 C107 C108 C109 -0.1(7) . . . . ?

C112 O15 C108 C107 -95.7(5) . . . . ?

C112 O15 C108 C109 87.1(5) . . . . ?

C113 O16 C109 C108 178.0(5) . . . . ?

C113 O16 C109 C110 -1.4(7) . . . . ?

C107 C108 C109 O16 -177.9(4) . . . . ?

O15 C108 C109 O16 -0.6(6) . . . . ?

C107 C108 C109 C110 1.5(7) . . . . ?

O15 C108 C109 C110 178.8(4) . . . . ?

C106 C105 C110 C109 1.6(7) . . . . ?

C104 C105 C110 C109 -177.4(4) . . . . ?

O16 C109 C110 C105 177.1(4) . . . . ?

C108 C109 C110 C105 -2.2(7) . . . . ?

C127 B1 C121 C122 6.8(7) . . . . ?

C133 B1 C121 C122 125.6(5) . . . . ?

C139 B1 C121 C122 -114.2(5) . . . . ?

C127 B1 C121 C126 -175.1(4) . . . . ?

C133 B1 C121 C126 -56.3(6) . . . . ?

C139 B1 C121 C126 63.9(6) . . . . ?

C126 C121 C122 C123 -1.6(8) . . . . ?

B1 C121 C122 C123 176.6(5) . . . . ?

C121 C122 C123 C124 0.9(9) . . . . ?

C122 C123 C124 C125 0.3(10) . . . . ?

C123 C124 C125 C126 -0.6(9) . . . . ?

C124 C125 C126 C121 -0.3(9) . . . . ?

C122 C121 C126 C125 1.4(8) . . . . ?

B1 C121 C126 C125 -176.9(5) . . . . ?

C133 B1 C127 C128 -60.2(6) . . . . ?

C121 B1 C127 C128 59.8(6) . . . . ?

C139 B1 C127 C128 175.1(4) . . . . ?

C133 B1 C127 C132 114.7(5) . . . . ?

C121 B1 C127 C132 -125.3(5) . . . . ?

C139 B1 C127 C132 -10.0(7) . . . . ?

C132 C127 C128 C129 0.5(8) . . . . ?

B1 C127 C128 C129 175.8(5) . . . . ?

C127 C128 C129 C130 -1.3(9) . . . . ?

C128 C129 C130 C131 1.3(10) . . . . ?

C129 C130 C131 C132 -0.5(9) . . . . ?

C128 C127 C132 C131 0.3(8) . . . . ?

B1 C127 C132 C131 -174.8(5) . . . . ?

C130 C131 C132 C127 -0.3(8) . . . . ?

C127 B1 C133 C138 -76.2(5) . . . . ?

C121 B1 C133 C138 161.9(4) . . . . ?

C139 B1 C133 C138 48.1(6) . . . . ?

C127 B1 C133 C134 99.6(5) . . . . ?

C121 B1 C133 C134 -22.2(7) . . . . ?

C139 B1 C133 C134 -136.0(5) . . . . ?

C138 C133 C134 C135 -0.7(7) . . . . ?

B1 C133 C134 C135 -176.9(5) . . . . ?

C133 C134 C135 C136 -1.1(8) . . . . ?

C134 C135 C136 C137 2.2(8) . . . . ?

C135 C136 C137 C138 -1.3(8) . . . . ?

C136 C137 C138 C133 -0.6(8) . . . . ?

C134 C133 C138 C137 1.6(7) . . . . ?

B1 C133 C138 C137 177.8(5) . . . . ?

C127 B1 C139 C144 130.9(5) . . . . ?

C133 B1 C139 C144 9.5(7) . . . . ?

C121 B1 C139 C144 -108.2(5) . . . . ?

C127 B1 C139 C140 -52.5(6) . . . . ?

C133 B1 C139 C140 -173.9(4) . . . . ?

C121 B1 C139 C140 68.4(6) . . . . ?

C144 C139 C140 C141 -1.5(7) . . . . ?

B1 C139 C140 C141 -178.4(5) . . . . ?

C139 C140 C141 C142 0.7(8) . . . . ?

C140 C141 C142 C143 1.8(8) . . . . ?

C141 C142 C143 C144 -3.4(8) . . . . ?

C140 C139 C144 C143 -0.1(7) . . . . ?

B1 C139 C144 C143 176.5(5) . . . . ?

C142 C143 C144 C139 2.6(8) . . . . ?

C169 B2 C151 C152 31.2(5) . . . . ?

C163 B2 C151 C152 146.5(3) . . . . ?

C157 B2 C151 C152 -93.0(4) . . . . ?

C169 B2 C151 C156 -156.2(4) . . . . ?

C163 B2 C151 C156 -40.9(5) . . . . ?

C157 B2 C151 C156 79.6(4) . . . . ?

C156 C151 C152 C153 0.0 . . . . ?

B2 C151 C152 C153 172.6(4) . . . . ?

C151 C152 C153 C154 0.0 . . . . ?

C152 C153 C154 C155 0.0 . . . . ?

C153 C154 C155 C156 0.0 . . . . ?

C154 C155 C156 C151 0.0 . . . . ?

C152 C151 C156 C155 0.0 . . . . ?

B2 C151 C156 C155 -172.5(4) . . . . ?

C169 B2 C157 C158 154.4(3) . . . . ?

C163 B2 C157 C158 37.2(5) . . . . ?

C151 B2 C157 C158 -81.7(4) . . . . ?

C169 B2 C157 C162 -27.2(6) . . . . ?

C163 B2 C157 C162 -144.4(3) . . . . ?

C151 B2 C157 C162 96.7(4) . . . . ?

C162 C157 C158 C159 0.0 . . . . ?

B2 C157 C158 C159 178.4(4) . . . . ?

C157 C158 C159 C160 0.0 . . . . ?

C158 C159 C160 C161 0.0 . . . . ?

C159 C160 C161 C162 0.0 . . . . ?

C160 C161 C162 C157 0.0 . . . . ?

C158 C157 C162 C161 0.0 . . . . ?

B2 C157 C162 C161 -178.4(4) . . . . ?

C169 B2 C163 C164 79.7(5) . . . . ?

C157 B2 C163 C164 -156.3(3) . . . . ?

C151 B2 C163 C164 -42.5(5) . . . . ?

C169 B2 C163 C168 -98.3(4) . . . . ?

C157 B2 C163 C168 25.6(6) . . . . ?

C151 B2 C163 C168 139.5(4) . . . . ?

C168 C163 C164 C165 0.0 . . . . ?

B2 C163 C164 C165 -178.1(4) . . . . ?

C163 C164 C165 C166 0.0 . . . . ?

C164 C165 C166 C167 0.0 . . . . ?

C165 C166 C167 C168 0.0 . . . . ?

C166 C167 C168 C163 0.0 . . . . ?

C164 C163 C168 C167 0.0 . . . . ?

B2 C163 C168 C167 178.0(4) . . . . ?

C163 B2 C169 C170 -82.1(5) . . . . ?

C157 B2 C169 C170 155.0(3) . . . . ?

C151 B2 C169 C170 37.8(5) . . . . ?

C163 B2 C169 C174 89.5(4) . . . . ?

C157 B2 C169 C174 -33.4(5) . . . . ?

C151 B2 C169 C174 -150.6(4) . . . . ?

C174 C169 C170 C171 0.0 . . . . ?

B2 C169 C170 C171 171.6(4) . . . . ?

C169 C170 C171 C172 0.0 . . . . ?

C170 C171 C172 C173 0.0 . . . . ?

C171 C172 C173 C174 0.0 . . . . ?

C172 C173 C174 C169 0.0 . . . . ?

C170 C169 C174 C173 0.0 . . . . ?

B2 C169 C174 C173 -171.5(4) . . . . ?

O22 S1 C181 F1 54.4(9) . . . . ?

O23 S1 C181 F1 176.7(8) . . . . ?

O21 S1 C181 F1 -62.2(9) . . . . ?

O22 S1 C181 F2 -174.4(7) . . . . ?

O23 S1 C181 F2 -52.1(8) . . . . ?

O21 S1 C181 F2 68.9(8) . . . . ?

O22 S1 C181 F3 -61.7(7) . . . . ?

O23 S1 C181 F3 60.6(7) . . . . ?

O21 S1 C181 F3 -178.3(6) . . . . ?

O32 S2 C191 F12 -176.2(9) . . . . ?

O33 S2 C191 F12 61.2(10) . . . . ?

O31 S2 C191 F12 -59.0(10) . . . . ?

O32 S2 C191 F11 -51.7(8) . . . . ?

O33 S2 C191 F11 -174.3(6) . . . . ?

O31 S2 C191 F11 65.5(7) . . . . ?

O32 S2 C191 F13 60.5(9) . . . . ?

O33 S2 C191 F13 -62.1(8) . . . . ?

O31 S2 C191 F13 177.7(7) . . . . ?

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_diffrn_reflns_theta_full 25.09

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