A Thermally Induced Two-Step, Two-Site Incomplete $^6A_1 \leftrightarrow {}^2T_2$ Crossover in a Mononuclear Iron(III) Phenolate-Pyridyl Schiff-Base Complex: A Rare Crystallographic Observation of the Coexistence of Pure $S = 5/2$ and $S = 1/2$ Metal Centers in the Asymmetric Unit

Musa S. Shongwe, *et al*. (FOUR CIF FILES)

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'Morris, Michael J.'
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'Hearne, Giovanni, G.'


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A thermally induced two-step, two-site 6A1 ↔ 2T2 crossover in a
mononuclear iron(III) complex: a rare crystallographic observation of
the coexistence of pure S = 5/2 and S = 1/2 metal centers in the
asymmetric unit
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data_musa294

$[Fe(salpm)_2]ClO_4 \cdot 0.5EtOH$ (at 294 K)

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
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 goodness of fit S are based on F^2^, conventional R-factors R are
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 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
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based
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and R-
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P=(Fo^2^+2Fc^2^)/3'
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O1 O 0.43521(19) 0.00455(15) 0.19271(16) 0.0611(8) Uani 1 1 d . . .
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O3 O 0.07589(19) 0.00971(16) 0.30076(18) 0.0677(9) Uani 1 1 d . . .
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O5 O 0.7775(4) 0.2598(3) 0.2753(3) 0.156(2) Uani 1 1 d . . .
O6 O 0.8287(5) 0.3017(3) 0.3808(4) 0.196(3) Uani 1 1 d . . .
O7 O 0.8155(3) 0.1860(2) 0.3730(3) 0.1294(17) Uani 1 1 d . . .
O8 O 0.7029(4) 0.2523(3) 0.3794(6) 0.268(5) Uani 1 1 d . . .
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O10 O 1.0163(3) 0.2635(3) 0.9623(3) 0.158(2) Uani 1 1 d . . .
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C2 C 0.3085(3) -0.0549(3) 0.1730(3) 0.0757(15) Uani 1 1 d . . .
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C3 C 0.2607(4) -0.1047(3) 0.1365(3) 0.0960(19) Uani 1 1 d . . .
H3 H 0.2046 -0.1127 0.1507 0.115 Uiso 1 1 calc R . .
C4 C 0.2949(4) -0.1441(3) 0.0779(4) 0.107(2) Uani 1 1 d . . .
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C5 C 0.3742(4) -0.1336(3) 0.0598(3) 0.0918(18) Uani 1 1 d . . .
H5 H 0.3973 -0.1611 0.0209 0.110 Uiso 1 1 calc R . .
C6 C 0.4248(3) -0.0827(2) 0.0969(3) 0.0640(13) Uani 1 1 d . . .
C7 C 0.5087(4) -0.0733(2) 0.0722(2) 0.0645(13) Uani 1 1 d . . .
H7 H 0.5260 -0.1037 0.0333 0.077 Uiso 1 1 calc R . .
C8 C 0.6454(3) -0.0313(3) 0.0627(3) 0.0710(14) Uani 1 1 d . . .
H8A H 0.6717 -0.0768 0.0732 0.085 Uiso 1 1 calc R . .
H8B H 0.6380 -0.0257 0.0063 0.085 Uiso 1 1 calc R . .
C9 C 0.7012(3) 0.0237(2) 0.0947(3) 0.0668(13) Uani 1 1 d . . .
C10 C 0.7830(4) 0.0312(3) 0.0731(4) 0.107(2) Uani 1 1 d . . .
H10 H 0.8048 0.0004 0.0367 0.129 Uiso 1 1 calc R . .
C11 C 0.8327(4) 0.0825(4) 0.1034(5) 0.119(2) Uani 1 1 d . . .
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C13 C 0.7189(3) 0.1162(3) 0.1775(3) 0.0697(13) Uani 1 1 d . . .
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C14 C 0.4498(3) 0.1747(2) 0.1342(2) 0.0490(10) Uani 1 1 d . . .
C15 C 0.3946(3) 0.2041(2) 0.0788(3) 0.0638(13) Uani 1 1 d . . .
H15 H 0.3891 0.1845 0.0289 0.077 Uiso 1 1 calc R . .
C16 C 0.3483(3) 0.2610(2) 0.0956(3) 0.0652(13) Uani 1 1 d . . .
H16 H 0.3100 0.2795 0.0573 0.078 Uiso 1 1 calc R . .
C17 C 0.3558(3) 0.2923(2) 0.1664(3) 0.0627(13) Uani 1 1 d . . .
H17 H 0.3250 0.3330 0.1764 0.075 Uiso 1 1 calc R . .
C18 C 0.4076(3) 0.2639(2) 0.2212(3) 0.0570(12) Uani 1 1 d . . .
H18 H 0.4124 0.2847 0.2706 0.068 Uiso 1 1 calc R . .
C19 C 0.4549(2) 0.20419(19) 0.2072(2) 0.0434(10) Uani 1 1 d . . .
C20 C 0.5051(3) 0.1747(2) 0.2706(2) 0.0506(11) Uani 1 1 d . . .
H20 H 0.5104 0.2011 0.3165 0.061 Uiso 1 1 calc R . .
C21 C 0.5864(3) 0.0956(2) 0.3433(2) 0.0635(13) Uani 1 1 d . . .
H21A H 0.5522 0.1091 0.3868 0.076 Uiso 1 1 calc R . .
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C22 C 0.5996(2) 0.0192(2) 0.3441(2) 0.0454(10) Uani 1 1 d . . .
C23 C 0.6144(3) -0.0175(2) 0.4102(2) 0.0530(11) Uani 1 1 d . . .
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C24 C 0.6296(3) -0.0869(2) 0.4075(3) 0.0619(12) Uani 1 1 d . . .
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C27 C 0.0030(3) -0.0183(2) 0.2807(3) 0.0589(12) Uani 1 1 d . . .
C28 C -0.0038(4) -0.0623(3) 0.2165(3) 0.0767(15) Uani 1 1 d . . .
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C33 C -0.0681(3) 0.0341(2) 0.3910(3) 0.0540(11) Uani 1 1 d . . .
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C34 C -0.0207(3) 0.1065(2) 0.4915(2) 0.0554(11) Uani 1 1 d . . .
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H34B H -0.0645 0.1416 0.4793 0.066 Uiso 1 1 calc R . .
C35 C 0.0578(2) 0.1413(2) 0.5221(2) 0.0486(10) Uani 1 1 d . . .
C36 C 0.0618(3) 0.1755(2) 0.5913(3) 0.0639(13) Uani 1 1 d . . .
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C39 C 0.1937(3) 0.1739(2) 0.5006(3) 0.0554(11) Uani 1 1 d . . .
H39 H 0.2408 0.1729 0.4691 0.066 Uiso 1 1 calc R . .
C40 C 0.2447(2) -0.0312(2) 0.4343(2) 0.0439(10) Uani 1 1 d . . .
C41 C 0.2608(3) -0.0924(2) 0.4742(2) 0.0450(10) Uani 1 1 d . . .
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C42 C 0.3341(3) -0.1277(2) 0.4681(2) 0.0524(11) Uani 1 1 d . . .
H42 H 0.3426 -0.1698 0.4954 0.063 Uiso 1 1 calc R . .
C43 C 0.3963(3) -0.1032(2) 0.4227(3) 0.0602(12) Uani 1 1 d . . .
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C44 C 0.3832(3) -0.0433(3) 0.3825(2) 0.0585(12) Uani 1 1 d . . .
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C47 C 0.2395(3) 0.1576(3) 0.2901(3) 0.0709(14) Uani 1 1 d . . .
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H47B H 0.2809 0.1895 0.3154 0.085 Uiso 1 1 calc R . .
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C49 C 0.1459(4) 0.2540(3) 0.2429(4) 0.111(2) Uani 1 1 d . . .
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C50 C 0.0680(4) 0.2848(4) 0.2376(4) 0.131(3) Uani 1 1 d . . .
H50 H 0.0610 0.3282 0.2129 0.157 Uiso 1 1 calc R . .
C51 C 0.0008(4) 0.2529(3) 0.2678(4) 0.111(2) Uani 1 1 d . . .
H51 H -0.0541 0.2724 0.2631 0.134 Uiso 1 1 calc R . .
C52 C 0.0155(3) 0.1921(3) 0.3050(3) 0.0782(16) Uani 1 1 d . . .
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O3 0.054(2) 0.074(2) 0.076(2) -0.0173(17) 0.0131(17) -0.0071(17)
O4 0.0381(16) 0.0514(17) 0.071(2) 0.0136(14) 0.0192(14) 0.0038(13)
O5 0.224(6) 0.144(4) 0.098(4) 0.029(3) -0.021(4) 0.045(4)
O6 0.261(8) 0.138(5) 0.184(6) -0.035(4) -0.032(5) -0.077(5)
O7 0.124(4) 0.106(3) 0.159(4) 0.068(3) 0.023(3) 0.035(3)
O8 0.146(5) 0.169(6) 0.506(14) 0.140(7) 0.188(8) 0.062(5)
O9 0.183(5) 0.214(6) 0.099(3) 0.044(4) 0.039(3) 0.124(5)
O10 0.068(3) 0.217(6) 0.188(5) 0.074(4) 0.001(3) -0.031(3)
O11 0.183(5) 0.130(4) 0.088(3) 0.019(3) 0.060(3) 0.031(3)
O12 0.158(8) 0.104(5) 0.138(5) -0.057(4) -0.010(5) -0.007(5)
O12' 0.147(10) 0.107(8) 0.140(7) -0.048(7) -0.016(8) -0.012(7)
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N2 0.061(2) 0.045(2) 0.065(2) 0.0047(18) 0.009(2) 0.0052(19)
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N4 0.049(2) 0.041(2) 0.046(2) -0.0016(15) -0.0023(16) -0.0023(16)
N5 0.036(2) 0.0441(19) 0.057(2) 0.0073(16) 0.0050(17) -0.0010(16)
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N7 0.042(2) 0.056(2) 0.052(2) 0.0113(17) 0.0091(17) -0.0042(18)
N8 0.044(2) 0.055(2) 0.064(2) 0.0166(18) 0.0048(18) 0.0026(18)
C1 0.060(3) 0.059(3) 0.047(3) -0.005(2) -0.008(2) 0.000(2)
C2 0.068(4) 0.080(4) 0.078(4) -0.025(3) -0.002(3) -0.008(3)
C3 0.076(4) 0.105(5) 0.106(5) -0.028(4) -0.003(4) -0.016(4)
C4 0.086(5) 0.103(5) 0.132(6) -0.055(4) -0.002(4) -0.019(4)
C5 0.102(5) 0.087(4) 0.085(4) -0.043(3) -0.007(4) -0.001(4)
C6 0.074(4) 0.064(3) 0.052(3) -0.021(2) -0.008(3) 0.003(3)
C7 0.092(4) 0.058(3) 0.044(3) -0.017(2) -0.001(3) 0.016(3)
C8 0.092(4) 0.061(3) 0.062(3) -0.008(2) 0.025(3) 0.007(3)
C9 0.073(4) 0.056(3) 0.073(3) 0.012(3) 0.029(3) 0.010(3)
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C11 0.080(5) 0.095(5) 0.186(7) 0.002(5) 0.058(5) -0.002(4)
C12 0.072(4) 0.070(4) 0.136(5) 0.000(4) 0.017(4) -0.007(3)
C13 0.067(4) 0.058(3) 0.084(4) 0.004(3) 0.011(3) 0.001(3)
C14 0.052(3) 0.045(2) 0.050(3) 0.004(2) 0.002(2) 0.007(2)
C15 0.075(3) 0.057(3) 0.058(3) 0.003(2) -0.016(3) 0.012(3)
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C17 0.064(3) 0.048(3) 0.077(4) 0.008(3) 0.021(3) 0.019(2)
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C19 0.050(3) 0.039(2) 0.042(2) 0.0031(18) 0.008(2) 0.0006(19)
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C23 0.060(3) 0.052(3) 0.046(3) 0.000(2) -0.008(2) -0.001(2)
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C26 0.067(3) 0.039(3) 0.057(3) -0.006(2) -0.006(2) 0.005(2)
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C35 0.039(2) 0.047(2) 0.061(3) 0.008(2) 0.006(2) 0.0096(19)
C36 0.062(3) 0.062(3) 0.069(3) -0.011(2) 0.012(3) 0.004(3)
C37 0.077(4) 0.068(3) 0.070(3) -0.018(3) -0.002(3) 0.003(3)
C38 0.056(3) 0.058(3) 0.085(4) -0.006(3) -0.005(3) 0.003(2)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Fe1 N4 2.181(3) . ?
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Fe2 N6 2.166(3) . ?
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O2 C14 1.325(5) . ?
O3 C27 1.311(5) . ?
O4 C40 1.315(4) . ?
O5 Cl1 1.399(5) . ?
O6 Cl1 1.355(5) . ?
O7 Cl1 1.386(4) . ?
O8 Cl1 1.302(5) . ?
O9 Cl2 1.404(5) . ?
O9 O12' 1.72(3) . ?
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N7 C47 1.463(5) . ?
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C15 C16 1.366(6) . ?
C16 C17 1.374(6) . ?
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O12' Cl2 O12 45.5(11) . . ?
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O10 Cl2 O9 107.1(4) . . ?
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END

data_musa150

$[Fe(salpm)_2]ClO_4 \cdot 0.5EtOH$ (at 150 K)

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_symmetry_space_group_name_H-M    P2(1)/n

loop_
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_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Bruker SMART'
_computing_cell_refinement        'Bruker SMART'
_computing_data_reduction         'Bruker SHELXTL'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

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

_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^)+(0.0508P)^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
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          7538
_refine_ls_number_parameters      696
_refine_ls_number_restraints      7
_refine_ls_R_factor_all           0.0625
_refine_ls_R_factor_gt            0.0400
_refine_ls_wR_factor_ref          0.0939
_refine_ls_wR_factor_gt           0.0878
_refine_ls_goodness_of_fit_ref    0.918
_refine_ls_restrained_S_all       0.918
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

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Fe2 Fe 0.12305(3) 0.08104(3) 0.37961(3) 0.03201(14) Uani 1 1 d . . .
O1 O 0.44614(15) 0.00869(11) 0.19391(12) 0.0373(6) Uani 1 1 d . . .
O2 O 0.50832(15) 0.12562(11) 0.11636(11) 0.0382(6) Uani 1 1 d . . .
O3 O 0.09690(18) 0.02744(15) 0.29368(15) 0.0605(8) Uani 1 1 d . . .
O4 O 0.16608(14) 0.00719(11) 0.44068(12) 0.0351(6) Uani 1 1 d . . .
O5 O 0.77791(18) 0.26220(13) 0.27521(14) 0.0588(8) Uani 1 1 d . . .
O6 O 0.83864(18) 0.30632(14) 0.38826(15) 0.0645(8) Uani 1 1 d . . .
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O7 O 0.81713(17) 0.18665(13) 0.37470(15) 0.0592(8) Uani 1 1 d . . .
O8 O 0.69845(18) 0.25901(14) 0.38564(18) 0.0740(9) Uani 1 1 d . . .
O9 O 0.91366(19) 0.32094(15) 0.93339(14) 0.0689(9) Uani 1 1 d . A .
O10 O 1.03011(17) 0.24764(15) 0.95196(16) 0.0703(9) Uani 1 1 d . A .
O11 O 0.92650(18) 0.25271(13) 1.04457(14) 0.0580(8) Uani 1 1 d . A .
O12 O 0.9234(15) 0.1878(6) 0.9324(12) 0.078(3) Uani 0.32(2) 1 d PDU A
1
O12' O 0.8835(8) 0.2078(6) 0.9246(5) 0.078(3) Uani 0.68(2) 1 d PDU A
2
N1 N 0.57877(18) -0.02313(13) 0.09595(14) 0.0317(7) Uani 1 1 d . . .
N2 N 0.68853(18) 0.07129(14) 0.14910(14) 0.0344(7) Uani 1 1 d . . .
N3 N 0.55640(17) 0.12200(13) 0.27125(14) 0.0287(6) Uani 1 1 d . . .
N4 N 0.60890(17) -0.00847(13) 0.27515(14) 0.0299(6) Uani 1 1 d . . .
N5 N 0.00615(17) 0.07014(13) 0.41868(15) 0.0306(7) Uani 1 1 d . . .
N6 N 0.13565(17) 0.14342(13) 0.47383(14) 0.0291(6) Uani 1 1 d . . .
N7 N 0.23880(17) 0.10009(13) 0.34012(14) 0.0287(6) Uani 1 1 d . . .
N8 N 0.09582(17) 0.16891(13) 0.31925(14) 0.0318(7) Uani 1 1 d . . .
C1 C 0.4004(2) -0.03797(17) 0.15491(18) 0.0329(8) Uani 1 1 d . . .
C2 C 0.3147(2) -0.05082(18) 0.1725(2) 0.0423(9) Uani 1 1 d . . .
H2 H 0.2899 -0.0251 0.2123 0.051 Uiso 1 1 calc R . .
C3 C 0.2653(2) -0.10003(19) 0.1333(2) 0.0495(10) Uani 1 1 d . . .
H3 H 0.2072 -0.1080 0.1466 0.059 Uiso 1 1 calc R . .
C4 C 0.2998(3) -0.13808(19) 0.0745(2) 0.0505(10) Uani 1 1 d . . .
H4 H 0.2656 -0.1720 0.0477 0.061 Uiso 1 1 calc R . .
C5 C 0.3831(3) -0.12634(19) 0.0554(2) 0.0465(10) Uani 1 1 d . . .
H5 H 0.4064 -0.1525 0.0152 0.056 Uiso 1 1 calc R . .
C6 C 0.4354(2) -0.07634(17) 0.09391(18) 0.0341(8) Uani 1 1 d . . .
C7 C 0.5213(2) -0.06654(17) 0.06918(18) 0.0365(9) Uani 1 1 d . . .
H7 H 0.5381 -0.0953 0.0283 0.044 Uiso 1 1 calc R . .
C8 C 0.6636(2) -0.02518(18) 0.06214(19) 0.0394(9) Uani 1 1 d . . .
H8A H 0.6562 -0.0175 0.0061 0.047 Uiso 1 1 calc R . .
H8B H 0.6898 -0.0715 0.0706 0.047 Uiso 1 1 calc R . .
C9 C 0.7230(2) 0.02910(17) 0.09686(19) 0.0370(9) Uani 1 1 d . . .
C10 C 0.8082(3) 0.0351(2) 0.0768(2) 0.0518(11) Uani 1 1 d . . .
H10 H 0.8312 0.0038 0.0410 0.062 Uiso 1 1 calc R . .
C11 C 0.8592(3) 0.0866(2) 0.1091(2) 0.0581(11) Uani 1 1 d . . .
H11 H 0.9174 0.0923 0.0949 0.070 Uiso 1 1 calc R . .
C12 C 0.8244(3) 0.13015(19) 0.1629(2) 0.0495(10) Uani 1 1 d . . .
H12 H 0.8584 0.1658 0.1867 0.059 Uiso 1 1 calc R . .
C13 C 0.7398(2) 0.12064(18) 0.1811(2) 0.0419(9) Uani 1 1 d . . .
H13 H 0.7163 0.1505 0.2181 0.050 Uiso 1 1 calc R . .
C14 C 0.4601(2) 0.17943(16) 0.13502(18) 0.0300(8) Uani 1 1 d . . .
C15 C 0.4023(2) 0.20821(17) 0.0795(2) 0.0392(9) Uani 1 1 d . . .
H15 H 0.3956 0.1874 0.0302 0.047 Uiso 1 1 calc R . .
C16 C 0.3554(2) 0.26607(18) 0.0957(2) 0.0413(9) Uani 1 1 d . . .
H16 H 0.3162 0.2846 0.0573 0.050 Uiso 1 1 calc R . .
C17 C 0.3633(2) 0.29854(17) 0.1666(2) 0.0369(9) Uani 1 1 d . . .
H17 H 0.3316 0.3396 0.1762 0.044 Uiso 1 1 calc R . .
C18 C 0.4177(2) 0.27024(16) 0.2224(2) 0.0354(9) Uani 1 1 d . . .
H18 H 0.4232 0.2917 0.2714 0.042 Uiso 1 1 calc R . .
C19 C 0.4659(2) 0.20952(16) 0.20846(18) 0.0285(8) Uani 1 1 d . . .
C20 C 0.5176(2) 0.18078(16) 0.27120(18) 0.0299(8) Uani 1 1 d . . .
H20 H 0.5236 0.2077 0.3168 0.036 Uiso 1 1 calc R . .
C21 C 0.5999(2) 0.09956(16) 0.34375(18) 0.0352(8) Uani 1 1 d . . .
H21A H 0.5657 0.1146 0.3873 0.042 Uiso 1 1 calc R . .
H21B H 0.6579 0.1212 0.3495 0.042 Uiso 1 1 calc R . .
C22 C 0.6087(2) 0.02223(16) 0.34458(18) 0.0274(8) Uani 1 1 d . . .
C23 C 0.6162(2) -0.01583(17) 0.41103(19) 0.0319(8) Uani 1 1 d . . .
H23 H 0.6138 0.0067 0.4593 0.038 Uiso 1 1 calc R . .
C24 C 0.6270(2) -0.08613(17) 0.40780(19) 0.0362(9) Uani 1 1 d . . .
H24 H 0.6312 -0.1129 0.4535 0.043 Uiso 1 1 calc R . .
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C25 C 0.6315(2) -0.11745(17) 0.33686(19) 0.0395(9) Uani 1 1 d . . .
H25 H 0.6415 -0.1659 0.3330 0.047 Uiso 1 1 calc R . .
C26 C 0.6213(2) -0.07731(17) 0.27215(19) 0.0345(8) Uani 1 1 d . . .
H26 H 0.6230 -0.0990 0.2234 0.041 Uiso 1 1 calc R . .
C27 C 0.0257(3) -0.0074(2) 0.2749(2) 0.0528(11) Uani 1 1 d . . .
C28 C 0.0227(3) -0.0474(2) 0.2077(2) 0.0740(15) Uani 1 1 d . . .
H28 H 0.0722 -0.0491 0.1774 0.089 Uiso 1 1 calc R . .
C29 C -0.0504(5) -0.0843(2) 0.1844(3) 0.0899(19) Uani 1 1 d . . .
H29 H -0.0502 -0.1107 0.1385 0.108 Uiso 1 1 calc R . .
C30 C -0.1238(4) -0.0836(2) 0.2265(3) 0.0815(17) Uani 1 1 d . . .
H30 H -0.1734 -0.1099 0.2104 0.098 Uiso 1 1 calc R . .
C31 C -0.1238(3) -0.0440(2) 0.2921(2) 0.0667(13) Uani 1 1 d . . .
H31 H -0.1747 -0.0421 0.3205 0.080 Uiso 1 1 calc R . .
C32 C -0.0505(3) -0.00649(17) 0.3181(2) 0.0445(10) Uani 1 1 d . . .
C33 C -0.0555(2) 0.03249(17) 0.38813(19) 0.0389(9) Uani 1 1 d . . .
H33 H -0.1083 0.0304 0.4139 0.047 Uiso 1 1 calc R . .
C34 C -0.0120(2) 0.10737(16) 0.48925(18) 0.0330(8) Uani 1 1 d . . .
H34A H -0.0325 0.0744 0.5279 0.040 Uiso 1 1 calc R . .
H34B H -0.0583 0.1420 0.4784 0.040 Uiso 1 1 calc R . .
C35 C 0.0682(2) 0.14304(15) 0.52021(18) 0.0298(8) Uani 1 1 d . . .
C36 C 0.0727(2) 0.17615(17) 0.59035(19) 0.0372(9) Uani 1 1 d . . .
H36 H 0.0253 0.1740 0.6230 0.045 Uiso 1 1 calc R . .
C37 C 0.1469(2) 0.21242(17) 0.6126(2) 0.0394(9) Uani 1 1 d . . .
H37 H 0.1514 0.2351 0.6609 0.047 Uiso 1 1 calc R . .
C38 C 0.2143(2) 0.21528(17) 0.56375(19) 0.0349(8) Uani 1 1 d . . .
H38 H 0.2647 0.2418 0.5767 0.042 Uiso 1 1 calc R . .
C39 C 0.2070(2) 0.17926(16) 0.49631(19) 0.0317(8) Uani 1 1 d . . .
H39 H 0.2547 0.1796 0.4638 0.038 Uiso 1 1 calc R . .
C40 C 0.2396(2) -0.02780(17) 0.43323(17) 0.0315(8) Uani 1 1 d . . .
C41 C 0.2524(2) -0.08912(16) 0.47476(18) 0.0354(9) Uani 1 1 d . . .
H41 H 0.2087 -0.1043 0.5074 0.042 Uiso 1 1 calc R . .
C42 C 0.3266(2) -0.12838(17) 0.46989(18) 0.0379(9) Uani 1 1 d . . .
H42 H 0.3326 -0.1702 0.4983 0.046 Uiso 1 1 calc R . .
C43 C 0.3924(2) -0.10725(17) 0.42389(18) 0.0366(9) Uani 1 1 d . . .
H43 H 0.4434 -0.1343 0.4204 0.044 Uiso 1 1 calc R . .
C44 C 0.3825(2) -0.04658(18) 0.38343(18) 0.0376(9) Uani 1 1 d . . .
H44 H 0.4279 -0.0317 0.3525 0.045 Uiso 1 1 calc R . .
C45 C 0.3071(2) -0.00566(16) 0.38630(17) 0.0285(8) Uani 1 1 d . . .
C46 C 0.3037(2) 0.05827(16) 0.34432(17) 0.0298(8) Uani 1 1 d . . .
H46 H 0.3534 0.0707 0.3174 0.036 Uiso 1 1 calc R . .
C47 C 0.2485(2) 0.16428(17) 0.2964(2) 0.0385(9) Uani 1 1 d . . .
H47A H 0.2706 0.1535 0.2454 0.046 Uiso 1 1 calc R . .
H47B H 0.2909 0.1951 0.3239 0.046 Uiso 1 1 calc R . .
C48 C 0.1626(2) 0.20006(17) 0.28677(18) 0.0332(8) Uani 1 1 d . . .
C49 C 0.1522(2) 0.26241(18) 0.2486(2) 0.0441(10) Uani 1 1 d . . .
H49 H 0.2001 0.2837 0.2259 0.053 Uiso 1 1 calc R . .
C50 C 0.0720(2) 0.29333(19) 0.2440(2) 0.0479(10) Uani 1 1 d . . .
H50 H 0.0638 0.3364 0.2183 0.057 Uiso 1 1 calc R . .
C51 C 0.0039(2) 0.26112(19) 0.2769(2) 0.0469(10) Uani 1 1 d . . .
H51 H -0.0522 0.2815 0.2740 0.056 Uiso 1 1 calc R . .
C52 C 0.0174(2) 0.19978(17) 0.31362(19) 0.0373(9) Uani 1 1 d . . .
H52 H -0.0301 0.1778 0.3362 0.045 Uiso 1 1 calc R . .
Cl1 Cl 0.78268(5) 0.25358(4) 0.35677(5) 0.0377(2) Uani 1 1 d . . .
Cl2 Cl 0.94116(5) 0.25462(5) 0.96490(5) 0.0385(2) Uani 1 1 d D . .

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Fe1 0.0382(3) 0.0264(3) 0.0254(3) -0.0027(2) -0.0021(2) 0.0075(2)
Fe2 0.0210(3) 0.0448(3) 0.0303(3) 0.0020(2) 0.0025(2) 0.0023(2)
O1 0.0387(14) 0.0387(14) 0.0345(14) -0.0101(11) 0.0005(11) 0.0025(12)
O2 0.0550(16) 0.0354(14) 0.0236(13) -0.0013(10) -0.0038(11)
0.0163(12)
O3 0.0488(18) 0.084(2) 0.0475(17) -0.0222(15) -0.0096(14) 0.0269(17)
O4 0.0351(14) 0.0345(13) 0.0363(14) 0.0032(10) 0.0084(11) -0.0080(11)
O5 0.074(2) 0.0569(18) 0.0435(17) 0.0046(13) -0.0147(14) -0.0035(15)
O6 0.068(2) 0.0684(19) 0.0564(18) -0.0139(15) -0.0026(15) -0.0275(16)
O7 0.0475(17) 0.0491(17) 0.081(2) 0.0321(14) 0.0080(15) 0.0094(13)
O8 0.0444(18) 0.0614(19) 0.119(3) 0.0170(17) 0.0324(17) 0.0049(15)
O9 0.074(2) 0.086(2) 0.0475(17) 0.0183(15) 0.0156(15) 0.0410(18)
O10 0.0314(16) 0.100(2) 0.081(2) 0.0359(17) 0.0194(14) 0.0179(15)
O11 0.071(2) 0.0623(18) 0.0422(16) 0.0060(13) 0.0206(14) 0.0142(15)
O12 0.058(7) 0.092(6) 0.082(5) -0.035(6) -0.009(7) -0.036(6)
O12' 0.056(6) 0.092(5) 0.086(3) -0.026(4) -0.011(4) -0.039(4)
N1 0.0398(18) 0.0281(16) 0.0270(16) -0.0044(12) -0.0023(14)
0.0078(14)
N2 0.0425(18) 0.0316(16) 0.0288(16) 0.0040(13) -0.0011(14) 0.0085(14)
N3 0.0397(17) 0.0208(15) 0.0252(16) -0.0001(12) -0.0026(13)
0.0028(13)
N4 0.0353(17) 0.0263(16) 0.0277(16) 0.0003(12) -0.0018(13) 0.0031(13)
N5 0.0294(16) 0.0258(15) 0.0363(17) -0.0046(12) -0.0009(13)
0.0023(13)
N6 0.0263(16) 0.0284(16) 0.0324(16) 0.0018(12) -0.0010(13) 0.0051(13)
N7 0.0260(16) 0.0325(16) 0.0278(16) 0.0034(12) 0.0027(12) -0.0031(13)
N8 0.0249(16) 0.0372(17) 0.0334(16) 0.0084(13) 0.0013(13) -0.0007(13)
C1 0.037(2) 0.031(2) 0.031(2) -0.0008(16) -0.0070(17) 0.0049(17)
C2 0.046(2) 0.044(2) 0.037(2) -0.0134(18) -0.0026(18) 0.0058(19)
C3 0.038(2) 0.055(3) 0.055(3) -0.013(2) 0.002(2) 0.003(2)
C4 0.052(3) 0.047(2) 0.051(3) -0.0159(19) -0.003(2) -0.005(2)
C5 0.054(3) 0.047(2) 0.038(2) -0.0166(18) -0.001(2) 0.006(2)
C6 0.043(2) 0.034(2) 0.0242(19) -0.0055(15) -0.0047(17) 0.0062(17)
C7 0.049(2) 0.035(2) 0.0248(19) -0.0078(16) -0.0013(18) 0.0124(18)
C8 0.041(2) 0.041(2) 0.036(2) -0.0019(17) 0.0079(18) 0.0113(18)
C9 0.046(2) 0.029(2) 0.036(2) 0.0047(16) 0.0018(18) 0.0073(17)
C10 0.048(3) 0.049(3) 0.060(3) -0.006(2) 0.016(2) 0.009(2)
C11 0.048(3) 0.047(3) 0.080(3) 0.003(2) 0.011(2) -0.001(2)
C12 0.047(3) 0.039(2) 0.063(3) 0.001(2) 0.000(2) -0.001(2)
C13 0.047(3) 0.031(2) 0.048(2) 0.0012(17) -0.0008(19) -0.0001(19)
C14 0.036(2) 0.0239(18) 0.031(2) 0.0021(15) 0.0028(16) 0.0070(16)
C15 0.046(2) 0.036(2) 0.034(2) -0.0015(16) -0.0100(18) 0.0093(18)
C16 0.032(2) 0.039(2) 0.052(3) 0.0096(19) -0.0062(18) 0.0050(17)
C17 0.035(2) 0.029(2) 0.048(2) 0.0048(17) 0.0107(18) 0.0079(16)
C18 0.041(2) 0.029(2) 0.037(2) 0.0054(16) 0.0132(18) 0.0039(17)
C19 0.0297(19) 0.0270(19) 0.029(2) 0.0030(15) 0.0059(16) 0.0016(15)
C20 0.040(2) 0.0240(19) 0.0262(19) -0.0030(14) 0.0062(16) -0.0067(16)
C21 0.047(2) 0.030(2) 0.027(2) -0.0018(15) -0.0085(17) 0.0009(16)
C22 0.0286(19) 0.0244(18) 0.029(2) -0.0003(15) -0.0067(15) -
0.0029(14)
C23 0.033(2) 0.034(2) 0.029(2) -0.0020(16) -0.0041(16) -0.0071(16)
C24 0.047(2) 0.029(2) 0.031(2) 0.0067(16) -0.0122(17) -0.0082(17)
C25 0.055(2) 0.0260(19) 0.036(2) 0.0005(17) -0.0111(18) 0.0013(17)
C26 0.040(2) 0.029(2) 0.034(2) -0.0056(16) -0.0065(17) 0.0021(16)
C27 0.077(3) 0.041(2) 0.039(2) -0.0036(19) -0.010(2) 0.032(2)
C28 0.094(4) 0.080(3) 0.046(3) -0.028(2) -0.028(3) 0.041(3)
C29 0.161(6) 0.053(3) 0.052(3) -0.018(3) -0.040(4) 0.039(4)
C30 0.141(5) 0.043(3) 0.057(3) -0.002(2) -0.039(3) -0.023(3)
C31 0.098(4) 0.045(3) 0.055(3) 0.004(2) -0.015(3) -0.018(3)
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C32 0.067(3) 0.027(2) 0.038(2) 0.0004(17) -0.015(2) -0.006(2)
C33 0.046(2) 0.031(2) 0.039(2) 0.0060(16) 0.0018(19) -0.0023(18)
C34 0.034(2) 0.0295(19) 0.036(2) -0.0004(15) 0.0044(17) 0.0013(16)
C35 0.032(2) 0.0255(18) 0.032(2) 0.0025(15) -0.0001(17) 0.0040(15)
C36 0.039(2) 0.039(2) 0.033(2) -0.0047(16) 0.0045(17) 0.0044(18)
C37 0.044(2) 0.036(2) 0.037(2) -0.0098(17) -0.0077(19) 0.0031(18)
C38 0.026(2) 0.033(2) 0.045(2) -0.0063(17) -0.0052(18) 0.0017(16)
C39 0.024(2) 0.0306(19) 0.040(2) 0.0013(16) -0.0007(16) 0.0032(16)
C40 0.036(2) 0.033(2) 0.026(2) -0.0090(15) 0.0002(16) -0.0100(17)
C41 0.044(2) 0.028(2) 0.034(2) -0.0003(16) 0.0019(17) -0.0133(18)
C42 0.057(3) 0.0255(19) 0.031(2) -0.0023(15) -0.0074(19) -0.0081(18)
C43 0.040(2) 0.037(2) 0.032(2) -0.0038(16) -0.0013(18) 0.0035(17)
C44 0.039(2) 0.045(2) 0.029(2) -0.0023(17) 0.0052(17) -0.0020(18)
C45 0.032(2) 0.0314(19) 0.0219(18) -0.0036(14) 0.0020(15) -0.0029(16)
C46 0.028(2) 0.039(2) 0.0221(18) 0.0002(15) 0.0051(15) -0.0068(17)
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Cl2 0.0305(5) 0.0471(6) 0.0384(5) -0.0079(4) 0.0078(4) -0.0056(4)

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 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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Fe1 N2 2.158(3) . ?
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Fe2 O4 1.882(2) . ?
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Fe2 N7 1.981(3) . ?
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O3 C27 1.316(5) . ?
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O12' Cl2 1.430(3) . ?
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N2 C9 1.351(4) . ?
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C16 C17 1.387(5) . ?
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O4 C40 C45 123.7(3) . . ?
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END

data_musa100

$[Fe(salpm)_2]ClO_4 \cdot 0.5EtOH$ (at 100 K)

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

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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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P=(Fo^2^+2Fc^2^)/3'
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N5 N 0.00850(17) 0.07085(12) 0.41849(14) 0.0244(6) Uani 1 1 d . . .
N6 N 0.13835(16) 0.14450(12) 0.47337(14) 0.0226(6) Uani 1 1 d . . .
N7 N 0.23941(17) 0.10086(12) 0.34120(14) 0.0237(6) Uani 1 1 d . . .
N8 N 0.09655(17) 0.17046(13) 0.32143(14) 0.0252(6) Uani 1 1 d . . .
C1 C 0.4021(2) -0.03730(16) 0.15464(18) 0.0284(8) Uani 1 1 d . . .
C2 C 0.3159(2) -0.05056(17) 0.17252(19) 0.0351(9) Uani 1 1 d . . .
H2 H 0.2911 -0.0252 0.2126 0.042 Uiso 1 1 calc R . .
C3 C 0.2662(2) -0.09981(18) 0.1331(2) 0.0404(9) Uani 1 1 d . . .
H3 H 0.2080 -0.1082 0.1467 0.048 Uiso 1 1 calc R . .
C4 C 0.3007(2) -0.13734(18) 0.0735(2) 0.0403(9) Uani 1 1 d . . .
H4 H 0.2663 -0.1709 0.0461 0.048 Uiso 1 1 calc R . .
C5 C 0.3843(2) -0.12523(18) 0.05509(19) 0.0373(9) Uani 1 1 d . . .
H5 H 0.4079 -0.1513 0.0150 0.045 Uiso 1 1 calc R . .
C6 C 0.4370(2) -0.07527(16) 0.09353(17) 0.0275(8) Uani 1 1 d . . .
C7 C 0.5227(2) -0.06530(16) 0.06882(18) 0.0301(8) Uani 1 1 d . . .
H7 H 0.5393 -0.0935 0.0275 0.036 Uiso 1 1 calc R . .
C8 C 0.6668(2) -0.02403(17) 0.06249(19) 0.0332(8) Uani 1 1 d . . .
H8A H 0.6595 -0.0160 0.0066 0.040 Uiso 1 1 calc R . .
H8B H 0.6931 -0.0704 0.0707 0.040 Uiso 1 1 calc R . .
C9 C 0.7263(2) 0.03001(16) 0.09767(19) 0.0314(8) Uani 1 1 d . . .
C10 C 0.8112(2) 0.03618(19) 0.0778(2) 0.0452(10) Uani 1 1 d . . .
H10 H 0.8340 0.0054 0.0414 0.054 Uiso 1 1 calc R . .
C11 C 0.8633(3) 0.0873(2) 0.1110(2) 0.0491(10) Uani 1 1 d . . .
H11 H 0.9219 0.0928 0.0974 0.059 Uiso 1 1 calc R . .
C12 C 0.8278(3) 0.13078(18) 0.1649(2) 0.0434(10) Uani 1 1 d . . .
H12 H 0.8619 0.1665 0.1889 0.052 Uiso 1 1 calc R . .
C13 C 0.7430(2) 0.12106(17) 0.1826(2) 0.0350(9) Uani 1 1 d . . .
H13 H 0.7192 0.1507 0.2197 0.042 Uiso 1 1 calc R . .
C14 C 0.4622(2) 0.17964(15) 0.13462(18) 0.0261(8) Uani 1 1 d . . .
C15 C 0.4040(2) 0.20899(17) 0.07889(19) 0.0338(9) Uani 1 1 d . . .
H15 H 0.3976 0.1884 0.0296 0.041 Uiso 1 1 calc R . .
C16 C 0.3565(2) 0.26670(17) 0.0948(2) 0.0351(9) Uani 1 1 d . . .
H16 H 0.3172 0.2851 0.0562 0.042 Uiso 1 1 calc R . .
C17 C 0.3640(2) 0.29911(17) 0.1656(2) 0.0321(8) Uani 1 1 d . . .
H17 H 0.3317 0.3400 0.1751 0.039 Uiso 1 1 calc R . .
C18 C 0.4188(2) 0.27112(15) 0.22181(19) 0.0292(8) Uani 1 1 d . . .
H18 H 0.4244 0.2929 0.2706 0.035 Uiso 1 1 calc R . .
C19 C 0.4672(2) 0.21035(15) 0.20816(17) 0.0233(7) Uani 1 1 d . . .
C20 C 0.5186(2) 0.18148(15) 0.27086(17) 0.0255(8) Uani 1 1 d . . .
H20 H 0.5239 0.2082 0.3165 0.031 Uiso 1 1 calc R . .
C21 C 0.6014(2) 0.10026(15) 0.34428(17) 0.0296(8) Uani 1 1 d . . .
H21A H 0.5670 0.1155 0.3876 0.036 Uiso 1 1 calc R . .
H21B H 0.6600 0.1215 0.3504 0.036 Uiso 1 1 calc R . .
C22 C 0.6095(2) 0.02278(15) 0.34468(17) 0.0229(7) Uani 1 1 d . . .
C23 C 0.6158(2) -0.01552(16) 0.41133(18) 0.0257(8) Uani 1 1 d . . .
H23 H 0.6131 0.0069 0.4595 0.031 Uiso 1 1 calc R . .
C24 C 0.6259(2) -0.08584(16) 0.40802(18) 0.0291(8) Uani 1 1 d . . .
H24 H 0.6292 -0.1128 0.4536 0.035 Uiso 1 1 calc R . .
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C25 C 0.6313(2) -0.11729(16) 0.33693(18) 0.0314(8) Uani 1 1 d . . .
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C26 C 0.6227(2) -0.07684(16) 0.27236(18) 0.0291(8) Uani 1 1 d . . .
H26 H 0.6252 -0.0984 0.2236 0.035 Uiso 1 1 calc R . .
C27 C 0.0297(3) -0.00510(17) 0.2750(2) 0.0370(9) Uani 1 1 d . . .
C28 C 0.0288(3) -0.04431(19) 0.2066(2) 0.0491(11) Uani 1 1 d . . .
H28 H 0.0783 -0.0439 0.1761 0.059 Uiso 1 1 calc R . .
C29 C -0.0430(3) -0.0829(2) 0.1841(2) 0.0572(12) Uani 1 1 d . . .
H29 H -0.0416 -0.1096 0.1385 0.069 Uiso 1 1 calc R . .
C30 C -0.1173(3) -0.08428(19) 0.2256(2) 0.0558(12) Uani 1 1 d . . .
H30 H -0.1661 -0.1115 0.2088 0.067 Uiso 1 1 calc R . .
C31 C -0.1192(3) -0.04531(19) 0.2922(2) 0.0504(11) Uani 1 1 d . . .
H31 H -0.1703 -0.0449 0.3206 0.060 Uiso 1 1 calc R . .
C32 C -0.0460(2) -0.00623(16) 0.31794(19) 0.0336(9) Uani 1 1 d . . .
C33 C -0.0520(2) 0.03230(16) 0.38779(19) 0.0310(8) Uani 1 1 d . . .
H33 H -0.1050 0.0291 0.4134 0.037 Uiso 1 1 calc R . .
C34 C -0.0100(2) 0.10823(16) 0.48892(17) 0.0269(8) Uani 1 1 d . . .
H34A H -0.0305 0.0753 0.5275 0.032 Uiso 1 1 calc R . .
H34B H -0.0565 0.1429 0.4780 0.032 Uiso 1 1 calc R . .
C35 C 0.0712(2) 0.14393(15) 0.51959(17) 0.0249(8) Uani 1 1 d . . .
C36 C 0.0755(2) 0.17699(16) 0.58974(18) 0.0294(8) Uani 1 1 d . . .
H36 H 0.0279 0.1746 0.6224 0.035 Uiso 1 1 calc R . .
C37 C 0.1499(2) 0.21366(16) 0.61180(19) 0.0320(8) Uani 1 1 d . . .
H37 H 0.1544 0.2363 0.6601 0.038 Uiso 1 1 calc R . .
C38 C 0.2172(2) 0.21690(16) 0.56325(18) 0.0287(8) Uani 1 1 d . . .
H38 H 0.2677 0.2436 0.5762 0.034 Uiso 1 1 calc R . .
C39 C 0.2102(2) 0.18061(15) 0.49533(18) 0.0246(8) Uani 1 1 d . . .
H39 H 0.2578 0.1811 0.4628 0.029 Uiso 1 1 calc R . .
C40 C 0.2379(2) -0.02669(15) 0.43363(17) 0.0236(7) Uani 1 1 d . . .
C41 C 0.2499(2) -0.08820(15) 0.47563(17) 0.0272(8) Uani 1 1 d . . .
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C42 C 0.3241(2) -0.12779(16) 0.47090(17) 0.0284(8) Uani 1 1 d . . .
H42 H 0.3299 -0.1694 0.4998 0.034 Uiso 1 1 calc R . .
C43 C 0.3906(2) -0.10804(16) 0.42468(18) 0.0299(8) Uani 1 1 d . . .
H43 H 0.4415 -0.1356 0.4213 0.036 Uiso 1 1 calc R . .
C44 C 0.3807(2) -0.04732(17) 0.38391(17) 0.0307(8) Uani 1 1 d . . .
H44 H 0.4262 -0.0331 0.3526 0.037 Uiso 1 1 calc R . .
C45 C 0.3062(2) -0.00556(15) 0.38674(16) 0.0236(7) Uani 1 1 d . . .
C46 C 0.3041(2) 0.05838(16) 0.34512(17) 0.0247(8) Uani 1 1 d . . .
H46 H 0.3542 0.0704 0.3184 0.030 Uiso 1 1 calc R . .
C47 C 0.2505(2) 0.16547(17) 0.29817(19) 0.0324(8) Uani 1 1 d . . .
H47A H 0.2733 0.1551 0.2475 0.039 Uiso 1 1 calc R . .
H47B H 0.2927 0.1961 0.3264 0.039 Uiso 1 1 calc R . .
C48 C 0.1632(2) 0.20114(17) 0.28817(17) 0.0279(8) Uani 1 1 d . . .
C49 C 0.1531(2) 0.26326(17) 0.24907(19) 0.0357(9) Uani 1 1 d . . .
H49 H 0.2011 0.2842 0.2260 0.043 Uiso 1 1 calc R . .
C50 C 0.0723(2) 0.29414(18) 0.2442(2) 0.0383(9) Uani 1 1 d . . .
H50 H 0.0639 0.3368 0.2178 0.046 Uiso 1 1 calc R . .
C51 C 0.0039(2) 0.26261(17) 0.27784(19) 0.0369(9) Uani 1 1 d . . .
H51 H -0.0523 0.2832 0.2749 0.044 Uiso 1 1 calc R . .
C52 C 0.0176(2) 0.20123(16) 0.31560(18) 0.0294(8) Uani 1 1 d . . .
H52 H -0.0301 0.1795 0.3385 0.035 Uiso 1 1 calc R . .
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0.0104(13)
O4 0.0258(13) 0.0271(12) 0.0304(13) 0.0024(10) 0.0046(10) -0.0024(10)
O5 0.0572(18) 0.0492(16) 0.0345(15) 0.0035(12) -0.0109(13) -
0.0058(13)
O6 0.0544(18) 0.0554(17) 0.0416(16) -0.0106(13) -0.0047(13) -
0.0201(14)
O7 0.0351(15) 0.0407(15) 0.0689(19) 0.0263(13) 0.0058(13) 0.0053(12)
O8 0.0365(16) 0.0514(17) 0.091(2) 0.0159(15) 0.0260(15) 0.0061(13)
O9 0.0518(18) 0.0625(18) 0.0387(16) 0.0107(13) 0.0081(13) 0.0272(14)
O10 0.0274(15) 0.0736(19) 0.0615(18) 0.0228(14) 0.0165(13) 0.0130(13)
O11 0.0541(17) 0.0518(16) 0.0340(15) 0.0055(12) 0.0162(13) 0.0125(13)
O12 0.043(7) 0.068(6) 0.070(5) -0.028(6) -0.011(7) -0.028(6)
O12' 0.044(5) 0.068(4) 0.071(3) -0.020(3) -0.011(4) -0.025(4)
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0.0005(12)
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N7 0.0220(16) 0.0264(15) 0.0228(15) 0.0014(11) 0.0023(12) -0.0017(12)
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C4 0.040(2) 0.039(2) 0.042(2) -0.0091(17) -0.0035(19) -0.0042(18)
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C17 0.029(2) 0.0242(18) 0.044(2) 0.0055(17) 0.0078(18) 0.0053(15)
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C19 0.0241(19) 0.0252(17) 0.0206(18) 0.0047(14) 0.0025(15) 0.0038(14)
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0.0020(14)
C23 0.0240(19) 0.0319(19) 0.0207(19) -0.0018(15) -0.0050(15) -
0.0061(15)
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C29 0.083(4) 0.038(2) 0.049(3) -0.010(2) -0.016(3) 0.012(2)
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C34 0.027(2) 0.0257(18) 0.0285(19) -0.0021(14) 0.0054(16) 0.0003(15)
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C36 0.028(2) 0.0320(19) 0.028(2) -0.0014(15) 0.0020(16) 0.0032(16)
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0.0057(15)
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C50 0.038(2) 0.035(2) 0.042(2) 0.0179(17) 0.0041(19) 0.0076(18)
C51 0.028(2) 0.040(2) 0.042(2) 0.0126(17) -0.0019(18) 0.0092(17)
C52 0.0212(19) 0.035(2) 0.032(2) 0.0071(16) 0.0005(16) -0.0007(16)
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Cl2 0.0251(5) 0.0381(5) 0.0329(5) -0.0066(4) 0.0062(4) -0.0039(4)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Fe1 N3 2.101(2) . ?
Fe1 N2 2.160(3) . ?
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Fe2 N6 2.010(2) . ?
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C10 C11 1.380(5) . ?
C11 C12 1.392(5) . ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
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 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-
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H1 H 0.3214 0.8575 0.3531 0.037 Uiso 1 1 calc R . .
C2 C 0.4533(5) 1.0181(4) 0.4062(3) 0.0356(12) Uani 1 1 d . . .
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C7 C 0.7048(4) 0.6170(4) 0.2857(2) 0.0224(10) Uani 1 1 d . . .
H7 H 0.7960 0.6545 0.2963 0.027 Uiso 1 1 calc R . .
C8 C 0.6575(4) 0.4843(4) 0.2622(2) 0.0190(10) Uani 1 1 d . . .
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C10 C 0.7165(4) 0.2971(4) 0.2397(2) 0.0189(10) Uani 1 1 d . . .
C11 C 0.5846(4) 0.2308(4) 0.2222(2) 0.0202(10) Uani 1 1 d . . .
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C14 C 0.3435(4) 0.2051(4) 0.2028(2) 0.0219(10) Uani 1 1 d . . .
C15 C 0.2661(4) 0.2210(4) 0.2738(2) 0.0295(11) Uani 1 1 d . . .
H15A H 0.2929 0.1835 0.3122 0.044 Uiso 1 1 calc R . .
H15B H 0.1733 0.1803 0.2582 0.044 Uiso 1 1 calc R . .
H15C H 0.2826 0.3093 0.2963 0.044 Uiso 1 1 calc R . .
C16 C 0.2849(4) 0.2428(4) 0.1380(2) 0.0310(11) Uani 1 1 d . . .
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H16B H 0.1942 0.1905 0.1249 0.046 Uiso 1 1 calc R . .
H16C H 0.3335 0.2324 0.0925 0.046 Uiso 1 1 calc R . .
C17 C 0.3265(4) 0.0673(4) 0.1754(3) 0.0350(12) Uani 1 1 d . . .
H17A H 0.3733 0.0538 0.1294 0.053 Uiso 1 1 calc R . .
H17B H 0.2342 0.0202 0.1628 0.053 Uiso 1 1 calc R . .
H17C H 0.3610 0.0397 0.2164 0.053 Uiso 1 1 calc R . .
C18 C 0.8231(4) 0.2370(4) 0.2410(2) 0.0241(11) Uani 1 1 d . . .
C19 C 0.7699(4) 0.0969(4) 0.2146(3) 0.0344(12) Uani 1 1 d . . .
H19A H 0.8401 0.0623 0.2181 0.052 Uiso 1 1 calc R . .
H19B H 0.7327 0.0731 0.1610 0.052 Uiso 1 1 calc R . .
H19C H 0.7026 0.0647 0.2475 0.052 Uiso 1 1 calc R . .
C20 C 0.9254(4) 0.2835(4) 0.1858(3) 0.0369(12) Uani 1 1 d . . .
H20A H 0.9625 0.3739 0.2019 0.055 Uiso 1 1 calc R . .
H20B H 0.8841 0.2593 0.1331 0.055 Uiso 1 1 calc R . .
H20C H 0.9943 0.2467 0.1874 0.055 Uiso 1 1 calc R . .
C21 C 0.8879(4) 0.2732(4) 0.3230(2) 0.0351(12) Uani 1 1 d . . .
H21A H 0.8227 0.2461 0.3583 0.053 Uiso 1 1 calc R . .
H21B H 0.9283 0.3633 0.3388 0.053 Uiso 1 1 calc R . .
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H21C H 0.9544 0.2335 0.3244 0.053 Uiso 1 1 calc R . .
C22 C 0.5427(4) 0.6623(4) 0.4587(2) 0.0267(11) Uani 1 1 d . . .
H22 H 0.6253 0.6913 0.4400 0.032 Uiso 1 1 calc R . .
C23 C 0.5371(4) 0.6590(4) 0.5355(2) 0.0305(11) Uani 1 1 d . . .
H23 H 0.6137 0.6861 0.5694 0.037 Uiso 1 1 calc R . .
C24 C 0.4156(5) 0.6149(4) 0.5614(2) 0.0338(12) Uani 1 1 d . . .
H24 H 0.4080 0.6113 0.6139 0.041 Uiso 1 1 calc R . .
C25 C 0.3075(4) 0.5768(4) 0.5119(2) 0.0293(11) Uani 1 1 d . . .
H25 H 0.2243 0.5454 0.5294 0.035 Uiso 1 1 calc R . .
C26 C 0.3190(4) 0.5838(4) 0.4355(2) 0.0230(10) Uani 1 1 d . . .
C27 C 0.2048(4) 0.5453(4) 0.3786(2) 0.0267(11) Uani 1 1 d . . .
H27A H 0.1697 0.4539 0.3628 0.032 Uiso 1 1 calc R . .
H27B H 0.1363 0.5762 0.4026 0.032 Uiso 1 1 calc R . .
C28 C 0.1537(4) 0.6165(4) 0.2733(2) 0.0232(11) Uani 1 1 d . . .
H28 H 0.0721 0.6037 0.2943 0.028 Uiso 1 1 calc R . .
C29 C 0.1659(4) 0.6587(4) 0.2029(2) 0.0196(10) Uani 1 1 d . . .
C30 C 0.0555(4) 0.6750(4) 0.1716(2) 0.0244(11) Uani 1 1 d . . .
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C31 C 0.0540(4) 0.7110(4) 0.1044(2) 0.0205(10) Uani 1 1 d . . .
C32 C 0.1726(4) 0.7340(3) 0.0683(2) 0.0235(10) Uani 1 1 d . . .
H32 H 0.1746 0.7611 0.0219 0.028 Uiso 1 1 calc R . .
C33 C 0.2833(4) 0.7202(3) 0.0949(2) 0.0183(10) Uani 1 1 d . . .
C34 C 0.2822(4) 0.6817(4) 0.1654(2) 0.0211(10) Uani 1 1 d . . .
C35 C 0.4062(4) 0.7431(4) 0.0512(2) 0.0221(10) Uani 1 1 d . . .
C36 C 0.5207(4) 0.8411(4) 0.1012(2) 0.0295(11) Uani 1 1 d . . .
H36A H 0.5004 0.9181 0.1182 0.044 Uiso 1 1 calc R . .
H36B H 0.5968 0.8558 0.0713 0.044 Uiso 1 1 calc R . .
H36C H 0.5391 0.8127 0.1463 0.044 Uiso 1 1 calc R . .
C37 C 0.4385(4) 0.6225(4) 0.0253(2) 0.0292(11) Uani 1 1 d . . .
H37A H 0.5177 0.6382 -0.0017 0.044 Uiso 1 1 calc R . .
H37B H 0.3667 0.5602 -0.0094 0.044 Uiso 1 1 calc R . .
H37C H 0.4518 0.5922 0.0706 0.044 Uiso 1 1 calc R . .
C38 C 0.3870(4) 0.7875(4) -0.0212(2) 0.0396(13) Uani 1 1 d . . .
H38A H 0.3679 0.8654 -0.0063 0.059 Uiso 1 1 calc R . .
H38B H 0.3147 0.7249 -0.0554 0.059 Uiso 1 1 calc R . .
H38C H 0.4663 0.8006 -0.0482 0.059 Uiso 1 1 calc R . .
C39 C -0.0655(4) 0.7226(4) 0.0659(2) 0.0274(11) Uani 1 1 d . . .
C40 C -0.0368(4) 0.8535(4) 0.0534(3) 0.0418(13) Uani 1 1 d . . .
H40A H -0.0146 0.9138 0.1034 0.063 Uiso 1 1 calc R . .
H40B H -0.1135 0.8591 0.0275 0.063 Uiso 1 1 calc R . .
H40C H 0.0360 0.8711 0.0213 0.063 Uiso 1 1 calc R . .
C41 C -0.1038(4) 0.6276(4) -0.0120(2) 0.0342(12) Uani 1 1 d . . .
H41A H -0.1817 0.6332 -0.0366 0.051 Uiso 1 1 calc R . .
H41B H -0.1215 0.5441 -0.0039 0.051 Uiso 1 1 calc R . .
H41C H -0.0328 0.6446 -0.0454 0.051 Uiso 1 1 calc R . .
C42 C -0.1816(4) 0.6975(4) 0.1149(2) 0.0361(12) Uani 1 1 d . . .
H42A H -0.1593 0.7570 0.1652 0.054 Uiso 1 1 calc R . .
H42B H -0.2036 0.6133 0.1223 0.054 Uiso 1 1 calc R . .
H42C H -0.2561 0.7061 0.0884 0.054 Uiso 1 1 calc R . .
N1S N 0.0345(5) 0.2747(5) 0.5513(3) 0.0558(12) Uani 1 1 d . . .
O1S O 0.0651(3) 0.3827(3) 0.5875(2) 0.0554(10) Uani 1 1 d . . .
O2S O 0.1243(4) 0.2288(4) 0.5346(2) 0.0886(14) Uani 1 1 d . . .
O3S O -0.0805(4) 0.2112(4) 0.5345(3) 0.0842(14) Uani 1 1 d . . .
O1W O 0.1403(4) 0.0221(3) 0.4295(2) 0.0776(13) Uani 1 1 d . . .
O2W O 0.0123(4) 0.9264(4) 0.2818(3) 0.1071(16) Uani 1 1 d . . .

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N3 0.017(2) 0.023(2) 0.026(2) 0.0072(18) 0.0009(17) 0.0035(18)
N4 0.017(2) 0.025(2) 0.021(2) 0.0077(18) 0.0026(16) 0.0067(18)
O1 0.0171(17) 0.0277(17) 0.0258(16) 0.0088(15) 0.0030(13) 0.0077(14)
O2 0.0167(17) 0.0310(17) 0.0244(16) 0.0126(15) 0.0022(13) 0.0097(14)
C1 0.030(3) 0.032(3) 0.032(3) 0.008(3) 0.005(2) 0.012(2)
C2 0.040(3) 0.030(3) 0.039(3) 0.007(3) 0.011(3) 0.015(3)
C3 0.043(3) 0.021(3) 0.040(3) 0.004(2) 0.007(3) 0.006(3)
C4 0.030(3) 0.030(3) 0.039(3) 0.015(3) -0.001(2) 0.004(3)
C5 0.032(3) 0.019(3) 0.022(3) 0.011(2) 0.002(2) 0.005(2)
C6 0.023(3) 0.025(3) 0.049(3) 0.015(3) 0.005(2) 0.009(2)
C7 0.014(2) 0.030(3) 0.026(3) 0.015(2) 0.003(2) 0.006(2)
C8 0.017(3) 0.020(2) 0.020(2) 0.008(2) 0.0020(19) 0.005(2)
C9 0.011(2) 0.029(3) 0.027(3) 0.011(2) 0.0014(19) 0.004(2)
C10 0.017(3) 0.025(3) 0.016(2) 0.008(2) 0.0008(19) 0.006(2)
C11 0.026(3) 0.019(2) 0.016(2) 0.007(2) 0.0036(19) 0.005(2)
C12 0.020(3) 0.026(3) 0.015(2) 0.007(2) 0.0000(19) 0.010(2)
C13 0.018(3) 0.029(3) 0.016(2) 0.009(2) 0.0025(19) 0.013(2)
C14 0.021(3) 0.023(3) 0.021(2) 0.003(2) -0.0007(19) 0.008(2)
C15 0.022(3) 0.031(3) 0.030(3) 0.006(2) 0.002(2) 0.003(2)
C16 0.017(3) 0.041(3) 0.029(3) 0.001(2) -0.003(2) 0.006(2)
C17 0.021(3) 0.033(3) 0.043(3) 0.000(3) -0.001(2) 0.004(2)
C18 0.022(3) 0.025(3) 0.026(3) 0.007(2) 0.004(2) 0.009(2)
C19 0.026(3) 0.033(3) 0.045(3) 0.006(3) 0.000(2) 0.012(2)
C20 0.027(3) 0.042(3) 0.049(3) 0.014(3) 0.014(2) 0.017(2)
C21 0.033(3) 0.035(3) 0.041(3) 0.009(3) 0.000(2) 0.017(2)
C22 0.025(3) 0.024(3) 0.030(3) 0.005(2) 0.000(2) 0.007(2)
C23 0.033(3) 0.030(3) 0.030(3) 0.009(2) -0.006(2) 0.012(2)
C24 0.054(4) 0.036(3) 0.017(3) 0.007(2) 0.007(3) 0.021(3)
C25 0.036(3) 0.028(3) 0.031(3) 0.015(2) 0.010(2) 0.013(2)
C26 0.029(3) 0.019(2) 0.024(3) 0.007(2) 0.005(2) 0.010(2)
C27 0.023(3) 0.031(3) 0.030(3) 0.015(2) 0.008(2) 0.009(2)
C28 0.013(3) 0.029(3) 0.026(3) 0.005(2) 0.005(2) 0.005(2)
C29 0.018(3) 0.023(2) 0.020(2) 0.005(2) 0.0043(19) 0.011(2)
C30 0.018(3) 0.031(3) 0.025(3) 0.006(2) 0.007(2) 0.010(2)
C31 0.013(2) 0.024(2) 0.025(2) 0.003(2) 0.0005(19) 0.009(2)
C32 0.022(3) 0.023(2) 0.025(2) 0.007(2) 0.003(2) 0.006(2)
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C34 0.018(3) 0.020(2) 0.028(3) 0.003(2) 0.003(2) 0.011(2)
C35 0.019(3) 0.028(3) 0.023(2) 0.010(2) 0.005(2) 0.009(2)
C36 0.021(3) 0.030(3) 0.040(3) 0.011(2) 0.008(2) 0.010(2)
C37 0.021(3) 0.030(3) 0.031(3) 0.003(2) 0.007(2) 0.005(2)
C38 0.028(3) 0.068(4) 0.034(3) 0.027(3) 0.015(2) 0.022(3)
C39 0.023(3) 0.031(3) 0.030(3) 0.007(2) 0.002(2) 0.011(2)
C40 0.029(3) 0.052(3) 0.051(3) 0.018(3) -0.009(2) 0.019(3)
C41 0.025(3) 0.050(3) 0.032(3) 0.017(3) -0.001(2) 0.013(2)
C42 0.017(3) 0.064(3) 0.036(3) 0.014(3) 0.002(2) 0.022(3)
N1S 0.049(4) 0.050(3) 0.068(3) 0.007(3) -0.001(3) 0.020(3)
O1S 0.047(2) 0.047(2) 0.063(3) -0.002(2) 0.013(2) 0.013(2)
O2S 0.063(3) 0.087(3) 0.112(4) -0.012(3) -0.002(3) 0.043(3)
O3S 0.044(3) 0.059(3) 0.125(4) 0.001(3) -0.026(3) -0.002(2)
O1W 0.081(3) 0.075(3) 0.084(3) 0.025(3) 0.030(2) 0.032(2)
O2W 0.062(3) 0.116(4) 0.111(4) -0.005(3) 0.019(3) 0.006(3)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Fe1 N3 2.206(3) . ?
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N1 C1 1.348(5) . ?
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N2 C6 1.456(5) . ?
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C10 C11 1.397(5) . ?
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C12 C14 1.542(5) . ?
C14 C16 1.529(5) . ?
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C18 C19 1.518(5) . ?
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C18 C20 1.547(5) . ?
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C28 C29 1.442(5) . ?
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C5 N1 C1 118.1(4) . . ?
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C7 N2 Fe1 125.3(3) . . ?
C6 N2 Fe1 117.8(2) . . ?
C22 N3 C26 119.0(3) . . ?
C22 N3 Fe1 125.5(3) . . ?
C26 N3 Fe1 115.5(3) . . ?
C28 N4 C27 117.4(3) . . ?
C28 N4 Fe1 125.4(3) . . ?
C27 N4 Fe1 117.0(3) . . ?
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C34 O2 Fe1 135.2(2) . . ?
N1 C1 C2 123.4(4) . . ?
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C5 C4 C3 119.4(4) . . ?
N1 C5 C4 121.4(4) . . ?
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O1 C13 C8 120.3(4) . . ?
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O2 C34 C29 120.9(3) . . ?
O2 C34 C33 120.9(3) . . ?
C29 C34 C33 118.2(4) . . ?
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C36 C35 C37 109.1(3) . . ?
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C31 C39 C42 111.9(3) . . ?
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C31 C39 C41 109.0(3) . . ?
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C42 C39 C41 108.0(3) . . ?
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O3S N1S O2S 121.2(5) . . ?

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N2 Fe1 N1 C5 -3.7(3) . . . . ?
N3 Fe1 N1 C5 89.0(3) . . . . ?
O1 Fe1 N1 C1 -159.2(3) . . . . ?
O2 Fe1 N1 C1 77.8(3) . . . . ?
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N2 Fe1 N1 C1 -176.4(3) . . . . ?
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O2 Fe1 N2 C7 -107.8(3) . . . . ?
N4 Fe1 N2 C7 101.0(6) . . . . ?
N1 Fe1 N2 C7 165.5(3) . . . . ?
N3 Fe1 N2 C7 83.9(3) . . . . ?
O1 Fe1 N2 C6 178.9(3) . . . . ?
O2 Fe1 N2 C6 80.7(3) . . . . ?
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N1 Fe1 N2 C6 -6.0(3) . . . . ?
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O1 Fe1 N3 C22 93.6(3) . . . . ?
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O2 Fe1 N3 C26 39.3(5) . . . . ?
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N1 Fe1 N3 C26 107.8(3) . . . . ?
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O2 Fe1 N4 C28 -13.2(3) . . . . ?
N2 Fe1 N4 C28 139.0(5) . . . . ?
N1 Fe1 N4 C28 76.8(3) . . . . ?
N3 Fe1 N4 C28 156.8(4) . . . . ?
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O2 Fe1 N4 C27 172.0(3) . . . . ?
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N1 Fe1 N4 C27 -98.0(3) . . . . ?
N3 Fe1 N4 C27 -18.0(3) . . . . ?
O2 Fe1 O1 C13 115.3(3) . . . . ?
N4 Fe1 O1 C13 -156.7(3) . . . . ?
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N3 Fe1 O2 C34 -12.8(6) . . . . ?
C5 N1 C1 C2 -1.6(6) . . . . ?
Fe1 N1 C1 C2 171.0(3) . . . . ?
N1 C1 C2 C3 -1.4(6) . . . . ?
C1 C2 C3 C4 2.3(6) . . . . ?
C2 C3 C4 C5 -0.2(6) . . . . ?
C1 N1 C5 C4 3.7(5) . . . . ?
Fe1 N1 C5 C4 -169.6(3) . . . . ?
C1 N1 C5 C6 -174.3(4) . . . . ?
Fe1 N1 C5 C6 12.4(4) . . . . ?
C3 C4 C5 N1 -2.9(6) . . . . ?
C3 C4 C5 C6 175.0(4) . . . . ?
C7 N2 C6 C5 -158.7(3) . . . . ?
Fe1 N2 C6 C5 13.6(4) . . . . ?
N1 C5 C6 N2 -16.7(5) . . . . ?
C4 C5 C6 N2 165.3(4) . . . . ?
C6 N2 C7 C8 179.2(4) . . . . ?
Fe1 N2 C7 C8 7.5(6) . . . . ?
N2 C7 C8 C9 -178.8(4) . . . . ?
N2 C7 C8 C13 -0.9(6) . . . . ?
C13 C8 C9 C10 -0.1(6) . . . . ?
C7 C8 C9 C10 177.7(4) . . . . ?
C8 C9 C10 C11 1.1(6) . . . . ?
C8 C9 C10 C18 -177.0(3) . . . . ?
C9 C10 C11 C12 -0.2(5) . . . . ?
C18 C10 C11 C12 177.9(3) . . . . ?
C10 C11 C12 C13 -1.7(6) . . . . ?
C10 C11 C12 C14 179.7(3) . . . . ?
Fe1 O1 C13 C12 172.2(3) . . . . ?
Fe1 O1 C13 C8 -7.1(5) . . . . ?
C11 C12 C13 O1 -176.7(3) . . . . ?
C14 C12 C13 O1 2.0(5) . . . . ?
C11 C12 C13 C8 2.7(5) . . . . ?
C14 C12 C13 C8 -178.7(3) . . . . ?
C9 C8 C13 O1 177.5(3) . . . . ?
C7 C8 C13 O1 -0.2(6) . . . . ?
C9 C8 C13 C12 -1.9(5) . . . . ?
C7 C8 C13 C12 -179.6(3) . . . . ?
C11 C12 C14 C16 -124.9(4) . . . . ?
C13 C12 C14 C16 56.5(5) . . . . ?
C11 C12 C14 C17 -5.2(5) . . . . ?
C13 C12 C14 C17 176.2(3) . . . . ?
C11 C12 C14 C15 114.5(4) . . . . ?
C13 C12 C14 C15 -64.1(5) . . . . ?
C9 C10 C18 C19 -177.1(3) . . . . ?
C11 C10 C18 C19 4.8(5) . . . . ?
C9 C10 C18 C21 61.7(4) . . . . ?
C11 C10 C18 C21 -116.3(4) . . . . ?
C9 C10 C18 C20 -58.0(5) . . . . ?
C11 C10 C18 C20 124.0(4) . . . . ?
C26 N3 C22 C23 -0.7(6) . . . . ?
Fe1 N3 C22 C23 177.0(3) . . . . ?
N3 C22 C23 C24 0.8(6) . . . . ?
C22 C23 C24 C25 0.0(6) . . . . ?
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C23 C24 C25 C26 -0.9(6) . . . . ?
C22 N3 C26 C25 -0.3(6) . . . . ?
Fe1 N3 C26 C25 -178.2(3) . . . . ?
C22 N3 C26 C27 180.0(4) . . . . ?
Fe1 N3 C26 C27 2.0(4) . . . . ?
C24 C25 C26 N3 1.1(6) . . . . ?
C24 C25 C26 C27 -179.2(4) . . . . ?
C28 N4 C27 C26 -151.0(4) . . . . ?
Fe1 N4 C27 C26 24.3(4) . . . . ?
N3 C26 C27 N4 -16.3(5) . . . . ?
C25 C26 C27 N4 163.9(4) . . . . ?
C27 N4 C28 C29 -176.6(4) . . . . ?
Fe1 N4 C28 C29 8.7(6) . . . . ?
N4 C28 C29 C30 179.1(4) . . . . ?
N4 C28 C29 C34 -0.1(7) . . . . ?
C34 C29 C30 C31 1.1(6) . . . . ?
C28 C29 C30 C31 -178.1(4) . . . . ?
C29 C30 C31 C32 -1.3(6) . . . . ?
C29 C30 C31 C39 176.3(4) . . . . ?
C30 C31 C32 C33 1.4(6) . . . . ?
C39 C31 C32 C33 -176.3(4) . . . . ?
C31 C32 C33 C34 -1.2(6) . . . . ?
C31 C32 C33 C35 178.1(4) . . . . ?
Fe1 O2 C34 C29 -13.9(6) . . . . ?
Fe1 O2 C34 C33 169.1(3) . . . . ?
C30 C29 C34 O2 -177.8(4) . . . . ?
C28 C29 C34 O2 1.3(6) . . . . ?
C30 C29 C34 C33 -0.7(6) . . . . ?
C28 C29 C34 C33 178.4(4) . . . . ?
C32 C33 C34 O2 177.8(4) . . . . ?
C35 C33 C34 O2 -1.4(6) . . . . ?
C32 C33 C34 C29 0.8(6) . . . . ?
C35 C33 C34 C29 -178.5(3) . . . . ?
C32 C33 C35 C36 122.4(4) . . . . ?
C34 C33 C35 C36 -58.4(5) . . . . ?
C32 C33 C35 C38 2.5(5) . . . . ?
C34 C33 C35 C38 -178.2(4) . . . . ?
C32 C33 C35 C37 -116.6(4) . . . . ?
C34 C33 C35 C37 62.6(5) . . . . ?
C30 C31 C39 C40 124.1(4) . . . . ?
C32 C31 C39 C40 -58.3(5) . . . . ?
C30 C31 C39 C42 3.9(6) . . . . ?
C32 C31 C39 C42 -178.5(4) . . . . ?
C30 C31 C39 C41 -115.5(4) . . . . ?
C32 C31 C39 C41 62.1(5) . . . . ?

_diffrn_measured_fraction_theta_max    0.995
_diffrn_reflns_theta_full              23.31
_diffrn_measured_fraction_theta_full   0.995
_refine_diff_density_max    0.388
_refine_diff_density_min   -0.401
_refine_diff_density_rms    0.063
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