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Tuning of the charge in octahedral ferric complexes based on pyridoxal-N-substituted thiosemicarbazone ligands

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# Supplementary Material (ESI) for Dalton Transactions
# This journal is (c) The Royal Society of Chemistry 2009
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_journal_codен_Cambridge    0222
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loop_
_publ_author_name
'Petra van Koningsbruggen'
'Christophe Faulmann'
'Auke Meetsma'
'Robby Roswanda'
'Eddy W. Yemeli Tido'

# Attachment 'q1126.cif'

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data_DATNAM
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_chemical_name_systematic
;
;
_chemical_name_common      ?
_chemical_melting_point    ?
_chemical_formula_moiety    'C18 H22 Fe N8 O4 S2, 0.5(S1 O4), 3.5(H2 O)'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_sum       'C18 H29 Fe1 N8 O9.5 S2.5'
_chemical_formula_iupac     ?
_chemical_formula_weight    645.49
_chemical_compound_source   'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scат_dispersiоn_real
_atom_type_scат_dispersiоn_imag
_atom_type_scат_source
S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe Fe 0.3463 0.8444 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

# 6. CRYSTAL DATA

```

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_symmetry_space_group_name_Hall	'-C 2yc'
_symmetry_space_group_name_H-M	'C 2/c'
_symmetry_Int_Tables_number	15

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loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z

```

_cell_length_a	27.416(2)
_cell_length_b	12.2927(8)
_cell_length_c	17.230(1)
_cell_angle_alpha	90
_cell_angle_beta	106.167(1)
_cell_angle_gamma	90
_cell_volume	5577.2(6)
_cell_formula_units_Z	8

_cell_measurement_temperature	100(1)
_cell_measurement_reflns_used	9741
_cell_measurement_theta_min	2.46
_cell_measurement_theta_max	29.61
_cell_special_details	

;

The final unit cell was obtained from the xyz centroids of 9741 reflections after integration using the SAINTPLUS software package (Bruker, 2000).

Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

;

_exptl_crystal_description	platelet
_exptl_crystal_colour	red
_exptl_crystal_size_max	0.39
_exptl_crystal_size_mid	0.27
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_exptl_crystal_size_rad	?
_exptl_crystal_density_meas	?
_exptl_crystal_density_diffn	1.537
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	2680
_exptl_absorpt_coefficient_mu	0.790
_exptl_absorpt_correction_type	Multi-Scan
_exptl_absorpt_process_details	'(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min	0.7348
_exptl_absorpt_correction_T_max	0.9240

#=====

7. EXPERIMENTAL DATA

```

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_diffn_ambient_temperature      100(1)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK\alpha
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_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean 66.06

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_diffn_standards_interval_time  ?
_diffn_standards_decay_%        0

loop_
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_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
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_diffn_reflns_av_sigmaI/netI    0.0551
_diffn_reflns_limit_h_min       -33
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_diffn_reflns_limit_k_min       -15
_diffn_reflns_limit_k_max       14
_diffn_reflns_limit_l_min       -19
_diffn_reflns_limit_l_max       21
_diffn_reflns_theta_min         2.84
_diffn_reflns_theta_max         26.02
_diffn_measured_fraction_theta_max 0.994
_diffn_reflns_theta_full        25.00
_diffn_measured_fraction_theta_full 0.994

_diffn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total            5471

```

```

_reflns_number_gt          4729
_reflns_threshold_expression I>2\s(I)

_computing_data_collection 'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement 'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction  'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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/[\s2(Fo2)+(0.0001P)2+149.39P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method none
_refine_ls_extinction_coef   ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration .

_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns      5471
_refine_ls_number_parameters  450
_refine_ls_number_restraints  0
_refine_ls_number_constraints  ?
_refine_ls_R_factor_all       0.1018
_refine_ls_R_factor_gt        0.0906
_refine_ls_wR_factor_ref      0.2062
_refine_ls_wR_factor_gt       0.2021
_refine_ls_goodness_of_fit_ref 1.294
_refine_ls_restrained_S_all    1.294
_refine_ls_shift/su_max        0.001
_refine_ls_shift/su_mean       0.000

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_refine_diff_density_min -0.588
_refine_diff_density_rms 0.144

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#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
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_atom_site_occupancy
_atom_site_U_iso_or_equiv
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_atom_site_refinement_flags
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S1 S Uani 0.36322(6) 0.05937(14) 0.20616(10) 1.0 0.0121(5) . .
S2 S Uani 0.25740(6) -0.01323(14) 0.24175(10) 1.0 0.0118(5) . .
O1 O Uani 0.24395(17) 0.2170(4) 0.2576(3) 1.0 0.0144(14) . .
O2 O Uani 0.0594(2) 0.2039(5) -0.0334(3) 1.0 0.0289(19) . .
O3 O Uani 0.32897(17) 0.2815(4) 0.2260(3) 1.0 0.0113(12) . .
O4A O Uani 0.4431(4) 0.4315(9) 0.5628(6) 0.5 0.024(3) . .
O4B O Uani 0.4103(5) 0.3164(12) 0.5455(8) 0.5 0.023(4) . .
N1 N Uani 0.2656(2) 0.1404(5) 0.1190(3) 1.0 0.0103(17) . .
N2 N Uani 0.1135(2) 0.2695(6) 0.2029(4) 1.0 0.023(2) . .
N3 N Uani 0.2926(2) 0.1069(5) 0.0654(3) 1.0 0.0115(17) . .
N4 N Uani 0.3663(2) 0.0309(5) 0.0555(4) 1.0 0.0161(19) . .
N5 N Uani 0.3256(2) 0.1303(5) 0.3492(3) 1.0 0.0116(17) . .
N6A N Uiso 0.4074(5) 0.4950(11) 0.3268(8) 0.5 0.011(3) . .
N6B N Uani 0.4259(5) 0.4650(11) 0.3173(7) 0.5 0.015(4) . .
N7 N Uani 0.3095(2) 0.0500(5) 0.3922(3) 1.0 0.0119(17) . .
N8 N Uani 0.2545(2) -0.0919(5) 0.3831(4) 1.0 0.0142(17) . .
C1 C Uani 0.2188(2) 0.1652(5) 0.0849(4) 1.0 0.0105(17) . .
C2 C Uani 0.1830(3) 0.2015(5) 0.1273(4) 1.0 0.0101(17) . .
C3 C Uani 0.1314(3) 0.2144(6) 0.0829(4) 1.0 0.0161(19) . .
C4 C Uani 0.0975(3) 0.2512(7) 0.1234(5) 1.0 0.026(2) . .
C5 C Uani 0.1607(3) 0.2577(5) 0.2482(4) 1.0 0.0132(19) . .
C6 C Uani 0.1982(2) 0.2243(5) 0.2111(4) 1.0 0.0095(17) . .
C7 C Uani 0.1123(3) 0.1895(7) -0.0053(4) 1.0 0.021(2) . .
C8 C Uani 0.1735(3) 0.2758(6) 0.3368(4) 1.0 0.016(2) . .
C9 C Uani 0.3387(3) 0.0688(6) 0.1017(4) 1.0 0.0136(17) . .
C10 C Uani 0.3564(3) 0.1984(7) 0.3936(4) 1.0 0.021(2) . .
C11 C Uani 0.3770(3) 0.2957(7) 0.3663(5) 1.0 0.033(3) . .
C12A C Uiso 0.4007(5) 0.3742(12) 0.4294(8) 0.5 0.009(3) . .
C12B C Uani 0.4236(6) 0.3363(14) 0.4182(8) 0.5 0.020(5) . .
C13A C Uani 0.4190(5) 0.4688(11) 0.4052(8) 0.5 0.011(4) . .
C13B C Uani 0.4448(6) 0.4263(14) 0.3931(9) 0.5 0.020(5) . .
C14 C Uani 0.3828(3) 0.4284(7) 0.2652(4) 1.0 0.022(2) . .
C15 C Uani 0.3610(3) 0.3314(6) 0.2842(4) 1.0 0.0150(19) . .
C16A C Uani 0.4155(7) 0.3458(16) 0.5151(11) 0.5 0.017(5) . .
C16B C Uani 0.4470(6) 0.2984(14) 0.5038(8) 0.5 0.020(5) . .
C17 C Uani 0.3693(3) 0.4755(6) 0.1829(4) 1.0 0.018(2) . .
C18 C Uani 0.2756(3) -0.0164(6) 0.3465(4) 1.0 0.0127(17) . .

S3 S Uani 0.000 0.2026(2) 0.25000 1.000 0.0138(7) . .
 O5 O Uani -0.04306(19) 0.2708(4) 0.2081(3) 1.0 0.0244(17) . .
 O6 O Uani 0.01511(18) 0.1342(4) 0.1904(3) 1.0 0.0196(16) . .
 O7 O Uani 0.0281(3) 0.4526(8) 0.3782(6) 1.0 0.052(3) . .
 O9 O Uani 0.0017(7) 0.6176(13) 0.4804(10) 0.5 0.052(6) . .
 O11 O Uani -0.0147(5) 0.5918(10) 0.2759(7) 0.5 0.030(4) . .
 O8 O Uani 0.0178(4) 0.9023(10) 0.3234(7) 0.5 0.029(4) . .
 O10 O Uani 0.0470(4) 0.7653(10) 0.2960(7) 0.5 0.027(4) . .
 O12 O Uani 0.3133(18) 0.428(3) 0.485(2) 0.5 0.24(2) . .
 H1 H Uiso 0.20702 0.15922 0.02772 1.0 0.0123 . .
 H161' H Uiso 0.43662 0.27926 0.52350 0.5 0.0204 . .
 H162' H Uiso 0.47831 0.34009 0.52899 0.5 0.0241 . .
 H4 H Uiso 0.06301 0.26348 0.09471 1.0 0.0311 . .
 H7 H Uiso 0.12924 0.23795 -0.03577 1.0 0.0249 . .
 H7' H Uiso 0.12098 0.11342 -0.01505 1.0 0.0249 . .
 H8 H Uiso 0.14234 0.29078 0.35222 1.0 0.0238 . .
 H8' H Uiso 0.19660 0.33801 0.35148 1.0 0.0238 . .
 H8'' H Uiso 0.18996 0.21070 0.36510 1.0 0.0238 . .
 H10 H Uiso 0.36682 0.18406 0.45002 1.0 0.0254 . .
 H17 H Uiso 0.39295 0.53448 0.18073 1.0 0.0265 . .
 H17' H Uiso 0.33461 0.50436 0.16958 1.0 0.0265 . .
 H17'' H Uiso 0.37133 0.41902 0.14377 1.0 0.0265 . .
 H21 H Uiso 0.053(4) 0.170(9) -0.083(7) 1.0 0.0500 . .
 H22 H Uiso 0.091(4) 0.282(10) 0.213(7) 1.0 0.0500 . .
 H24 H Uiso 0.347(4) 0.005(9) 0.011(7) 1.0 0.0500 . .
 H24' H Uiso 0.389(4) -0.001(9) 0.079(7) 1.0 0.0500 . .
 H28 H Uiso 0.229(4) -0.141(9) 0.358(7) 1.0 0.0500 . .
 H28' H Uiso 0.258(4) -0.100(9) 0.431(7) 1.0 0.0500 . .
 H41 H Uiso 0.47360 0.42844 0.56231 0.5 0.0353 . .
 H42 H Uiso 0.39457 0.25822 0.54742 0.5 0.0348 . .
 H61 H Uiso 0.41630 0.55999 0.31416 0.5 0.0134 . .
 H62 H Uiso 0.44265 0.51722 0.30101 0.5 0.0183 . .
 H131 H Uiso 0.43995 0.51570 0.44436 0.5 0.0134 . .
 H132 H Uiso 0.47288 0.46144 0.42932 0.5 0.0241 . .
 H161 H Uiso 0.38465 0.33013 0.53241 0.5 0.0204 . .
 H162 H Uiso 0.45577 0.22015 0.50462 0.5 0.0241 . .
 H31 H Uiso 0.030(4) 0.394(10) 0.353(7) 1.0 0.0500 . .
 H31' H Uiso 0.013(5) 0.485(11) 0.380(8) 1.0 0.0500 . .
 H33 H Uiso 0.020(8) 0.648(18) 0.434(13) 0.5 0.0500 . .
 H33' H Uiso 0.028(9) 0.572(19) 0.494(14) 0.5 0.0500 . .
 H35 H Uiso 0.016(8) 0.531(18) 0.312(13) 0.5 0.0500 . .
 H35' H Uiso -0.049(8) 0.597(18) 0.244(13) 0.5 0.0500 . .

loop_

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 _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

Fe 0.0105(4) 0.0080(5) 0.0065(4) 0.0001(4) 0.0026(3) -0.0003(4)
 S1 0.0119(8) 0.0146(9) 0.0093(8) 0.0009(7) 0.0023(6) 0.0030(6)
 S2 0.0166(8) 0.0102(8) 0.0087(8) -0.0014(6) 0.0035(6) -0.0024(7)
 O1 0.013(2) 0.018(3) 0.012(2) -0.005(2) 0.0033(19) 0.001(2)
 O2 0.018(3) 0.047(4) 0.018(3) -0.005(3) -0.001(2) 0.007(3)
 O3 0.013(2) 0.008(2) 0.012(2) 0.0033(19) 0.0019(18) 0.0005(18)
 O4A 0.028(6) 0.020(6) 0.017(5) -0.006(5) -0.003(5) -0.011(5)
 O4B 0.016(6) 0.043(9) 0.014(7) -0.005(6) 0.009(5) -0.009(6)
 N1 0.013(3) 0.008(3) 0.011(3) 0.000(2) 0.005(2) 0.002(2)
 N2 0.013(3) 0.036(4) 0.024(4) -0.009(3) 0.014(3) -0.002(3)

N3 0.012(3) 0.018(3) 0.006(3) 0.000(2) 0.005(2) 0.003(2)
 N4 0.016(3) 0.022(4) 0.010(3) -0.004(3) 0.003(2) 0.006(3)
 N5 0.014(3) 0.010(3) 0.011(3) 0.002(2) 0.004(2) 0.000(2)
 N6B 0.013(6) 0.016(7) 0.017(7) 0.002(5) 0.005(5) -0.007(5)
 N7 0.013(3) 0.010(3) 0.013(3) 0.000(2) 0.004(2) -0.004(2)
 N8 0.017(3) 0.012(3) 0.013(3) -0.003(2) 0.003(2) -0.008(2)
 C1 0.011(3) 0.012(3) 0.008(3) -0.001(3) 0.002(2) 0.000(3)
 C2 0.013(3) 0.009(3) 0.010(3) 0.000(3) 0.006(3) 0.001(3)
 C3 0.017(3) 0.020(4) 0.012(3) -0.004(3) 0.005(3) 0.000(3)
 C4 0.011(3) 0.038(5) 0.027(4) -0.012(4) 0.004(3) 0.004(3)
 C5 0.017(3) 0.007(3) 0.018(4) 0.001(3) 0.009(3) -0.003(3)
 C6 0.012(3) 0.003(3) 0.012(3) -0.002(2) 0.001(3) 0.002(2)
 C7 0.016(4) 0.029(4) 0.017(4) -0.002(3) 0.004(3) 0.008(3)
 C8 0.023(4) 0.013(4) 0.016(4) 0.001(3) 0.011(3) -0.003(3)
 C9 0.018(3) 0.008(3) 0.015(3) -0.002(3) 0.005(3) -0.003(3)
 C10 0.029(4) 0.026(4) 0.006(3) 0.006(3) 0.001(3) -0.010(3)
 C11 0.047(5) 0.032(5) 0.012(4) 0.007(3) -0.004(4) -0.029(4)
 C12B 0.022(8) 0.029(9) 0.005(7) -0.006(6) -0.001(6) -0.004(7)
 C13A 0.009(7) 0.008(7) 0.011(7) -0.001(5) -0.007(5) 0.001(6)
 C13B 0.012(7) 0.023(9) 0.020(8) 0.001(7) -0.004(6) -0.009(7)
 C14 0.023(4) 0.024(4) 0.015(4) 0.003(3) -0.001(3) -0.010(3)
 C15 0.017(3) 0.013(4) 0.013(3) 0.001(3) 0.001(3) -0.007(3)
 C16A 0.017(8) 0.023(10) 0.014(10) -0.004(8) 0.008(7) -0.013(7)
 C16B 0.019(8) 0.032(9) 0.009(7) -0.002(6) 0.003(6) -0.015(7)
 C17 0.020(4) 0.017(4) 0.016(4) 0.001(3) 0.005(3) 0.000(3)
 C18 0.014(3) 0.011(3) 0.012(3) 0.002(3) 0.002(3) 0.003(3)
 S3 0.0114(11) 0.0097(12) 0.0187(12) 0.00 0.0016(9) 0.0000
 O5 0.014(3) 0.023(3) 0.040(3) 0.012(3) 0.014(2) 0.007(2)
 O6 0.016(2) 0.021(3) 0.020(3) -0.003(2) 0.002(2) 0.001(2)
 O7 0.033(4) 0.064(6) 0.065(5) -0.050(5) 0.025(4) -0.018(4)
 O9 0.079(11) 0.037(9) 0.048(9) -0.017(7) 0.033(9) -0.007(8)
 O11 0.031(6) 0.032(7) 0.026(6) -0.008(5) 0.006(5) -0.003(5)
 O8 0.035(7) 0.025(6) 0.027(6) 0.003(5) 0.007(5) 0.010(5)
 O10 0.026(6) 0.035(7) 0.019(6) 0.003(5) 0.005(5) -0.005(5)
 O12 0.32(5) 0.13(3) 0.17(3) -0.04(2) -0.10(3) 0.15(3)

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10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Fe S1 2.2222(19) . . yes

Fe S2 2.205(2) . . yes

Fe O1 1.884(5) . . yes

Fe O3 1.962(5) . . yes

Fe N1 1.926(5) . . yes

Fe N5 1.927(5) . . yes
 S1 C9 1.741(7) . . yes
 S2 C18 1.734(7) . . yes
 S3 O5 1.464(5) . 2_555 yes
 S3 O6 1.473(5) . 2_555 yes
 S3 O5 1.464(5) . . yes
 S3 O6 1.473(5) . . yes
 O1 C6 1.290(8) . . yes
 O2 C7 1.407(10) . . yes
 O3 C15 1.289(9) . . yes
 O4A O4B 1.658(18) . . yes
 O4A C16A 1.42(2) . . yes
 O4B C16A 0.68(2) . . yes
 O4B C16B 1.41(2) . . yes
 O2 H21 0.92(11) . . no
 O4A H41 0.84 . . no
 O4B H161' 1.01 . . no
 O4B H161 0.70 . . no
 O4B H42 0.84 . . no
 O7 H31 0.85(12) . . no
 O7 H31' 0.58(14) . . no
 O9 H33 1.1(2) . . no
 O9 H33' 0.9(3) . . no
 O11 H35 1.2(2) . . no
 O11 H35' 1.0(2) . . no
 N1 C1 1.290(8) . . yes
 N1 N3 1.397(8) . . yes
 N2 C4 1.336(11) . . yes
 N2 C5 1.320(10) . . yes
 N3 C9 1.330(10) . . yes
 N4 C9 1.326(10) . . yes
 N5 N7 1.379(8) . . yes
 N5 C10 1.280(10) . . yes
 N6A C13A 1.338(19) . . yes
 N6A C14 1.361(15) . . yes
 N6A C13B 1.56(2) . . yes
 N6A N6B 0.68(2) . . yes
 N6B C13B 1.350(19) . . yes
 N6B C14 1.347(15) . . yes
 N6B C13A 1.578(18) . . yes
 N7 C18 1.320(9) . . yes
 N8 C18 1.341(10) . . yes
 N2 H22 0.70(12) . . no
 N4 H24' 0.75(12) . . no
 N4 H24 0.86(11) . . no
 N6A H61 0.88 . . no
 N6A H62 1.20 . . no
 N6B H62 0.88 . . no
 N6B H61 1.19 . . no
 N8 H28 0.93(11) . . no
 N8 H28' 0.81(11) . . no
 C1 C2 1.448(10) . . no
 C2 C6 1.415(9) . . no
 C2 C3 1.417(11) . . no
 C3 C4 1.384(12) . . no
 C3 C7 1.495(9) . . no
 C5 C6 1.414(10) . . no
 C5 C8 1.485(9) . . no
 C10 C11 1.456(12) . . no
 C11 C12B 1.430(18) . . no
 C11 C15 1.429(11) . . no

C11 C12A 1.464(16) . . no
 C12A C13B 1.64(2) . . no
 C12A C12B 0.85(2) . . no
 C12A C13A 1.38(2) . . no
 C12A C16B 1.79(2) . . no
 C12A C16A 1.46(2) . . no
 C12B C13A 1.64(2) . . no
 C12B C13B 1.37(2) . . no
 C12B C16B 1.509(19) . . no
 C12B C16A 1.75(2) . . no
 C13A C13B 0.95(2) . . no
 C14 C17 1.480(10) . . no
 C14 C15 1.413(11) . . no
 C16A C16B 1.10(3) . . no
 C1 H1 0.95 . . no
 C4 H4 0.95 . . no
 C7 H7 0.99 . . no
 C7 H7' 0.99 . . no
 C8 H8 0.98 . . no
 C8 H8' 0.98 . . no
 C8 H8" 0.98 . . no
 C10 H10 0.95 . . no
 C13A H132 1.42 . . no
 C13A H131 0.95 . . no
 C13B H131 1.44 . . no
 C13B H132 0.95 . . no
 C16A H161' 0.99 . . no
 C16A H161 0.99 . . no
 C16A H42 1.41 . . no
 C16B H162 0.99 . . no
 C16B H162' 0.99 . . no
 C16B H161' 0.55 . . no
 C17 H17 0.98 . . no
 C17 H17' 0.98 . . no
 C17 H17" 0.98 . . no

loop_
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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 S1 Fe S2 94.57(7) . . . yes
 S1 Fe O1 176.33(16) . . . yes
 S1 Fe O3 88.98(15) . . . yes
 S1 Fe N1 86.82(18) . . . yes
 S1 Fe N5 94.44(18) . . . yes
 S2 Fe O1 89.07(16) . . . yes
 S2 Fe O3 176.30(16) . . . yes
 S2 Fe N1 88.55(19) . . . yes
 S2 Fe N5 86.86(19) . . . yes
 O1 Fe O3 87.4(2) . . . yes
 O1 Fe N1 93.7(2) . . . yes
 O1 Fe N5 85.3(2) . . . yes
 O3 Fe N1 90.6(2) . . . yes
 O3 Fe N5 93.9(2) . . . yes
 N1 Fe N5 175.3(3) . . . yes
 Fe S1 C9 95.1(3) . . . yes

Fe S2 C18 94.6(3) . . . yes
 O5 S3 O6 109.1(3) 2_555 . 2_555 yes
 O6 S3 O6 110.4(3) . . 2_555 yes
 O5 S3 O6 109.0(3) 2_555 . . yes
 O5 S3 O6 109.1(3) . . . yes
 O5 S3 O5 110.1(3) . . 2_555 yes
 O5 S3 O6 109.0(3) . . 2_555 yes
 Fe O1 C6 125.5(4) . . . yes
 Fe O3 C15 125.9(5) . . . yes
 O4B O4A C16A 24.1(9) . . . yes
 C16A O4B C16B 50(2) . . . yes
 O4A O4B C16B 78.3(10) . . . yes
 O4A O4B C16A 57.9(19) . . . yes
 C7 O2 H21 100(7) . . . no
 C16A O4A H41 109 . . . no
 O4B O4A H41 117 . . . no
 C16B O4B H161' 19 . . . no
 C16A O4B H161' 68 . . . no
 C16A O4B H42 134 . . . no
 O4A O4B H161 107 . . . no
 O4A O4B H42 168 . . . no
 O4A O4B H161' 93 . . . no
 C16A O4B H161 92 . . . no
 H42 O4B H161 75 . . . no
 C16B O4B H161 132 . . . no
 H161' O4B H161 138 . . . no
 C16B O4B H42 110 . . . no
 H161' O4B H42 93 . . . no
 H31 O7 H31' 139(14) . . . no
 H33 O9 H33' 85(18) . . . no
 H35 O11 H35' 143(17) . . . no
 N3 N1 C1 114.3(5) . . . yes
 Fe N1 N3 120.4(4) . . . yes
 Fe N1 C1 125.3(5) . . . yes
 C4 N2 C5 125.2(7) . . . yes
 N1 N3 C9 113.7(5) . . . yes
 Fe N5 N7 120.2(4) . . . yes
 Fe N5 C10 125.7(5) . . . yes
 N7 N5 C10 113.8(5) . . . yes
 C13A N6A C13B 37.3(9) . . . yes
 C13A N6A C14 124.7(12) . . . yes
 C13B N6A C14 109.2(11) . . . yes
 N6B N6A C13B 60.1(15) . . . yes
 N6B N6A C14 74.2(16) . . . yes
 N6B N6A C13A 97.4(18) . . . yes
 N6A N6B C14 76.6(16) . . . yes
 C13A N6B C13B 36.7(9) . . . yes
 N6A N6B C13B 94.0(18) . . . yes
 C13B N6B C14 123.8(13) . . . yes
 C13A N6B C14 109.4(11) . . . yes
 N6A N6B C13A 57.2(15) . . . yes
 N5 N7 C18 113.6(5) . . . yes
 C5 N2 H22 131(9) . . . no
 C4 N2 H22 103(9) . . . no
 H24 N4 H24' 120(12) . . . no
 C9 N4 H24 111(8) . . . no
 C9 N4 H24' 113(8) . . . no
 C13B N6A H61 120 . . . no
 N6B N6A H62 46 . . . no
 C13A N6A H61 118 . . . no
 N6B N6A H61 99 . . . no

C14 N6A H61 118 . . . no
C14 N6A H62 97 . . . no
C13B N6A H62 88 . . . no
H61 N6A H62 53 . . . no
C13A N6A H62 116 . . . no
N6A N6B H62 100 . . . no
N6A N6B H61 47 . . . no
C13B N6B H61 114 . . . no
C13A N6B H61 86 . . . no
C13A N6B H62 120 . . . no
C14 N6B H62 118 . . . no
H61 N6B H62 53 . . . no
C13B N6B H62 118 . . . no
C14 N6B H61 99 . . . no
C18 N8 H28' 128(8) . . . no
H28 N8 H28' 105(11) . . . no
C18 N8 H28 127(8) . . . no
N1 C1 C2 124.8(6) . . . yes
C1 C2 C3 118.5(6) . . . no
C3 C2 C6 119.7(7) . . . no
C1 C2 C6 121.9(7) . . . no
C2 C3 C4 118.3(6) . . . no
C2 C3 C7 122.7(7) . . . no
C4 C3 C7 119.0(7) . . . no
N2 C4 C3 119.8(7) . . . yes
N2 C5 C6 118.8(6) . . . yes
C6 C5 C8 121.0(7) . . . no
N2 C5 C8 120.2(7) . . . yes
O1 C6 C5 116.3(6) . . . yes
C2 C6 C5 118.3(6) . . . no
O1 C6 C2 125.4(6) . . . yes
O2 C7 C3 111.1(6) . . . yes
S1 C9 N3 123.6(6) . . . yes
S1 C9 N4 118.5(6) . . . yes
N3 C9 N4 117.9(6) . . . yes
N5 C10 C11 126.5(6) . . . yes
C10 C11 C12B 116.4(9) . . . no
C12B C11 C15 119.1(9) . . . no
C12A C11 C12B 34.0(9) . . . no
C12A C11 C15 118.9(9) . . . no
C10 C11 C12A 115.7(8) . . . no
C10 C11 C15 122.2(7) . . . no
C11 C12A C16B 105.5(10) . . . no
C12B C12A C13A 92.3(17) . . . no
C12B C12A C13B 57.0(15) . . . no
C11 C12A C12B 70.8(14) . . . no
C11 C12A C13A 117.1(11) . . . no
C11 C12A C13B 101.3(10) . . . no
C12B C12A C16B 56.9(13) . . . no
C13A C12A C13B 35.3(9) . . . no
C13A C12A C16A 119.1(14) . . . no
C13A C12A C16B 114.2(12) . . . no
C13B C12A C16A 116.9(13) . . . no
C13B C12A C16B 91.5(10) . . . no
C16A C12A C16B 37.9(10) . . . no
C12B C12A C16A 94.8(16) . . . no
C11 C12A C16A 122.3(13) . . . no
C11 C12B C13B 117.8(12) . . . no
C11 C12B C16A 107.0(12) . . . no
C11 C12B C16B 124.5(14) . . . no
C12A C12B C13A 56.8(15) . . . no

C12A C12B C13B 92.0(18) . . . no
C11 C12B C12A 75.2(15) . . . no
C13A C12B C13B 35.2(10) . . . no
C13A C12B C16A 92.2(11) . . . no
C13A C12B C16B 115.8(12) . . . no
C13B C12B C16A 115.1(13) . . . no
C13B C12B C16B 117.0(14) . . . no
C16A C12B C16B 38.7(10) . . . no
C12A C12B C16A 56.4(14) . . . no
C12A C12B C16B 95.0(16) . . . no
C11 C12B C13A 103.8(11) . . . no
N6A C13A N6B 25.4(8) . . . yes
N6A C13A C13B 83.9(14) . . . yes
N6B C13A C12B 94.4(10) . . . yes
N6B C13A C13B 58.4(13) . . . yes
C12A C13A C12B 31.0(9) . . . no
N6A C13A C12A 120.3(13) . . . yes
N6A C13A C12B 111.3(11) . . . yes
C12B C13A C13B 56.7(14) . . . no
C12A C13A C13B 87.6(15) . . . no
N6B C13A C12A 114.6(12) . . . yes
N6A C13B C12B 114.7(14) . . . yes
N6A C13B N6B 26.0(8) . . . yes
N6B C13B C12A 112.4(13) . . . yes
N6B C13B C12B 120.4(15) . . . yes
N6A C13B C13A 58.8(13) . . . yes
C12A C13B C12B 31.1(9) . . . no
N6A C13B C12A 95.0(11) . . . yes
C12B C13B C13A 88.1(16) . . . no
C12A C13B C13A 57.1(13) . . . no
N6B C13B C13A 84.8(15) . . . yes
N6A C14 C15 118.5(8) . . . yes
N6A C14 C17 116.7(9) . . . yes
C15 C14 C17 122.9(7) . . . no
N6B C14 C17 116.5(8) . . . yes
N6A C14 N6B 29.2(8) . . . yes
N6B C14 C15 118.5(8) . . . yes
C11 C15 C14 117.1(7) . . . no
O3 C15 C14 117.5(6) . . . yes
O3 C15 C11 125.4(7) . . . yes
O4A C16A C12A 111.2(15) . . . yes
O4A C16A C12B 114.5(14) . . . yes
O4A C16A C16B 100.2(17) . . . yes
O4A C16A O4B 98(2) . . . yes
C12A C16A C16B 87.6(15) . . . no
C12B C16A C16B 58.8(12) . . . no
O4B C16A C16B 101(3) . . . yes
O4B C16A C12A 147(3) . . . yes
O4B C16A C12B 144(3) . . . yes
C12A C16A C12B 28.8(9) . . . no
O4B C16B C12A 79.6(11) . . . yes
O4B C16B C12B 106.3(13) . . . yes
C12A C16B C12B 28.0(8) . . . no
C12A C16B C16A 54.5(12) . . . no
C12B C16B C16A 82.5(15) . . . no
O4B C16B C16A 28.4(12) . . . yes
S2 C18 N8 117.9(6) . . . yes
N7 C18 N8 118.2(6) . . . yes
S2 C18 N7 123.9(6) . . . yes
C2 C1 H1 118 . . . no
N1 C1 H1 117 . . . no

N2 C4 H4 120 . . . no
C3 C4 H4 120 . . . no
O2 C7 H7' 109 . . . no
C3 C7 H7 109 . . . no
O2 C7 H7 109 . . . no
H7 C7 H7' 108 . . . no
C3 C7 H7' 109 . . . no
C5 C8 H8' 109 . . . no
C5 C8 H8" 109 . . . no
H8 C8 H8" 110 . . . no
H8' C8 H8" 110 . . . no
H8 C8 H8' 109 . . . no
C5 C8 H8 109 . . . no
N5 C10 H10 117 . . . no
C11 C10 H10 117 . . . no
C12B C13A H132 82 . . . no
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C12B C13B H131 108 . . . no
C12B C13B H132 120 . . . no
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C13A C13B H132 97 . . . no
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C12A C13B H131 82 . . . no
O4A C16A H161 109 . . . no
O4B C16A H161' 72 . . . no
O4B C16A H42 25 . . . no
O4B C16A H161 45 . . . no
C12A C16A H161' 109 . . . no
C12A C16A H42 124 . . . no
O4A C16A H161' 109 . . . no
O4A C16A H42 123 . . . no
H42 C16A H161 42 . . . no
C12B C16A H161' 82 . . . no
C12B C16A H42 120 . . . no
C12B C16A H161 128 . . . no
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C12A C16A H161 109 . . . no
H161' C16A H161 108 . . . no
H161' C16A H42 66 . . . no
O4B C16B H162' 111 . . . no
O4B C16B H162 111 . . . no
C12A C16B H162' 114 . . . no
C12A C16B H162 129 . . . no
C12A C16B H161' 106 . . . no
O4B C16B H161' 36 . . . no

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C12B C16B H162' 110 . . . no
C12B C16B H162 110 . . . no
C16A C16B H161' 64 . . . no
C16A C16B H162' 106 . . . no
C16A C16B H162 135 . . . no
H161' C16B H162' 119 . . . no
C12B C16B H161' 125 . . . no
H162' C16B H162 109 . . . no
H161' C16B H162 75 . . . no
C14 C17 H17' 109 . . . no
C14 C17 H17" 110 . . . no
H17 C17 H17" 109 . . . no
H17' C17 H17" 109 . . . no
H17 C17 H17' 109 . . . no
C14 C17 H17 110 . . . no

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_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
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S2 Fe S1 C9 93.4(3) . . . . no
O3 Fe S1 C9 -85.6(3) . . . . no
N1 Fe S1 C9 5.1(3) . . . . no
N5 Fe S1 C9 -179.4(3) . . . . no
S1 Fe S2 C18 101.1(3) . . . . no
O1 Fe S2 C18 -78.5(3) . . . . no
N1 Fe S2 C18 -172.3(3) . . . . no
N5 Fe S2 C18 6.9(3) . . . . no
S2 Fe O1 C6 -67.8(5) . . . . no
O3 Fe O1 C6 111.1(5) . . . . no
N1 Fe O1 C6 20.7(5) . . . . no
N5 Fe O1 C6 -154.8(5) . . . . no
S1 Fe O3 C15 -88.0(6) . . . . no
O1 Fe O3 C15 91.5(6) . . . . no
N1 Fe O3 C15 -174.8(6) . . . . no
N5 Fe O3 C15 6.4(6) . . . . no
S1 Fe N1 N3 -6.5(5) . . . . no
S1 Fe N1 C1 170.2(6) . . . . no
S2 Fe N1 N3 -101.2(5) . . . . no
S2 Fe N1 C1 75.5(6) . . . . no
O1 Fe N1 N3 169.9(5) . . . . no
O1 Fe N1 C1 -13.5(6) . . . . no
O3 Fe N1 N3 82.4(5) . . . . no
O3 Fe N1 C1 -100.9(6) . . . . no
S1 Fe N5 N7 -100.5(5) . . . . no
S1 Fe N5 C10 85.4(6) . . . . no
S2 Fe N5 N7 -6.1(5) . . . . no
S2 Fe N5 C10 179.8(7) . . . . no
O1 Fe N5 N7 83.2(5) . . . . no
O1 Fe N5 C10 -90.9(7) . . . . no
O3 Fe N5 N7 170.3(5) . . . . no
O3 Fe N5 C10 -3.9(7) . . . . no
Fe S1 C9 N3 -4.8(7) . . . . no
Fe S1 C9 N4 178.8(6) . . . . no

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Fe S2 C18 N7 -9.4(7) no
 Fe S2 C18 N8 171.7(6) no
 Fe O1 C6 C2 -17.6(9) no
 Fe O1 C6 C5 162.2(4) no
 Fe O3 C15 C11 -4.1(11) no
 Fe O3 C15 C14 174.8(5) no
 C16A O4A O4B C16B 50(2) no
 O4B O4A C16A C12A 166(3) no
 O4B O4A C16A C12B -163(3) no
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O3 H28 2.06(11) . 6_555 no
O3 H17" 2.67 . . no
O4A H131 2.27 . . no
O4A H7' 2.82 . 6_555 no
O4A H17 2.78 . 4_565 no
O4A H132 2.67 . . no
O4B H8 2.89 . 7_556 no
O4B H10 2.38 . . no
O5 H8 2.64 . 2_555 no
O5 H22 2.14(12) . 2_555 no
O5 H42 2.84 . 8_454 no
O5 H31 1.93(12) . 2_555 no
O6 H62 1.83 . 6_545 no
O6 H41 2.32 . 8_454 no
O6 H4 2.86 . . no
O6 H61 2.11 . 6_545 no
O6 H162' 2.70 . 8_454 no
O6 H22 2.71(12) . . no
O7 H33 2.6(2) . . no
O7 H33' 2.5(2) . . no
O7 H24' 2.26(12) . 6_555 no
O7 H162 2.88 . 7_556 no
O8 H21 1.86(12) . 4_565 no
O9 H4 2.65 . 4_565 no
O9 H31' 2.46(13) . . no
O10 H21 2.19(12) . 4_565 no
O10 H17" 2.89 . 6_555 no
O11 H33 2.7(2) . . no
O11 H31 2.88(12) . . no
O11 H31' 2.18(13) . . no
O12 H7' 2.86 . 6_555 no
O12 H161 2.25 . . no
O12 H1 2.89 . 6_555 no
N1 O3 2.764(7) . . no
N1 C9 2.283(10) . . no
N1 O1 2.781(7) . . no
N1 S2 2.891(6) . . no
N1 C6 2.938(8) . . no
N1 S1 2.859(6) . . no
N2 O5 2.780(8) . 2_555 no
N2 S3 3.525(6) . . no
N2 S3 3.525(6) . . no
N2 O6 3.125(8) . . no
N3 S1 2.712(5) . . no
N3 N8 3.027(8) . 4_554 no
N4 O7 2.962(11) . 6_545 no
N4 N7 2.982(8) . 4_554 no
N5 S1 3.052(6) . . no
N5 S2 2.848(6) . . no
N5 C18 2.258(10) . . no

N5 O1 2.583(7) . . no
 N5 O3 2.842(7) . . no
 N5 C15 2.985(10) . . no
 N6A C4 3.277(16) . 6_555 no
 N6A O6 2.807(15) . 6_555 no
 N6A C3 3.428(16) . 6_555 no
 N6B O6 2.661(15) . 6_555 no
 N7 N4 2.982(8) . 4_555 no
 N7 S2 2.702(5) . . no
 N7 O1 3.241(7) . . no
 N8 O3 2.966(8) . 6_545 no
 N8 N3 3.027(8) . 4_555 no
 N8 C17 3.369(10) . 6_545 no
 N8 C6 3.255(9) . 6_545 no
 N8 C2 3.097(9) . 6_545 no
 N8 C1 3.087(9) . 6_545 no
 N1 H28 2.71(11) . 6_555 no
 N2 H61 2.69 . 6_545 no
 N3 H28' 2.25(12) . 4_554 no
 N4 H7 2.87 . 7_555 no
 N7 H24 2.13(12) . 4_555 no
 N8 H17' 2.64 . 6_545 no
 C1 N8 3.087(9) . 6_555 no
 C1 O12 3.18(4) . 6_545 no
 C2 S2 3.575(7) . . no
 C2 N8 3.097(9) . 6_555 no
 C3 C13A 3.350(16) . 6_545 no
 C3 N6A 3.428(16) . 6_545 no
 C4 O6 3.155(10) . . no
 C4 C13A 3.518(16) . 6_545 no
 C4 N6A 3.277(16) . 6_545 no
 C5 S2 3.576(7) . 6_555 no
 C6 N8 3.255(9) . 6_555 no
 C6 S2 3.464(6) . 6_555 no
 C6 C18 3.473(10) . 6_555 no
 C7 C13A 3.449(16) . 6_545 no
 C8 S1 3.647(8) . 6_555 no
 C8 S2 3.684(8) . 6_555 no
 C10 O4B 2.997(15) . . no
 C12A O12 2.89(5) . . no
 C13A C3 3.350(16) . 6_555 no
 C13A C4 3.518(16) . 6_555 no
 C13A C7 3.449(16) . 6_555 no
 C13B O6 3.270(17) . 6_555 no
 C14 O10 3.157(14) . 6_545 no
 C15 O10 3.297(14) . 6_545 no
 C15 S2 3.685(8) . 6_555 no
 C16A O12 2.89(5) . . no
 C16B O2 3.318(18) . 8_555 no
 C16B O6 3.342(15) . 8_555 no
 C17 O10 3.407(14) . 6_545 no
 C17 O8 3.254(14) . 6_545 no
 C17 N8 3.369(10) . 6_555 no
 C18 C6 3.473(10) . 6_545 no
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 C1 H28 2.81(11) . 6_555 no
 C1 H7' 2.83 . . no
 C1 H28' 2.99(11) . 6_555 no
 C2 H28 3.05(11) . 6_555 no
 C3 H131 3.08 . 6_545 no
 C4 H61 2.66 . 6_545 no

C6 H28 3.08(11) . 6_555 no
C7 H131 2.93 . 6_545 no
C7 H17" 2.88 . 7_555 no
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C9 H7 2.87 . 7_555 no
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C10 H162 2.87 . . no
C10 H161' 2.84 . . no
C10 H161 2.81 . . no
C13A H7' 3.02 . 6_555 no
C13A H41 2.75 . . no
C13B H41 2.80 . . no
C15 H28 2.97(11) . 6_555 no
C16A H10 2.48 . . no
C16B H10 2.56 . . no
C17 H28 2.96(11) . 6_555 no
C18 H17' 2.97 . 6_545 no
C18 H24 2.97(12) . 4_555 no
H1 C7 2.53 . . no
H1 O12 2.89 . 6_545 no
H1 H7' 2.34 . . no
H1 H28' 2.56 . 4_554 no
H1 H7 2.32 . . no
H161' C10 2.84 . . no
H161' H10 2.30 . . no
H162' H132 2.25 . . no
H162' H41 1.25 . . no
H162' O6 2.70 . 8_555 no
H162' O2 2.78 . 8_555 no
H4 O6 2.86 . . no
H4 O9 2.65 . 4_564 no
H4 O2 2.30 . . no
H7 C9 2.87 . 7_555 no
H7 N4 2.87 . 7_555 no
H7 H1 2.32 . . no
H7 C1 2.88 . . no
H7' H17" 2.32 . 7_555 no
H7' O12 2.86 . 6_545 no
H7' O4A 2.82 . 6_545 no
H7' H1 2.34 . . no
H7' C1 2.83 . . no
H7' C13A 3.02 . 6_545 no
H8 H42 2.31 . 7_556 no
H8 O4B 2.89 . 7_556 no
H8 H22 2.42 . . no
H8 O5 2.64 . 2_555 no
H8' O1 2.77 . . no
H8' S1 3.19 . 6_555 no
H8' S2 2.94 . 6_555 no
H8" O1 2.67 . . no
H10 O4B 2.38 . . no
H10 H162 2.40 . . no
H10 H161 2.26 . . no
H10 H161' 2.30 . . no
H10 H42 1.87 . . no
H10 C16B 2.56 . . no
H10 C16A 2.48 . . no
H17 H62 2.15 . . no
H17 O4A 2.78 . 4_564 no
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H17" H7' 2.32 . 7_555 no
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H21 O10 2.19(11) . 4_564 no
H22 O5 2.14(12) . 2_555 no
H22 O6 2.71(12) . . no
H22 S3 2.91(12) . . no
H22 H8 2.42 . . no
H22 S3 2.91(12) . . no
H24 C18 2.97(12) . 4_554 no
H24 N7 2.13(12) . 4_554 no
H24' H31 2.55(16) . 6_545 no
H24' O7 2.26(11) . 6_545 no
H24' H31' 2.59(18) . 6_545 no
H28 C15 2.97(12) . 6_545 no
H28 O3 2.06(12) . 6_545 no
H28 H17' 2.45 . 6_545 no
H28 C17 2.96(11) . 6_545 no
H28 C1 2.81(11) . 6_545 no
H28 Fe 3.10(11) . 6_545 no
H28 N1 2.71(11) . 6_545 no
H28 O1 2.90(11) . 6_545 no
H28 C6 3.08(11) . 6_545 no
H28 C2 3.05(11) . 6_545 no
H28' N3 2.25(12) . 4_555 no
H28' H1 2.56 . 4_555 no
H28' C1 2.99(11) . 6_545 no
H31 S3 2.92(12) . . no
H31 H35 1.8(2) . . no
H31 O11 2.88(12) . . no
H31 O5 1.93(12) . 2_555 no
H31 H24' 2.55(16) . 6_555 no
H31 S3 2.92(12) . . no
H31' H24' 2.59(18) . 6_555 no
H31' H33' 2.2(3) . . no
H31' H35 1.3(3) . . no
H31' H33 2.2(3) . . no
H31' O11 2.18(13) . . no
H31' O9 2.46(13) . . no
H33 O7 2.6(2) . . no
H33 H21 2.5(2) . 4_565 no
H33 O11 2.7(2) . . no
H33 H31' 2.2(3) . . no
H33 O2 2.1(2) . 4_565 no
H33 H35 2.5(3) . . no
H33' O7 2.5(2) . . no
H33' H31' 2.2(3) . . no
H35 H33 2.5(3) . . no
H35 H31 1.8(2) . . no
H35 H31' 1.3(3) . . no
H35 O7 1.5(2) . . no
H41 C13A 2.75 . . no
H41 H131 2.26 . . no
H41 H132 2.32 . . no
H41 O6 2.32 . 8_555 no
H41 H162' 1.25 . . no

H41 C13B 2.80 . . no
 H42 H10 1.87 . . no
 H42 C10 2.67 . . no
 H42 O5 2.84 . 8_555 no
 H42 H8 2.31 . 7_556 no
 H61 N2 2.69 . 6_555 no
 H61 O6 2.11 . 6_555 no
 H61 H17 2.23 . . no
 H61 C4 2.66 . 6_555 no
 H62 H17 2.15 . . no
 H62 S3 3.03 . 5_555 no
 H62 O6 1.83 . 6_555 no
 H62 S3 3.03 . 6_555 no
 H131 H41 2.26 . . no
 H131 O4A 2.27 . . no
 H131 C7 2.93 . 6_555 no
 H131 O2 2.77 . 6_555 no
 H131 C3 3.08 . 6_555 no
 H132 H41 2.32 . . no
 H132 O4A 2.67 . . no
 H132 H162' 2.25 . . no
 H161 H10 2.26 . . no
 H161 C10 2.81 . . no
 H161 O12 2.25 . . no
 H162 H10 2.40 . . no
 H162 O7 2.88 . 7_556 no
 H162 C10 2.87 . . no

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 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
 _geom_hbond_publ_flag

#

#D H A D - H H...A D...A D - H...A symm(A)

#

O2 H21 O8 0.92(11) 1.86(12) 2.743(13) 160(11) 4_564 yes
 O2 H21 O10 0.92(11) 2.19(11) 2.888(13) 131(9) 4_564 yes
 N2 H22 O5 0.70(12) 2.14(12) 2.780(8) 152(12) 2_555 yes
 N4 H24 N7 0.86(11) 2.13(12) 2.982(8) 170(8) 4_554 yes
 N4 H24' O7 0.75(12) 2.26(11) 2.962(11) 156(11) 6_545 yes
 N8 H28 O3 0.93(11) 2.06(12) 2.966(8) 163(10) 6_545 yes
 N8 H28' N3 0.81(11) 2.25(12) 3.027(8) 162(10) 4_555 yes
 O7 H31 O5 0.85(12) 1.93(12) 2.777(11) 171(15) 2_555 yes
 O7 H31' O9 0.58(14) 2.46(13) 2.907(19) 136(14) . yes
 O7 H31' O11 0.58(14) 2.18(13) 2.502(16) 117(15) . yes
 O9 H33 O2 1.1(2) 2.1(2) 2.754(18) 113(14) 4_565 yes
 O9 H33' O7 0.9(3) 2.5(2) 2.907(19) 110(17) . yes
 O11 H35 O7 1.2(2) 1.5(2) 2.502(16) 144(18) . yes
 O4A H41 O6 0.8400 2.3200 2.639(12) 103 8_555 yes
 N6A H61 O6 0.8800 2.1100 2.807(15) 135 6_555 yes
 N6A H62 O6 1.2000 1.8300 2.807(15) 135 6_555 yes
 O4B H161 O12 0.7000 2.2500 2.92(5) 161 . yes
 C4 H4 O2 0.9500 2.3000 2.675(10) 103 . yes
 C10 H10 O4B 0.9500 2.3800 2.997(15) 122 . yes
 C13A H131 O4A 0.9500 2.2700 2.650(17) 103 . yes

```

# Loop Mechanism for Extra Tables(s)

#loop_
#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
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#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'

#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
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# ? ? ?

#
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# ? ? ?

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

===END of Crystallographic Information File

# Attachment 'q1138.cif'

# CIF-file generated for C18H28FeN9O10S2 P21/c q1138

data_q1138

```

_database_code_depnum_ccdc_archive 'CCDC 732215'

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety 'C18 H22 Fe N8 O4 S2, N O3, 3(H2 O)'

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)₃, (C6 N6 Cr 3-)₂, 2(H2 O)'

_chemical_formula_structural ?

_chemical_formula_sum 'C18 H28 Fe N9 O10 S2'

_chemical_formula_iupac ?

_chemical_formula_weight 650.45

_chemical_compound_source 'see text'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

Fe Fe 0.3463 0.8444 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

6. CRYSTAL DATA

_symmetry_cell_setting Monoclinic

_symmetry_space_group_name_Hall '-P 2ybc'

_symmetry_space_group_name_H-M 'P 21/c'

_symmetry_Int_Tables_number 14

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

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

3 -x,-y,-z

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

_cell_length_a 9.3807(6)

_cell_length_b 19.045(1)

_cell_length_c 15.885(1)

_cell_angle_alpha 90

_cell_angle_beta 107.057(1)

_cell_angle_gamma 90

_cell_volume 2713.1(3)

_cell_formula_units_Z 4

_cell_measurement_temperature 100(1)

_cell_measurement_reflns_used 6065

_cell_measurement_theta_min 2.51

_cell_measurement_theta_max 29.60

_cell_special_details

```
;  
The final unit cell was obtained from the xyz centroids of  
6065 reflections after integration using the SAINTPLUS  
software package (Bruker, 2000).
```

Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

```
;
```

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_exptl_crystal_description      block  
_exptl_crystal_colour          red  
_exptl_crystal_size_max        0.47  
_exptl_crystal_size_mid        0.39  
_exptl_crystal_size_min        0.28  
_exptl_crystal_size_rad        ?  
_exptl_crystal_density_meas    ?  
_exptl_crystal_density_diffn   1.592  
_exptl_crystal_density_method  'not measured'  
_exptl_crystal_F_000           1348  
_exptl_absorpt_coefficient_mu   0.778  
_exptl_absorpt_correction_type  Multi-Scan  
_exptl_absorpt_process_details  '(SADABS, Sheldrick, Bruker, 2001))'  
_exptl_absorpt_correction_T_min 0.7164  
_exptl_absorpt_correction_T_max 0.8115
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```
#=====
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7. EXPERIMENTAL DATA

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;  
;  
_diffrn_ambient_temperature    100(1)  
_diffrn_radiation_wavelength   0.71073  
_diffrn_radiation_type         MoK\alpha  
_diffrn_radiation_source       'fine focus sealed Siemens Mo tube '  
_diffrn_radiation_monochromator 'parallel mounted graphite'  
_diffrn_radiation_detector  
;  
CCD area-detector  
;  
_diffrn_measurement_device_type  
;  
Bruker Smart Apex; CCD area detector  
;  
_diffrn_measurement_method      '\f and \w scans'  
_diffrn_special_details  
;  
Crystal into the cold nitrogen stream of the low-temperature unit  
(KRYOFLEX, (Bruker, 2000)).  
;  
_diffrn_detector_area_resol_mean 66.06  
  
_diffrn_standards_number        0  
_diffrn_standards_interval_count ?  
_diffrn_standards_interval_time ?  
_diffrn_standards_decay_%       0  
  
loop_  
_diffrn_standard_refl_index_h
```

```

_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_refl_number      24468
_diffrn_refl_av_R_equivalents 0.0225
_diffrn_refl_av_sigmaI/netI 0.0239
_diffrn_refl_limit_h_min -12
_diffrn_refl_limit_h_max 12
_diffrn_refl_limit_k_min -25
_diffrn_refl_limit_k_max 25
_diffrn_refl_limit_l_min -21
_diffrn_refl_limit_l_max 21
_diffrn_refl_theta_min 2.51
_diffrn_refl_theta_max 28.28
_diffrn_measured_fraction_theta_max 0.998
_diffrn_refl_theta_full 25.00
_diffrn_measured_fraction_theta_full 0.999

_diffrn_refl_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_refl_number_total      6727
_refl_number_gt         6032
_refl_threshold_expression I>2\sigma(I)

_computing_data_collection 'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement 'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction 'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_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
 $F^2 > 2\sigma(F^2)$  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^)+(0.0347P)^2^+1.4799P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment refall
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration .
_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 6727
_refine_ls_number_parameters 473
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0349
_refine_ls_R_factor_gt 0.0302
_refine_ls_wR_factor_ref 0.0745
_refine_ls_wR_factor_gt 0.0724
_refine_ls_goodness_of_fit_ref 1.060
_refine_ls_restrained_S_all 1.060
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

_refine_diff_density_max 0.444
_refine_diff_density_min -0.272
_refine_diff_density_rms 0.062

_vrn_publ_code_frame_time_sec 10.0
_vrn_publ_code_meas_time_hour 9.7

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#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_U_iso_or_equiv
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Fe Fe Uani 0.98803(2) 0.25170(1) 0.18570(1) 1.000 0.0100(1) . .
S1 S Uani 1.09871(4) 0.18742(2) 0.30702(2) 1.000 0.0142(1) . .
S2 S Uani 0.88259(4) 0.31746(2) 0.26884(2) 1.000 0.0136(1) . .
O1 O Uani 0.89531(11) 0.30792(5) 0.08375(7) 1.000 0.0141(3) . .
O2 O Uani 1.42827(13) 0.38475(6) 0.05258(7) 1.000 0.0190(3) . .
O3 O Uani 1.07717(11) 0.19494(5) 0.11573(7) 1.000 0.0148(3) . .
O4 O Uani 0.54600(13) 0.10919(7) -0.09530(8) 1.000 0.0236(4) . .
N1 N Uani 1.17375(13) 0.30357(6) 0.21356(8) 1.000 0.0118(3) . .
N2 N Uani 0.93927(14) 0.42458(6) -0.07994(8) 1.000 0.0133(3) . .
N3 N Uani 1.28928(14) 0.29003(7) 0.28983(8) 1.000 0.0155(3) . .
N4 N Uani 1.37424(16) 0.21804(8) 0.40794(9) 1.000 0.0199(4) . .

```


N5	N	Uani	0.80185(14)	0.19968(6)	0.15296(8)	1.000	0.0121(3)	. .
N6	N	Uani	1.02940(15)	0.07752(7)	-0.06176(8)	1.000	0.0148(4)	. .
N7	N	Uani	0.68838(14)	0.21461(7)	0.19077(8)	1.000	0.0148(3)	. .
N8	N	Uani	0.61134(16)	0.28997(8)	0.28036(10)	1.000	0.0198(4)	. .
C1	C	Uani	1.21122(16)	0.34880(7)	0.16226(9)	1.000	0.0127(4)	. .
C2	C	Uani	1.11552(16)	0.37259(7)	0.07801(9)	1.000	0.0119(4)	. .
C3	C	Uani	1.17463(16)	0.41996(7)	0.02720(9)	1.000	0.0126(4)	. .
C4	C	Uani	1.08416(17)	0.44481(8)	-0.05149(10)	1.000	0.0141(4)	. .
C5	C	Uani	0.87648(16)	0.37950(7)	-0.03667(9)	1.000	0.0126(4)	. .
C6	C	Uani	0.96413(16)	0.35123(7)	0.04519(9)	1.000	0.0125(4)	. .
C7	C	Uani	1.33568(17)	0.44380(8)	0.05571(10)	1.000	0.0147(4)	. .
C8	C	Uani	0.71621(18)	0.35974(9)	-0.07459(10)	1.000	0.0174(4)	. .
C9	C	Uani	1.26384(16)	0.23597(8)	0.33531(9)	1.000	0.0142(4)	. .
C10	C	Uani	0.76336(17)	0.15258(7)	0.09073(9)	1.000	0.0138(4)	. .
C11	C	Uani	0.85815(16)	0.12727(7)	0.03954(9)	1.000	0.0127(4)	. .
C12	C	Uani	0.79935(17)	0.07771(7)	-0.02934(9)	1.000	0.0142(4)	. .
C13	C	Uani	0.88733(18)	0.05363(8)	-0.07890(10)	1.000	0.0159(4)	. .
C14	C	Uani	1.09207(17)	0.12433(7)	0.00086(9)	1.000	0.0140(4)	. .
C15	C	Uani	1.00780(16)	0.15068(7)	0.05546(9)	1.000	0.0127(4)	. .
C16	C	Uani	0.63978(18)	0.05216(8)	-0.05302(10)	1.000	0.0184(4)	. .
C17	C	Uani	1.24704(18)	0.14924(9)	0.01220(11)	1.000	0.0202(5)	. .
C18	C	Uani	0.71645(16)	0.26990(8)	0.24344(9)	1.000	0.0140(4)	. .
O5	O	Uani	0.25185(13)	0.46473(6)	0.35604(7)	1.000	0.0211(3)	. .
O6	O	Uani	0.24887(12)	0.51108(6)	0.22997(7)	1.000	0.0189(3)	. .
O7	O	Uani	0.04134(13)	0.49361(7)	0.26157(8)	1.000	0.0305(4)	. .
N9	N	Uani	0.17861(14)	0.48982(7)	0.28235(8)	1.000	0.0155(4)	. .
O8	O	Uani	0.50557(14)	0.09578(7)	0.19389(8)	1.000	0.0226(3)	. .
O9	O	Uani	0.70368(13)	0.05885(7)	0.63047(8)	1.000	0.0206(3)	. .
O10	O	Uani	0.27212(15)	0.04920(6)	0.24894(9)	1.000	0.0243(4)	. .
H1	H	Uiso	1.310(2)	0.3666(9)	0.1820(11)	1.000	0.010(4)	. .
H4	H	Uiso	1.1154(19)	0.4744(9)	-0.0860(11)	1.000	0.012(4)	. .
H7	H	Uiso	1.3609(19)	0.4624(9)	0.1123(12)	1.000	0.013(4)	. .
H7'	H	Uiso	1.3498(19)	0.4801(9)	0.0154(11)	1.000	0.013(4)	. .
H8	H	Uiso	0.670(2)	0.3821(11)	-0.1273(14)	1.000	0.027(5)	. .
H8'	H	Uiso	0.665(2)	0.3712(11)	-0.0346(14)	1.000	0.031(5)	. .
H10	H	Uiso	0.666(2)	0.1347(9)	0.0773(11)	1.000	0.015(4)	. .
H13	H	Uiso	0.8564(19)	0.0229(9)	-0.1246(12)	1.000	0.012(4)	. .
H16	H	Uiso	0.615(2)	0.0361(10)	-0.0004(13)	1.000	0.023(5)	. .
H16'	H	Uiso	0.626(2)	0.0129(10)	-0.0925(12)	1.000	0.016(4)	. .
H17	H	Uiso	1.249(2)	0.2012(11)	0.0188(14)	1.000	0.031(5)	. .
H17'	H	Uiso	1.276(2)	0.1370(12)	-0.0346(15)	1.000	0.036(6)	. .
H17''	H	Uiso	1.312(2)	0.1282(11)	0.0614(15)	1.000	0.032(6)	. .
H18''	H	Uiso	0.710(3)	0.3076(12)	-0.0808(15)	1.000	0.041(6)	. .
H22	H	Uiso	1.515(2)	0.3984(12)	0.0750(14)	1.000	0.030(6)	. .
H24	H	Uiso	0.461(3)	0.0940(12)	-0.1159(15)	1.000	0.037(6)	. .
H32	H	Uiso	0.878(2)	0.4430(10)	-0.1300(14)	1.000	0.027(5)	. .
H34	H	Uiso	1.367(2)	0.1854(11)	0.4431(14)	1.000	0.028(5)	. .
H34'	H	Uiso	1.444(3)	0.2455(11)	0.4224(14)	1.000	0.031(6)	. .
H36	H	Uiso	1.081(2)	0.0634(11)	-0.0917(14)	1.000	0.027(5)	. .
H38	H	Uiso	0.622(2)	0.3256(12)	0.3146(14)	1.000	0.030(5)	. .
H38'	H	Uiso	0.526(2)	0.2718(10)	0.2640(13)	1.000	0.020(5)	. .
H28	H	Uiso	0.553(3)	0.1360(15)	0.1971(17)	1.000	0.055(8)	. .
H28'	H	Uiso	0.574(3)	0.0662(13)	0.2139(16)	1.000	0.042(7)	. .
H29	H	Uiso	0.704(2)	0.0301(12)	0.6648(14)	1.000	0.028(6)	. .
H29'	H	Uiso	0.759(3)	0.0898(13)	0.6586(16)	1.000	0.041(7)	. .
H210	H	Uiso	0.346(2)	0.0676(11)	0.2394(14)	1.000	0.029(6)	. .
H211	H	Uiso	0.216(3)	0.0802(13)	0.2567(15)	1.000	0.040(7)	. .

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_atom_site_aniso_label

_atom_site_aniso_U_11

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Fe 0.0091(1) 0.0105(1) 0.0106(1) 0.0001(1) 0.0032(1) -0.0010(1)
S1 0.0126(2) 0.0141(2) 0.0158(2) 0.0038(1) 0.0040(1) 0.0000(1)
S2 0.0121(2) 0.0137(2) 0.0156(2) -0.0028(1) 0.0047(1) -0.0008(1)
O1 0.0106(5) 0.0174(5) 0.0131(5) 0.0036(4) 0.0016(4) -0.0029(4)
O2 0.0114(5) 0.0223(5) 0.0227(5) -0.0059(5) 0.0043(4) 0.0000(4)
O3 0.0116(5) 0.0179(5) 0.0154(5) -0.0056(4) 0.0048(4) -0.0022(4)
O4 0.0123(6) 0.0334(7) 0.0225(6) 0.0052(5) 0.0009(5) -0.0037(5)
N1 0.0094(6) 0.0136(5) 0.0118(5) -0.0007(4) 0.0021(4) 0.0004(4)
N2 0.0161(6) 0.0139(6) 0.0103(5) 0.0017(5) 0.0045(5) 0.0018(5)
N3 0.0106(6) 0.0204(6) 0.0132(6) 0.0031(5) 0.0001(5) -0.0015(5)
N4 0.0133(7) 0.0258(7) 0.0185(6) 0.0085(6) 0.0012(5) 0.0003(6)
N5 0.0114(6) 0.0127(5) 0.0131(5) 0.0023(4) 0.0049(5) -0.0001(4)
N6 0.0179(7) 0.0157(6) 0.0118(6) 0.0000(5) 0.0058(5) 0.0036(5)
N7 0.0117(6) 0.0165(6) 0.0187(6) -0.0011(5) 0.0084(5) -0.0015(5)
N8 0.0152(7) 0.0218(7) 0.0252(7) -0.0044(6) 0.0104(6) -0.0013(6)
C1 0.0098(7) 0.0139(6) 0.0137(6) -0.0007(5) 0.0025(5) -0.0025(5)
C2 0.0120(7) 0.0118(6) 0.0119(6) -0.0002(5) 0.0037(5) -0.0003(5)
C3 0.0132(7) 0.0123(6) 0.0136(6) -0.0017(5) 0.0061(5) -0.0010(5)
C4 0.0161(7) 0.0135(7) 0.0146(7) 0.0015(5) 0.0076(6) -0.0002(5)
C5 0.0133(7) 0.0133(6) 0.0113(6) -0.0013(5) 0.0040(5) 0.0003(5)
C6 0.0125(7) 0.0122(6) 0.0131(6) -0.0002(5) 0.0043(5) 0.0001(5)
C7 0.0137(7) 0.0155(7) 0.0159(7) -0.0009(6) 0.0058(6) -0.0032(5)
C8 0.0146(7) 0.0219(8) 0.0140(7) 0.0033(6) 0.0018(6) -0.0017(6)
C9 0.0122(7) 0.0177(7) 0.0140(6) 0.0007(5) 0.0058(5) 0.0017(5)
C10 0.0108(7) 0.0147(7) 0.0156(7) 0.0001(5) 0.0036(5) -0.0029(5)
C11 0.0140(7) 0.0124(6) 0.0115(6) 0.0009(5) 0.0033(5) -0.0003(5)
C12 0.0160(7) 0.0127(6) 0.0125(6) 0.0014(5) 0.0019(5) -0.0017(5)
C13 0.0210(8) 0.0136(7) 0.0117(6) -0.0002(5) 0.0027(6) -0.0008(6)
C14 0.0155(7) 0.0138(6) 0.0123(6) 0.0017(5) 0.0037(5) 0.0022(5)
C15 0.0120(7) 0.0138(6) 0.0119(6) 0.0018(5) 0.0030(5) 0.0015(5)
C16 0.0188(8) 0.0197(7) 0.0159(7) -0.0023(6) 0.0041(6) -0.0067(6)
C17 0.0159(8) 0.0279(9) 0.0187(7) -0.0047(7) 0.0079(6) -0.0005(7)
C18 0.0127(7) 0.0151(6) 0.0148(6) 0.0023(5) 0.0048(5) 0.0003(5)
O5 0.0202(6) 0.0279(6) 0.0150(5) 0.0084(5) 0.0047(4) 0.0030(5)
O6 0.0195(6) 0.0246(6) 0.0140(5) 0.0037(4) 0.0070(4) -0.0023(4)
O7 0.0138(6) 0.0476(8) 0.0293(7) 0.0137(6) 0.0052(5) 0.0026(5)
N9 0.0170(7) 0.0155(6) 0.0150(6) 0.0019(5) 0.0062(5) 0.0003(5)
O8 0.0160(6) 0.0209(6) 0.0298(6) 0.0028(5) 0.0048(5) -0.0024(5)
O9 0.0175(6) 0.0192(6) 0.0232(6) -0.0033(5) 0.0031(5) -0.0002(5)
O10 0.0221(6) 0.0197(6) 0.0346(7) -0.0031(5) 0.0136(5) -0.0016(5)

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``` # 10. MOLECULAR GEOMETRY ```

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_geom_special_details
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Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles
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loop_
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Fe S1 2.2620(4) . . yes
Fe S2 2.2489(4) . . yes
Fe O1 1.9234(11) . . yes
Fe O3 1.9101(11) . . yes
Fe N1 1.9377(13) . . yes
Fe N5 1.9415(13) . . yes
S1 C9 1.7459(16) . . yes
S2 C18 1.7445(16) . . yes
O1 C6 1.3055(18) . . yes
O2 C7 1.431(2) . . yes
O3 C15 1.2981(17) . . yes
O4 C16 1.435(2) . . yes
O2 H22 0.83(2) . . no
O4 H24 0.82(3) . . no
O5 N9 1.2644(17) . . yes
O6 N9 1.2698(17) . . yes
O7 N9 1.2341(19) . . yes
O8 H28' 0.84(3) . . no
O8 H28 0.88(3) . . no
O9 H29' 0.83(3) . . no
O9 H29 0.77(2) . . no
O10 H211 0.82(3) . . no
O10 H210 0.83(2) . . no
N1 N3 1.3923(18) . . yes
N1 C1 1.3029(18) . . yes
N2 C4 1.356(2) . . yes
N2 C5 1.3394(19) . . yes
N3 C9 1.319(2) . . yes
N4 C9 1.349(2) . . yes
N5 N7 1.3963(19) . . yes
N5 C10 1.3049(18) . . yes
N6 C13 1.358(2) . . yes
N6 C14 1.3367(19) . . yes
N7 C18 1.323(2) . . yes
N8 C18 1.342(2) . . yes
N2 H32 0.90(2) . . no
N4 H34 0.85(2) . . no
N4 H34' 0.82(3) . . no
N6 H36 0.82(2) . . no
N8 H38' 0.840(19) . . no
N8 H38 0.86(2) . . no
C1 C2 1.448(2) . . no
C2 C3 1.427(2) . . no
C2 C6 1.421(2) . . no
C3 C7 1.514(2) . . no
C3 C4 1.373(2) . . no
C5 C8 1.495(2) . . no
C5 C6 1.425(2) . . no
C10 C11 1.452(2) . . no
C11 C12 1.4277(19) . . no
C11 C15 1.423(2) . . no
C12 C16 1.513(2) . . no
C12 C13 1.376(2) . . no
C14 C15 1.425(2) . . no
C14 C17 1.489(2) . . no
C1 H1 0.949(19) . . no

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C4 H4 0.893(18) . . no
 C7 H7 0.930(18) . . no
 C7 H7' 0.977(17) . . no
 C8 H8 0.93(2) . . no
 C8 H8' 0.93(2) . . no
 C8 H18" 1.00(2) . . no
 C10 H10 0.939(19) . . no
 C13 H13 0.911(18) . . no
 C16 H16' 0.960(19) . . no
 C16 H16 0.98(2) . . no
 C17 H17" 0.93(2) . . no
 C17 H17 1.00(2) . . no
 C17 H17' 0.89(2) . . no

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 S1 Fe S2 88.40(1) . . . yes
 S1 Fe O1 178.94(3) . . . yes
 S1 Fe O3 91.12(3) . . . yes
 S1 Fe N1 85.65(4) . . . yes
 S1 Fe N5 95.97(4) . . . yes
 S2 Fe O1 90.93(3) . . . yes
 S2 Fe O3 179.37(3) . . . yes
 S2 Fe N1 95.90(4) . . . yes
 S2 Fe N5 85.72(4) . . . yes
 O1 Fe O3 89.55(4) . . . yes
 O1 Fe N1 93.60(5) . . . yes
 O1 Fe N5 84.80(5) . . . yes
 O3 Fe N1 84.47(5) . . . yes
 O3 Fe N5 93.92(5) . . . yes
 N1 Fe N5 177.75(5) . . . yes
 Fe S1 C9 94.79(5) . . . yes
 Fe S2 C18 95.28(5) . . . yes
 Fe O1 C6 125.67(10) . . . yes
 Fe O3 C15 125.90(10) . . . yes
 C7 O2 H22 105.6(15) . . . no
 C16 O4 H24 108.1(16) . . . no
 H28 O8 H28' 104(3) . . . no
 H29 O9 H29' 105(2) . . . no
 H210 O10 H211 109(2) . . . no
 N3 N1 C1 112.50(12) . . . yes
 Fe N1 C1 125.71(10) . . . yes
 Fe N1 N3 121.50(9) . . . yes
 C4 N2 C5 124.03(13) . . . yes
 N1 N3 C9 113.67(12) . . . yes
 Fe N5 N7 121.35(9) . . . yes
 N7 N5 C10 112.92(13) . . . yes
 Fe N5 C10 125.52(11) . . . yes
 C13 N6 C14 124.34(14) . . . yes
 N5 N7 C18 113.51(13) . . . yes
 C4 N2 H32 119.9(13) . . . no
 C5 N2 H32 116.0(13) . . . no
 C9 N4 H34 123.8(14) . . . no
 H34 N4 H34' 120(2) . . . no

C9 N4 H34' 115.4(15) . . . no
 C13 N6 H36 119.1(14) . . . no
 C14 N6 H36 116.5(15) . . . no
 C18 N8 H38' 120.2(13) . . . no
 H38 N8 H38' 116.5(19) . . . no
 C18 N8 H38 122.6(13) . . . no
 O6 N9 O7 120.50(13) . . . yes
 O5 N9 O6 118.79(13) . . . yes
 O5 N9 O7 120.71(13) . . . yes
 N1 C1 C2 125.24(14) . . . yes
 C3 C2 C6 119.07(13) . . . no
 C1 C2 C6 122.09(13) . . . no
 C1 C2 C3 118.83(13) . . . no
 C2 C3 C4 119.61(14) . . . no
 C2 C3 C7 122.67(13) . . . no
 C4 C3 C7 117.72(13) . . . no
 N2 C4 C3 119.80(14) . . . yes
 C6 C5 C8 121.05(13) . . . no
 N2 C5 C6 119.19(14) . . . yes
 N2 C5 C8 119.76(13) . . . yes
 O1 C6 C2 125.96(13) . . . yes
 O1 C6 C5 115.76(13) . . . yes
 C2 C6 C5 118.28(13) . . . no
 O2 C7 C3 108.46(12) . . . yes
 S1 C9 N4 119.13(12) . . . yes
 N3 C9 N4 116.69(14) . . . yes
 S1 C9 N3 124.18(11) . . . yes
 N5 C10 C11 125.00(14) . . . yes
 C12 C11 C15 118.85(13) . . . no
 C10 C11 C15 122.05(12) . . . no
 C10 C11 C12 119.10(14) . . . no
 C13 C12 C16 117.80(13) . . . no
 C11 C12 C13 119.82(15) . . . no
 C11 C12 C16 122.34(14) . . . no
 N6 C13 C12 119.46(14) . . . yes
 C15 C14 C17 120.68(13) . . . no
 N6 C14 C17 120.21(14) . . . yes
 N6 C14 C15 119.10(14) . . . yes
 C11 C15 C14 118.42(12) . . . no
 O3 C15 C14 115.46(13) . . . yes
 O3 C15 C11 126.12(13) . . . yes
 O4 C16 C12 107.40(12) . . . yes
 N7 C18 N8 117.89(14) . . . yes
 S2 C18 N8 118.17(12) . . . yes
 S2 C18 N7 123.94(12) . . . yes
 N1 C1 H1 116.5(10) . . . no
 C2 C1 H1 118.3(10) . . . no
 C3 C4 H4 123.4(12) . . . no
 N2 C4 H4 116.9(11) . . . no
 C3 C7 H7 110.6(12) . . . no
 C3 C7 H7' 109.3(11) . . . no
 O2 C7 H7' 109.5(11) . . . no
 O2 C7 H7 110.4(11) . . . no
 H7 C7 H7' 108.6(15) . . . no
 H8' C8 H18" 106(2) . . . no
 C5 C8 H8 113.4(13) . . . no
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loop_

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#===END of Crystallographic Information File

# Attachment 'ql438.cif'

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_chemical_compound_source 'see text'

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6. CRYSTAL DATA

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_symmetry_equiv_pos_as_xyz	
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3	-x,-y,-z
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6	1/2-x,1/2+y,1/2-z
7	1/2-x,1/2-y,-z
8	1/2+x,1/2-y,1/2+z

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_cell_formula_units_Z	8

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;

The final unit cell was obtained from the xyz centroids of 4660 reflections after integration using the SAINTPLUS software package (Bruker, 2007).

Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

;

_exptl_crystal_description	platelet
_exptl_crystal_colour	red
_exptl_crystal_size_max	0.47
_exptl_crystal_size_mid	0.41
_exptl_crystal_size_min	0.07
_exptl_crystal_size_rad	?
_exptl_crystal_density_meas	?
_exptl_crystal_density_diffn	1.465
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	3096
_exptl_absorpt_coefficient_mu	0.647

```

_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_process_details    '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min    0.7438
_exptl_absorpt_correction_T_max    0.9557

#=====

# 7. EXPERIMENTAL DATA

_exptl_special_details
;
;
_diffn_ambient_temperature        100(1)
_diffn_radiation_wavelength        0.71073
_diffn_radiation_type              MoK\alpha
_diffn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator      'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method          '\f and \w scans'
_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2006)).
;
_diffn_detector_area_resol_mean    66.06

_diffn_standards_number            0
_diffn_standards_interval_count    .
_diffn_standards_interval_time     .
_diffn_standards_decay_%           0

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number                25391
_diffn_reflns_av_R_equivalents      0.0614
_diffn_reflns_av_sigmaI/netI        0.0614
_diffn_reflns_limit_h_min           -30
_diffn_reflns_limit_h_max           30
_diffn_reflns_limit_k_min           -14
_diffn_reflns_limit_k_max           14
_diffn_reflns_limit_l_min           -31
_diffn_reflns_limit_l_max           32
_diffn_reflns_theta_min              2.91
_diffn_reflns_theta_max              26.37
_diffn_measured_fraction_theta_max   0.988
_diffn_reflns_theta_full             25.00
_diffn_measured_fraction_theta_full  0.992

_diffn_reflns_reduction_process

```

```

;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
_reflns_number_total      6726
_reflns_number_gt         5085
_reflns_threshold_expression  I>2\|s(I)

_computing_data_collection 'SMART (Bruker, 2007)'
_computing_cell_refinement 'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction  'SAINT-Plus (Bruker, 2007)'
_computing_structure_solution
;
DIRDIF-07 (Beurskens et al., 2007)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLATON (Spek, 2003)
PLUTO (Meetsma, 2007)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_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
 $F^2 > 2\sigma(F^2)$  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)+(0.0607P)^2+64.9281P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration .
_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 6726
_refine_ls_number_parameters 489
_refine_ls_number_restraints 26
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0955
_refine_ls_R_factor_gt 0.0709

```

_refine_ls_wR_factor_ref	0.1847
_refine_ls_wR_factor_gt	0.1731
_refine_ls_goodness_of_fit_ref	1.097
_refine_ls_restrained_S_all	1.095
_refine_ls_shift/su_max	0.019
_refine_ls_shift/su_mean	0.002
_refine_diff_density_max	0.915
_refine_diff_density_min	-0.569
_refine_diff_density_rms	0.112

_vrn_publ_code_number_frames	1800
_vrn_publ_code_frame_time_sec	10.0
_vrn_publ_code_meas_time_hour	7.8

#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Fe Fe Uani 0.15209(3) 0.11125(6) 0.05172(3) 1.0 0.0173(2) . .
S1 S Uani 0.11524(5) 0.26229(11) -0.00644(6) 1.0 0.0224(4) . .
S2 S Uani 0.13062(5) -0.00877(11) -0.02245(5) 1.0 0.0210(3) . .
O1 O Uani 0.18698(14) -0.0171(3) 0.10358(14) 1.0 0.0207(10) . .
O2A O Uani 0.0189(4) -0.1739(9) 0.2011(5) 0.5 0.055(4) . .
O2B O Uani 0.0109(4) -0.0080(9) 0.1706(4) 0.5 0.054(3) . .
O3 O Uani 0.17177(14) 0.2051(3) 0.11859(14) 1.0 0.0234(10) . .
O4A O Uani 0.4128(4) 0.4423(8) 0.1913(4) 0.5 0.049(3) . .
O4B O Uani 0.4083(3) 0.2804(7) 0.1863(3) 0.5 0.032(3) . .
N1 N Uani 0.17185(19) -0.2326(4) 0.19225(19) 1.0 0.0232(12) . .
N2 N Uani 0.07442(15) 0.0995(3) 0.05174(16) 1.0 0.0145(11) . .
N3 N Uani 0.02898(17) 0.1778(4) 0.02188(18) 1.0 0.0220(11) . .
N4 N Uani 0.00540(18) 0.3378(4) -0.03598(19) 1.0 0.0267(14) . .
N5 N Uani 0.25265(18) 0.4465(4) 0.20123(17) 1.0 0.0225(12) . .
N6 N Uani 0.22987(16) 0.1296(3) 0.05306(16) 1.0 0.0153(11) . .
N7 N Uani 0.24771(17) 0.0597(4) 0.01971(17) 1.0 0.0198(11) . .
N8 N Uani 0.21365(17) -0.0703(4) -0.05491(17) 1.0 0.0213(11) . .
C1 C Uani 0.1602(2) -0.0792(4) 0.1267(2) 1.0 0.0194(14) . .
C2 C Uani 0.1946(2) -0.1703(4) 0.1634(2) 1.0 0.0198(14) . .
C3 C Uani 0.1163(2) -0.2142(5) 0.1885(2) 1.0 0.0274(17) . .
C4 C Uani 0.0794(2) -0.1321(5) 0.1523(2) 1.0 0.0249(16) . .
C5 C Uani 0.0999(2) -0.0621(4) 0.1196(2) 1.0 0.0211(16) . .
C6 C Uani 0.0601(2) 0.0250(4) 0.0818(2) 1.0 0.0230(16) . .
C7 C Uani 0.0447(2) 0.2567(4) -0.0060(2) 1.0 0.0197(16) . .
C8 C Uani -0.0544(2) 0.3489(5) -0.0389(2) 1.0 0.0308(16) . .
C9 C Uani -0.0880(2) 0.4448(5) -0.0791(3) 1.0 0.0321(17) . .
C10 C Uani 0.2567(2) -0.1951(5) 0.1705(2) 1.0 0.0249(16) . .
C11 C Uani 0.0177(2) -0.1175(5) 0.1504(3) 1.0 0.0324(17) . .
C12 C Uani 0.2143(2) 0.2829(4) 0.1371(2) 1.0 0.0201(14) . .
C13 C Uani 0.2101(2) 0.3678(4) 0.1752(2) 1.0 0.0204(14) . .
C14 C Uani 0.3029(2) 0.4430(4) 0.1924(2) 1.0 0.0216(16) . .
C15 C Uani 0.3109(2) 0.3659(4) 0.1560(2) 1.0 0.0206(14) . .

```


C16 C Uani 0.2646(2) 0.2853(4) 0.1251(2) 1.0 0.0198(14) . .
C17 C Uani 0.2711(2) 0.2040(4) 0.0857(2) 1.0 0.0193(16) . .
C18 C Uani 0.2037(2) -0.0042(4) -0.0177(2) 1.0 0.0180(14) . .
C19 C Uani 0.2731(2) -0.0810(4) -0.0549(2) 1.0 0.0222(16) . .
C20 C Uani 0.3070(2) -0.1849(5) -0.0207(2) 1.0 0.0296(17) . .
C21 C Uani 0.1548(2) 0.3658(5) 0.1856(2) 1.0 0.0258(17) . .
C22 C Uani 0.3699(2) 0.3658(5) 0.1520(2) 1.0 0.0250(16) . .
O31 O Uani 0.11917(19) 0.2272(4) 0.36647(18) 1.0 0.0397(12) . .
O32 O Uani 0.0375(2) 0.4537(6) 0.2230(2) 1.0 0.065(2) . .
O33 O Uani 0.0178(2) 0.2489(4) 0.3963(2) 1.0 0.0499(17) . .
O34 O Uani 0.0508(3) 0.2102(8) 0.2374(3) 1.0 0.107(3) . .
O35 O Uani 0.14388(15) 0.4663(3) 0.39151(16) 1.0 0.0297(11) . .
O36 O Uani 0.26232(15) 0.0993(3) 0.22893(15) 1.0 0.0248(11) . .
O37 O Uani 0.46673(18) -0.0131(4) 0.10554(18) 1.0 0.0396(14) . .
O38 O Uani 0.36223(17) 0.0771(4) 0.20491(16) 1.0 0.0326(11) . .
H1 H Uiso 0.193(2) -0.281(5) 0.216(2) 1.0 0.015(13) . .
H3 H Uiso 0.10288 -0.25908 0.21127 1.0 0.0331 . .
H6 H Uiso 0.02039 0.02843 0.07846 1.0 0.0274 . .
H8 H Uiso -0.05092 0.36484 0.00019 1.0 0.0370 . .
H8' H Uiso -0.07677 0.27575 -0.05277 1.0 0.0370 . .
H9 H Uiso -0.06676 0.51765 -0.06429 1.0 0.0477 . .
H9' H Uiso -0.12869 0.45001 -0.08184 1.0 0.0477 . .
H9" H Uiso -0.09066 0.42960 -0.11752 1.0 0.0477 . .
H10 H Uiso 0.27182 -0.26537 0.19340 1.0 0.0368 . .
H10' H Uiso 0.28323 -0.13043 0.19034 1.0 0.0368 . .
H10" H Uiso 0.25563 -0.20568 0.13237 1.0 0.0368 . .
H11 H Uiso -0.0145(18) -0.136(5) 0.1109(11) 1.0 0.037(16) . .
H14 H Uiso 0.33414 0.49689 0.21248 1.0 0.0264 . .
H17 H Uiso 0.30815 0.20430 0.08312 1.0 0.0234 . .
H19 H Uiso 0.29695 -0.01065 -0.03793 1.0 0.0270 . .
H19' H Uiso 0.26746 -0.08789 -0.09522 1.0 0.0270 . .
H20 H Uiso 0.31721 -0.17361 0.02025 1.0 0.0438 . .
H20' H Uiso 0.34403 -0.19479 -0.02511 1.0 0.0438 . .
H20" H Uiso 0.28180 -0.25370 -0.03506 1.0 0.0438 . .
H21 H Uiso 0.15594 0.29751 0.20837 1.0 0.0392 . .
H21' H Uiso 0.11875 0.36323 0.14840 1.0 0.0392 . .
H21" H Uiso 0.15392 0.43526 0.20674 1.0 0.0392 . .
H22 H Uiso 0.361(2) 0.362(5) 0.1102(7) 1.0 0.028(15) . .
H24 H Uiso 0.01619 0.38789 -0.05524 1.0 0.0319 . .
H28 H Uiso 0.18327 -0.10959 -0.08076 1.0 0.0251 . .
H231 H Uiso 0.04533 -0.14314 0.23106 0.5 0.0830 . .
H232 H Uiso -0.02366 -0.00261 0.16892 0.5 0.0803 . .
H241 H Uiso 0.01859 -0.15601 0.18527 0.5 0.16(15) . .
H242 H Uiso 0.01240 -0.04024 0.16458 0.5 0.0350 . .
H251 H Uiso 0.44458 0.43906 0.18730 0.5 0.0730 . .
H252 H Uiso 0.44053 0.28216 0.18302 0.5 0.0469 . .
H261 H Uiso 0.40031 0.41958 0.17935 0.5 0.0350 . .
H262 H Uiso 0.39801 0.30454 0.17660 0.5 0.0350 . .
H31 H Uiso 0.125(3) 0.2977(10) 0.3742(19) 1.0 0.0351 . .
H31' H Uiso 0.104(3) 0.215(4) 0.3307(4) 1.0 0.0360 . .
H32 H Uiso 0.030(3) 0.5226(17) 0.212(2) 1.0 0.0350 . .
H32' H Uiso 0.034(2) 0.441(4) 0.2532(14) 1.0 0.0350 . .
H33 H Uiso 0.010(2) 0.220(5) 0.4221(13) 1.0 0.0358 . .
H33' H Uiso -0.006(2) 0.225(5) 0.3633(8) 1.0 0.0355 . .
H34 H Uiso 0.048(2) 0.18052 0.2067(7) 1.0 0.0359 . .
H34' H Uiso 0.0853(11) 0.202(5) 0.2648(13) 1.0 0.0354 . .
H35 H Uiso 0.1754(13) 0.473(5) 0.4226(10) 1.0 0.0359 . .
H35' H Uiso 0.145(2) 0.508(4) 0.3653(14) 1.0 0.0353 . .
H36 H Uiso 0.2329(13) 0.119(4) 0.1980(13) 1.0 0.0357 . .
H36' H Uiso 0.2523(19) 0.052(4) 0.2475(18) 1.0 0.0355 . .
H37 H Uiso 0.4321(11) -0.022(4) 0.103(2) 1.0 0.0350 . .

H37' H Uiso 0.4829(19) 0.048(3) 0.123(2) 1.0 0.0350 . .
H38 H Uiso 0.3338(14) 0.081(5) 0.2143(19) 1.0 0.0350 . .
H38' H Uiso 0.3925(13) 0.044(5) 0.2303(16) 1.0 0.0350 . .

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

Fe 0.0128(3) 0.0211(4) 0.0185(4) 0.0001(3) 0.0074(3) 0.0011(3)
S1 0.0161(6) 0.0249(7) 0.0277(7) 0.0040(5) 0.0111(5) 0.0023(5)
S2 0.0146(5) 0.0258(7) 0.0224(6) -0.0018(5) 0.0080(5) 0.0005(5)
O1 0.0137(15) 0.0243(19) 0.0254(18) 0.0046(14) 0.0098(14) 0.0035(14)
O2A 0.031(5) 0.086(8) 0.058(6) 0.049(6) 0.028(5) 0.019(5)
O2B 0.037(5) 0.075(7) 0.061(6) -0.017(5) 0.033(5) -0.007(5)
O3 0.0164(16) 0.032(2) 0.0235(18) -0.0061(15) 0.0103(15) -0.0030(14)
O4A 0.044(5) 0.049(6) 0.065(6) -0.019(5) 0.035(5) -0.023(4)
O4B 0.017(3) 0.040(5) 0.043(5) 0.027(4) 0.018(3) 0.018(3)
N1 0.021(2) 0.024(2) 0.019(2) 0.0017(19) 0.0039(18) 0.0035(18)
N2 0.0102(17) 0.017(2) 0.0161(19) -0.0042(16) 0.0057(16) 0.0009(15)
N3 0.0128(19) 0.025(2) 0.027(2) -0.0003(18) 0.0077(17) 0.0035(16)
N4 0.017(2) 0.030(2) 0.034(3) 0.009(2) 0.0120(19) 0.0044(18)
N5 0.022(2) 0.025(2) 0.020(2) 0.0017(18) 0.0089(18) 0.0025(18)
N6 0.0105(17) 0.022(2) 0.0125(18) 0.0025(16) 0.0042(15) 0.0029(15)
N7 0.0171(19) 0.026(2) 0.020(2) -0.0011(18) 0.0115(17) 0.0018(17)
N8 0.0151(19) 0.028(2) 0.019(2) -0.0021(17) 0.0060(17) 0.0018(17)
C1 0.016(2) 0.024(3) 0.014(2) -0.0046(19) 0.0028(19) -0.0014(19)
C2 0.018(2) 0.020(3) 0.019(2) -0.002(2) 0.006(2) 0.0009(19)
C3 0.027(3) 0.031(3) 0.030(3) 0.002(2) 0.018(2) -0.001(2)
C4 0.020(2) 0.031(3) 0.024(3) -0.004(2) 0.010(2) -0.005(2)
C5 0.017(2) 0.026(3) 0.020(3) -0.006(2) 0.008(2) 0.000(2)
C6 0.018(2) 0.026(3) 0.028(3) -0.002(2) 0.013(2) 0.000(2)
C7 0.013(2) 0.022(3) 0.022(3) 0.000(2) 0.006(2) 0.0001(19)
C8 0.015(2) 0.039(3) 0.034(3) -0.003(3) 0.007(2) 0.005(2)
C9 0.025(3) 0.031(3) 0.039(3) 0.005(3) 0.013(3) 0.008(2)
C10 0.020(2) 0.030(3) 0.024(3) 0.003(2) 0.009(2) 0.006(2)
C11 0.024(3) 0.042(3) 0.038(3) 0.009(3) 0.020(3) 0.002(2)
C12 0.018(2) 0.021(3) 0.018(2) 0.0024(19) 0.005(2) 0.0026(19)
C13 0.019(2) 0.023(3) 0.018(2) 0.003(2) 0.007(2) 0.0047(19)
C14 0.019(2) 0.023(3) 0.020(3) 0.001(2) 0.006(2) 0.000(2)
C15 0.018(2) 0.020(3) 0.021(2) 0.006(2) 0.006(2) -0.0015(19)
C16 0.023(2) 0.022(3) 0.016(2) 0.0034(19) 0.010(2) 0.001(2)
C17 0.011(2) 0.027(3) 0.021(3) 0.004(2) 0.008(2) 0.0038(19)
C18 0.013(2) 0.022(3) 0.017(2) 0.0063(19) 0.0048(19) 0.0006(19)
C19 0.022(2) 0.025(3) 0.023(3) -0.001(2) 0.013(2) 0.002(2)
C20 0.024(3) 0.034(3) 0.035(3) 0.004(2) 0.017(2) 0.007(2)
C21 0.024(3) 0.028(3) 0.028(3) 0.001(2) 0.014(2) 0.001(2)
C22 0.021(2) 0.030(3) 0.024(3) -0.001(2) 0.010(2) -0.007(2)
O31 0.036(2) 0.036(2) 0.037(2) 0.0062(19) 0.007(2) -0.0015(19)
O32 0.040(3) 0.111(5) 0.043(3) 0.007(3) 0.018(2) -0.010(3)
O33 0.052(3) 0.055(3) 0.056(3) -0.001(3) 0.036(3) -0.011(2)
O34 0.089(5) 0.160(7) 0.067(4) -0.019(5) 0.030(4) -0.037(5)
O35 0.0192(18) 0.039(2) 0.027(2) 0.0062(17) 0.0067(16) -0.0031(16)
O36 0.0241(18) 0.024(2) 0.0242(19) 0.0026(15) 0.0087(15) -0.0036(15)
O37 0.030(2) 0.053(3) 0.037(2) -0.001(2) 0.016(2) -0.0013(19)
O38 0.0246(19) 0.042(2) 0.033(2) 0.0010(18) 0.0143(18) 0.0058(17)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Fe S1 2.2241(15) . . yes

Fe S2 2.2326(14) . . yes

Fe O1 1.932(3) . . yes

Fe O3 1.912(3) . . yes

Fe N2 1.930(4) . . yes

Fe N6 1.924(4) . . yes

S1 C7 1.754(6) . . yes

S2 C18 1.761(6) . . yes

O1 C1 1.291(6) . . yes

O2A C11 1.451(13) . . yes

O2B C11 1.412(12) . . yes

O3 C12 1.307(6) . . yes

O4A C22 1.411(11) . . yes

O4B C22 1.388(9) . . yes

O2A H241 0.46 . . no

O2A H231 0.84 . . no

O2B H242 0.41 . . no

O2B H232 0.84 . . no

O4A H251 0.84 . . no

O4A H261 0.42 . . no

O4B H262 0.39 . . no

O4B H252 0.84 . . no

O31 H31' 0.840(14) . . no

O31 H31 0.840(18) . . no

O32 H32 0.84(2) . . no

O32 H32' 0.83(4) . . no

O33 H33' 0.84(3) . . no

O33 H33 0.84(4) . . no

O34 H34' 0.84(3) . . no

O34 H34 0.84(2) . . no

N1 C3 1.353(8) . . yes

N1 C2 1.329(7) . . yes

N2 C6 1.311(6) . . yes

N2 N3 1.385(6) . . yes

N3 C7 1.325(7) . . yes

N4 C7 1.329(7) . . yes

N4 C8 1.456(7) . . yes

N5 C14 1.362(7) . . yes

N5 C13 1.330(7) . . yes

N6 N7 1.390(6) . . yes

N6 C17 1.318(6) . . yes

N7 C18 1.318(7) . . yes

N8 C18 1.335(7) . . yes
 N8 C19 1.478(7) . . yes
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 N8 H28 0.88 . . no
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 O37 H37 0.84(4) . . no
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 O38 H38 0.84(4) . . no
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 C5 C6 1.447(7) . . no
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 C13 C21 1.509(8) . . no
 C14 C15 1.374(7) . . no
 C15 C16 1.420(7) . . no
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S1 Fe N6 91.90(12) . . . yes
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S2 Fe N2 95.58(12) . . . yes
S2 Fe N6 86.61(12) . . . yes
O1 Fe O3 87.59(15) . . . yes
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O1 Fe N6 86.32(16) . . . yes
O3 Fe N2 84.01(16) . . . yes
O3 Fe N6 93.89(16) . . . yes
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Fe S1 C7 94.52(16) . . . yes
Fe S2 C18 94.27(16) . . . yes
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Fe N2 C6 125.3(3) . . . yes
Fe N2 N3 121.2(3) . . . yes
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Fe N6 C17 124.8(3) . . . yes
Fe N6 N7 121.0(3) . . . yes
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C18 N8 C19 123.4(4) . . . yes
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C1 C5 C4 118.1(4) . . . no
C1 C5 C6 122.8(4) . . . no
C4 C5 C6 119.0(5) . . . no
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S1 C7 N4 116.4(4) . . . yes
N3 C7 N4 119.3(5) . . . yes
S1 C7 N3 124.2(4) . . . yes
N4 C8 C9 110.0(5) . . . yes
O2B C11 C4 111.8(6) . . . yes
O2A C11 C4 107.6(6) . . . yes
O2A C11 O2B 91.8(7) . . . yes
O3 C12 C13 115.8(5) . . . yes
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 Fe S1 C7 N3 -1.6(4) no
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 Fe S2 C18 N7 -2.3(4) no
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C10 C21 3.446(7) . 6_545 no
C11 O4A 3.284(12) . 5_445 no
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 O36 H36 O3 0.84(3) 2.18(3) 2.998(5) 166(4) . yes
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SHELXL-97


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[c.f. r.h. blessing, acta cryst. (1995), a51, 33-38]
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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 $F^2 > 2\sigma(F^2)$ 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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loop_

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N1 N	0.5969(3) 0.4110(2) 0.0313(2) 0.0410(7) Uani 1 1 d . . .
H1N H	0.5551 0.3891 -0.0255 0.049 Uiso 1 1 calc R . .

N2 N 0.6309(3) 0.4115(2) 0.18388(19) 0.0355(7) Uani 1 1 d . . .
 H2N H 0.6965 0.4438 0.1999 0.043 Uiso 1 1 calc R . .
 N3 N 0.5899(2) 0.3898(2) 0.24949(18) 0.0295(6) Uani 1 1 d . . .
 N4 N 0.5749(3) 0.3955(3) 0.5617(2) 0.0466(8) Uani 1 1 d . . .
 H4N H 0.5622 0.3879 0.6102 0.056 Uiso 1 1 calc R . .
 N5 N 0.1266(3) 0.3093(3) 0.1940(3) 0.0493(9) Uani 1 1 d . . .
 H5N H 0.1130 0.3681 0.1995 0.059 Uiso 1 1 calc R . .
 N6 N 0.2512(3) 0.2014(2) 0.1861(2) 0.0445(8) Uani 1 1 d . . .
 H6N H 0.2033 0.1552 0.1843 0.053 Uiso 1 1 calc R . .
 N7 N 0.3541(3) 0.1834(2) 0.1807(2) 0.0358(7) Uani 1 1 d . . .
 N8 N 0.6464(3) -0.0087(3) 0.1259(3) 0.0526(9) Uani 1 1 d . . .
 H8N H 0.7039 -0.0313 0.1181 0.063 Uiso 1 1 calc R . .
 C1 C 0.6948(4) 0.4770(4) 0.0483(3) 0.0573(12) Uani 1 1 d . . .
 H1A H 0.6925 0.5336 0.0858 0.086 Uiso 1 1 calc R . .
 H1B H 0.6933 0.4937 -0.0096 0.086 Uiso 1 1 calc R . .
 H1C H 0.7640 0.4478 0.0801 0.086 Uiso 1 1 calc R . .
 C2 C 0.5656(3) 0.3811(2) 0.0948(2) 0.0337(8) Uani 1 1 d . . .
 C3 C 0.6444(3) 0.4365(3) 0.3310(2) 0.0341(8) Uani 1 1 d . . .
 H3 H 0.7047 0.4817 0.3399 0.041 Uiso 1 1 calc R . .
 C4 C 0.6160(3) 0.4217(3) 0.4091(2) 0.0344(8) Uani 1 1 d . . .
 C5 C 0.5445(3) 0.3414(3) 0.4074(2) 0.0364(8) Uani 1 1 d . . .
 C6 C 0.5265(4) 0.3297(3) 0.4891(3) 0.0430(9) Uani 1 1 d . . .
 C7 C 0.6421(4) 0.4733(3) 0.5650(2) 0.0452(10) Uani 1 1 d . . .
 H7 H 0.6723 0.5171 0.6183 0.054 Uiso 1 1 calc R . .
 C8 C 0.6663(3) 0.4884(3) 0.4903(2) 0.0391(8) Uani 1 1 d . . .
 C9 C 0.4530(5) 0.2458(4) 0.4931(3) 0.0599(12) Uani 1 1 d . . .
 H9A H 0.4580 0.2454 0.5552 0.090 Uiso 1 1 calc R . .
 H9B H 0.4789 0.1879 0.4746 0.090 Uiso 1 1 calc R . .
 H9C H 0.3746 0.2501 0.4519 0.090 Uiso 1 1 calc R . .
 C10 C 0.7419(4) 0.5751(3) 0.4941(3) 0.0485(10) Uani 1 1 d . . .
 H10A H 0.8077 0.5551 0.4831 0.058 Uiso 1 1 calc R . .
 H10B H 0.6995 0.6126 0.4452 0.058 Uiso 1 1 calc R . .
 C11 C 0.0376(5) 0.2373(4) 0.1854(5) 0.0787(17) Uani 1 1 d . . .
 H11A H 0.0228 0.1918 0.1322 0.118 Uiso 1 1 calc R . .
 H11B H -0.0312 0.2669 0.1783 0.118 Uiso 1 1 calc R . .
 H11C H 0.0618 0.2052 0.2401 0.118 Uiso 1 1 calc R . .
 C12 C 0.2278(3) 0.2919(3) 0.1942(3) 0.0382(8) Uani 1 1 d . . .
 C13 C 0.3636(4) 0.0946(3) 0.1584(3) 0.0423(9) Uani 1 1 d . . .
 H13 H 0.3020 0.0499 0.1478 0.051 Uiso 1 1 calc R . .
 C14 C 0.4642(4) 0.0613(3) 0.1493(3) 0.0414(9) Uani 1 1 d . . .
 C15 C 0.5675(4) 0.1191(3) 0.1796(3) 0.0397(9) Uani 1 1 d . . .
 C16 C 0.6611(4) 0.0812(3) 0.1663(3) 0.0483(10) Uani 1 1 d . . .
 C17 C 0.5499(4) -0.0652(3) 0.0972(3) 0.0525(11) Uani 1 1 d . . .
 H17 H 0.5465 -0.1270 0.0693 0.063 Uiso 1 1 calc R . .
 C18 C 0.4550(4) -0.0348(3) 0.1075(3) 0.0461(10) Uani 1 1 d . . .
 C19 C 0.7720(4) 0.1383(4) 0.1934(4) 0.0658(13) Uani 1 1 d . . .
 H19A H 0.8244 0.1001 0.1791 0.099 Uiso 1 1 calc R . .
 H19B H 0.8033 0.1590 0.2588 0.099 Uiso 1 1 calc R . .
 H19C H 0.7607 0.1932 0.1600 0.099 Uiso 1 1 calc R . .
 C20 C 0.3463(4) -0.1005(3) 0.0751(4) 0.0567(12) Uani 1 1 d . . .
 H20A H 0.3286 -0.1112 0.1280 0.068 Uiso 1 1 calc R . .
 H20B H 0.2835 -0.0699 0.0325 0.068 Uiso 1 1 calc R . .
 S3 S -0.03544(9) 0.48292(8) 0.29703(7) 0.0455(3) Uani 1 1 d . . .
 O5 O -0.0075(3) 0.4072(3) 0.3557(2) 0.0679(9) Uani 1 1 d . . .
 O6 O -0.1535(3) 0.5050(3) 0.2710(2) 0.0633(9) Uani 1 1 d . . .
 O7 O -0.0055(3) 0.4660(2) 0.2182(2) 0.0587(8) Uani 1 1 d . . .
 C21 C 0.0486(3) 0.5872(3) 0.3655(3) 0.0455(9) Uani 1 1 d . . .
 C22 C 0.0485(4) 0.6151(3) 0.4516(3) 0.0551(11) Uani 1 1 d . . .
 H22 H 0.0031 0.5789 0.4730 0.066 Uiso 1 1 calc R . .
 C23 C 0.1138(4) 0.6945(4) 0.5053(4) 0.0621(12) Uani 1 1 d . . .
 H23 H 0.1126 0.7113 0.5631 0.075 Uiso 1 1 calc R . .

C24 C 0.1819(4) 0.7510(3) 0.4762(4) 0.0601(12) Uani 1 1 d . . .
 C25 C 0.1811(4) 0.7237(4) 0.3900(4) 0.0652(13) Uani 1 1 d . . .
 H25 H 0.2253 0.7611 0.3685 0.078 Uiso 1 1 calc R . .
 C26 C 0.1164(4) 0.6425(4) 0.3349(3) 0.0577(11) Uani 1 1 d . . .
 H26 H 0.1184 0.6250 0.2775 0.069 Uiso 1 1 calc R . .
 C27 C 0.2539(6) 0.8394(4) 0.5362(5) 0.0857(18) Uani 1 1 d . . .
 H27A H 0.2952 0.8692 0.5048 0.129 Uiso 1 1 calc R . .
 H27B H 0.3075 0.8219 0.5938 0.129 Uiso 1 1 calc R . .
 H27C H 0.2049 0.8833 0.5483 0.129 Uiso 1 1 calc R . .
 S4 S -0.12136(10) 0.92019(8) 0.06020(10) 0.0571(3) Uani 1 1 d . . .
 O8 O -0.1239(3) 0.9568(3) -0.0236(3) 0.0746(10) Uani 1 1 d . . .
 O9 O -0.2350(3) 0.8919(3) 0.0539(3) 0.0741(11) Uani 1 1 d . . .
 O10 O -0.0545(4) 0.9840(3) 0.1428(3) 0.0811(11) Uani 1 1 d . . .
 C28 C -0.0519(4) 0.8142(3) 0.0689(3) 0.0485(10) Uani 1 1 d . . .
 C29 C 0.0531(5) 0.8188(4) 0.0640(5) 0.0780(18) Uani 1 1 d . . .
 H29 H 0.0849 0.8757 0.0545 0.094 Uiso 1 1 calc R . .
 C30 C 0.1120(5) 0.7368(4) 0.0735(5) 0.0816(18) Uani 1 1 d . . .
 H30 H 0.1844 0.7396 0.0718 0.098 Uiso 1 1 calc R . .
 C31 C 0.0645(4) 0.6524(3) 0.0851(4) 0.0578(12) Uani 1 1 d . . .
 C32 C -0.0416(5) 0.6498(4) 0.0879(4) 0.0667(14) Uani 1 1 d . . .
 H32 H -0.0748 0.5929 0.0959 0.080 Uiso 1 1 calc R . .
 C33 C -0.1002(4) 0.7308(4) 0.0790(4) 0.0595(12) Uani 1 1 d . . .
 H33 H -0.1729 0.7278 0.0801 0.071 Uiso 1 1 calc R . .
 C34 C 0.1305(6) 0.5652(4) 0.0961(5) 0.0856(19) Uani 1 1 d . . .
 H34A H 0.1319 0.5420 0.0376 0.128 Uiso 1 1 calc R . .
 H34B H 0.0938 0.5163 0.1164 0.128 Uiso 1 1 calc R . .
 H34C H 0.2078 0.5819 0.1411 0.128 Uiso 1 1 calc R . .
 O14 O 0.8283(4) -0.0329(3) 0.7712(3) 0.0918(13) Uani 1 1 d . . .
 H14 H 0.8986 -0.0231 0.7949 0.138 Uiso 1 1 calc R . .
 C42 C 0.7858(9) 0.0030(12) 0.6857(9) 0.207(7) Uani 1 1 d . . .
 H42A H 0.8023 -0.0391 0.6415 0.248 Uiso 1 1 calc R . .
 H42B H 0.8267 0.0651 0.6924 0.248 Uiso 1 1 calc R . .
 C43 C 0.6641(11) 0.0131(11) 0.6481(9) 0.201(6) Uani 1 1 d . . .
 H43A H 0.6235 -0.0437 0.6536 0.302 Uiso 1 1 calc R . .
 H43B H 0.6386 0.0225 0.5839 0.302 Uiso 1 1 calc R . .
 H43C H 0.6493 0.0673 0.6816 0.302 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_12

S5A 0.0559(13) 0.0462(12) 0.0304(11) 0.0089(9) 0.0167(9) 0.0132(9)
 O11A 0.098(5) 0.070(4) 0.029(2) -0.004(2) 0.024(3) 0.006(3)
 O12A 0.068(5) 0.053(5) 0.040(5) 0.019(4) 0.026(4) 0.014(4)
 O13A 0.055(4) 0.077(5) 0.121(9) 0.034(5) 0.007(5) 0.018(3)
 S5B 0.074(3) 0.061(3) 0.0291(19) 0.0056(18) 0.022(2) 0.003(2)
 O11B 0.122(11) 0.102(11) 0.027(5) -0.004(5) 0.025(6) -0.029(9)
 O12B 0.13(3) 0.11(2) 0.062(17) -0.007(12) 0.070(18) -0.025(14)
 O13B 0.074(7) 0.100(9) 0.072(8) 0.009(6) 0.030(6) 0.024(6)
 C35 0.072(3) 0.055(3) 0.041(2) 0.018(2) 0.013(2) 0.005(2)
 C36 0.124(6) 0.065(4) 0.094(5) 0.006(3) 0.050(4) 0.037(4)
 C37 0.073(4) 0.128(7) 0.134(7) 0.030(6) 0.053(5) 0.031(5)
 C38 0.080(4) 0.093(5) 0.088(5) 0.031(4) 0.024(4) -0.004(4)
 C39 0.108(5) 0.059(3) 0.082(4) -0.008(3) 0.031(4) -0.002(3)
 C40 0.073(4) 0.063(3) 0.074(3) 0.003(3) 0.031(3) 0.013(3)
 C41 0.099(7) 0.228(13) 0.149(9) 0.057(9) 0.017(6) -0.062(7)
 Fe 0.0416(3) 0.0301(3) 0.0240(3) 0.00104(19) 0.0153(2) 0.0061(2)

S1 0.0466(6) 0.0475(5) 0.0224(4) -0.0017(4) 0.0120(4) -0.0034(4)
 S2 0.0448(5) 0.0307(4) 0.0421(5) 0.0026(4) 0.0203(4) 0.0071(4)
 O1 0.0528(16) 0.0379(13) 0.0292(12) 0.0042(10) 0.0218(12) 0.0061(11)
 O2 0.069(2) 0.070(2) 0.0373(16) -0.0206(15) 0.0115(15) 0.0016(18)
 O3 0.0473(15) 0.0378(14) 0.0404(14) 0.0012(11) 0.0203(12) 0.0097(11)
 O4 0.098(3) 0.0371(16) 0.085(3) -0.0066(16) 0.045(2) 0.0081(17)
 N1 0.0505(19) 0.0492(19) 0.0246(15) 0.0013(13) 0.0177(14) -0.0023(15)
 N2 0.0401(17) 0.0458(17) 0.0208(13) 0.0013(12) 0.0136(12) -0.0003(13)
 N3 0.0358(16) 0.0348(15) 0.0198(13) 0.0044(11) 0.0124(11) 0.0089(12)
 N4 0.056(2) 0.067(2) 0.0216(15) 0.0074(15) 0.0185(14) 0.0179(18)
 N5 0.047(2) 0.0435(19) 0.062(2) -0.0067(16) 0.0294(18) 0.0032(15)
 N6 0.050(2) 0.0324(16) 0.060(2) -0.0022(15) 0.0336(17) 0.0014(14)
 N7 0.0442(18) 0.0330(15) 0.0346(16) 0.0002(12) 0.0212(14) 0.0053(13)
 N8 0.065(2) 0.047(2) 0.062(2) 0.0105(17) 0.040(2) 0.0219(18)
 C1 0.061(3) 0.074(3) 0.040(2) 0.013(2) 0.024(2) -0.006(2)
 C2 0.044(2) 0.0354(18) 0.0228(16) 0.0006(13) 0.0145(15) 0.0049(15)
 C3 0.0374(19) 0.0373(18) 0.0252(16) -0.0002(14) 0.0111(14) 0.0030(15)
 C4 0.039(2) 0.0424(19) 0.0213(16) 0.0030(14) 0.0110(14) 0.0119(16)
 C5 0.042(2) 0.046(2) 0.0249(17) 0.0066(15) 0.0153(15) 0.0167(16)
 C6 0.052(2) 0.055(2) 0.0293(18) 0.0117(17) 0.0218(17) 0.0170(19)
 C7 0.049(2) 0.061(3) 0.0218(17) -0.0010(16) 0.0110(16) 0.014(2)
 C8 0.041(2) 0.051(2) 0.0224(16) 0.0008(15) 0.0087(15) 0.0138(17)
 C9 0.079(3) 0.070(3) 0.043(2) 0.013(2) 0.035(2) 0.009(3)
 C10 0.054(2) 0.055(2) 0.0285(19) -0.0072(17) 0.0109(17) 0.001(2)
 C11 0.063(3) 0.062(3) 0.124(5) -0.014(3) 0.058(4) -0.006(3)
 C12 0.045(2) 0.040(2) 0.0335(18) -0.0015(15) 0.0200(16) 0.0057(16)
 C13 0.053(2) 0.0333(19) 0.045(2) 0.0018(16) 0.0247(19) 0.0049(17)
 C14 0.059(3) 0.0350(19) 0.039(2) 0.0074(16) 0.0277(19) 0.0142(18)
 C15 0.056(2) 0.0366(19) 0.0343(19) 0.0090(15) 0.0240(18) 0.0148(17)
 C16 0.067(3) 0.046(2) 0.046(2) 0.0127(18) 0.034(2) 0.024(2)
 C17 0.081(3) 0.036(2) 0.056(3) 0.0084(19) 0.041(2) 0.022(2)
 C18 0.067(3) 0.035(2) 0.045(2) 0.0090(17) 0.030(2) 0.0140(19)
 C19 0.060(3) 0.065(3) 0.082(4) 0.002(3) 0.038(3) 0.015(2)
 C20 0.077(3) 0.032(2) 0.069(3) 0.001(2) 0.038(3) 0.013(2)
 S3 0.0399(5) 0.0532(6) 0.0412(5) 0.0023(4) 0.0146(4) 0.0046(4)
 O5 0.076(2) 0.061(2) 0.055(2) 0.0146(16) 0.0144(17) -0.0044(17)
 O6 0.0381(16) 0.081(2) 0.061(2) -0.0136(17) 0.0142(15) 0.0031(15)
 O7 0.072(2) 0.0575(19) 0.0559(19) 0.0002(15) 0.0370(17) 0.0091(16)
 C21 0.036(2) 0.051(2) 0.045(2) 0.0050(18) 0.0119(17) 0.0053(17)
 C22 0.057(3) 0.054(3) 0.056(3) 0.003(2) 0.024(2) 0.006(2)
 C23 0.068(3) 0.060(3) 0.054(3) -0.001(2) 0.021(2) 0.009(2)
 C24 0.057(3) 0.050(3) 0.058(3) 0.004(2) 0.007(2) 0.011(2)
 C25 0.059(3) 0.062(3) 0.071(3) 0.016(3) 0.021(3) -0.002(2)
 C26 0.054(3) 0.066(3) 0.050(3) 0.005(2) 0.018(2) 0.001(2)
 C27 0.088(4) 0.057(3) 0.085(4) -0.001(3) 0.009(3) 0.002(3)
 S4 0.0516(7) 0.0452(6) 0.0748(8) 0.0027(5) 0.0258(6) 0.0113(5)
 O8 0.067(2) 0.070(2) 0.090(3) 0.032(2) 0.030(2) 0.0152(18)
 O9 0.071(2) 0.058(2) 0.109(3) 0.003(2) 0.052(2) 0.0179(17)
 O10 0.086(3) 0.058(2) 0.085(3) -0.0194(19) 0.025(2) 0.0099(19)
 C28 0.051(2) 0.045(2) 0.055(3) 0.0035(19) 0.026(2) 0.0147(19)
 C29 0.072(4) 0.046(3) 0.138(6) 0.014(3) 0.064(4) 0.010(2)
 C30 0.063(3) 0.060(3) 0.145(6) 0.016(3) 0.065(4) 0.014(3)
 C31 0.065(3) 0.054(3) 0.071(3) 0.015(2) 0.041(3) 0.021(2)
 C32 0.065(3) 0.050(3) 0.098(4) 0.019(3) 0.044(3) 0.012(2)
 C33 0.048(3) 0.059(3) 0.081(3) 0.015(2) 0.032(2) 0.011(2)
 C34 0.091(4) 0.067(3) 0.128(6) 0.027(4) 0.068(4) 0.032(3)
 O14 0.089(3) 0.089(3) 0.098(3) 0.020(3) 0.038(3) -0.012(3)
 C42 0.105(7) 0.346(19) 0.164(10) 0.164(12) 0.024(7) -0.008(9)
 C43 0.167(12) 0.251(16) 0.167(12) 0.102(12) 0.033(9) 0.011(11)

_geom_special_details

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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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S5A O12A 1.429(10) . ?
S5A O13A 1.436(7) . ?
S5A O11A 1.442(6) . ?
S5A C35 1.733(6) . ?
S5B O12B 1.411(17) . ?
S5B O11B 1.434(11) . ?
S5B O13B 1.444(14) . ?
S5B C35 1.870(8) . ?
C35 C36 1.378(8) . ?
C35 C40 1.385(7) . ?
C36 C37 1.376(10) . ?
C36 H36 0.9300 . ?
C37 C38 1.341(11) . ?
C37 H37 0.9300 . ?
C38 C39 1.357(10) . ?
C38 C41 1.523(10) . ?
C39 C40 1.345(8) . ?
C39 H39 0.9300 . ?
C40 H40 0.9300 . ?
C41 H41A 0.9600 . ?
C41 H41B 0.9600 . ?
C41 H41C 0.9600 . ?
Fe N7 1.907(3) . ?
Fe O3 1.913(3) . ?
Fe N3 1.915(3) . ?
Fe O1 1.917(2) . ?
Fe S1 2.2545(10) . ?
Fe S2 2.2635(10) . ?
S1 C2 1.718(4) . ?
S2 C12 1.712(4) . ?
O1 C5 1.292(4) . ?
O2 C10 1.417(5) . ?
O2 H2 0.8200 . ?
O3 C15 1.300(5) . ?
O4 C20 1.413(5) . ?
O4 H4 0.8200 . ?
N1 C2 1.311(4) . ?
N1 C1 1.435(5) . ?
N1 H1N 0.8600 . ?
N2 C2 1.338(4) . ?
N2 N3 1.383(4) . ?
N2 H2N 0.8600 . ?
N3 C3 1.293(4) . ?
N4 C6 1.323(5) . ?
N4 C7 1.339(6) . ?
N4 H4N 0.8600 . ?

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N5 C12 1.321(5) . ?
N5 C11 1.436(6) . ?
N5 H5N 0.8600 . ?
N6 C12 1.332(5) . ?
N6 N7 1.380(4) . ?
N6 H6N 0.8600 . ?
N7 C13 1.295(5) . ?
N8 C17 1.319(6) . ?
N8 C16 1.336(6) . ?
N8 H8N 0.8600 . ?
C1 H1A 0.9600 . ?
C1 H1B 0.9600 . ?
C1 H1C 0.9600 . ?
C3 C4 1.444(5) . ?
C3 H3 0.9300 . ?
C4 C5 1.407(6) . ?
C4 C8 1.420(5) . ?
C5 C6 1.420(5) . ?
C6 C9 1.490(6) . ?
C7 C8 1.365(5) . ?
C7 H7 0.9300 . ?
C8 C10 1.497(6) . ?
C9 H9A 0.9600 . ?
C9 H9B 0.9600 . ?
C9 H9C 0.9600 . ?
C10 H10A 0.9700 . ?
C10 H10B 0.9700 . ?
C11 H11A 0.9600 . ?
C11 H11B 0.9600 . ?
C11 H11C 0.9600 . ?
C13 C14 1.441(6) . ?
C13 H13 0.9300 . ?
C14 C15 1.394(6) . ?
C14 C18 1.431(5) . ?
C15 C16 1.411(5) . ?
C16 C19 1.472(7) . ?
C17 C18 1.366(6) . ?
C17 H17 0.9300 . ?
C18 C20 1.502(6) . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
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C26 H26 0.9300 . ?
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 H41A C41 H41B 109.5 . . ?
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C14 C15 C16 118.4(4) . . ?
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