Study of neutral Fe(III) complexes of pyridoxal-N-substituted thiosemicarbazone with desolvation-induced spin-state transformation above room temperature

Tido, Eddy W. Yemeli; van Ekenstein, Gert O. R. Alberda; Meetsma, Auke; van Koningsbruggen, Petra J.

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# CIF-file generated for C19H31FeN8O8S2               P-1        q1115
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# 0. AUDIT DETAILS

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_audit_update_record
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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
     Crystal Structure Center,
     Chemical Physics,
     Zernike Institute for Advanced Materials,
     University of Groningen,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Inorganic Chemistry'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2006-08-20  14:04:48

 Consider this CIF submission for deposition of the second
 X-ray structure of a manuscript to be submitted to : Inorganic Chemistry
  (Our Compound_Identification_Code : Q1115)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?
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_journal_date_printers_final        ?
_journal_date_proofs_out            ?
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_journal_coeditor_name              ?
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_journal_page_last                  ?


_journal_suppl_publ_number          ?
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# 3. TITLE AND AUTHOR LIST

_publ_section_title
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;
_publ_section_title_footnote
;
 ?
;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


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_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
;   # author related footnote
;
;   # Address of this author
;
   'Meetsma, Auke'
```

```
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Chemical Physics,
     Zernike Institute for Advanced Materials
     University of Groningen,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;

#===============================================================================

# 4. TEXT

_publ_section_synopsis
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 ?
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
 The asymmetric unit consists of five moieties: a Fe-complex,
   an highly disordered methanol solvate molecule and three water solvate
   molecules.
;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
 The structure was solved by direct methods using the program SIR2002.
 The positional and anisotropic displacement parameters for the non-hydrogen
   atoms were refined. A subsequent difference Fourier synthesis resulted in
   the location of the hydrogen atoms of the Fe-complex, which coordinates
   and isotropic displacement parameters were refined.
 Refinement was frustrated by a disorder problem: from the solution,
   it was clear that the atom positions of the solvate molecules were
   highly disordered: suggesting dynamic disorder (dynamic means that
   the smeared electron density is due to fluctuations of the atomic positions
   within each unit cell) as a consequence of translational- and rotational-
   disorder);
   the disorder is compensated by the larger the displacement parameters).
 The electron density for methanol solvate molecule has been described by
  two sites: each with an s.o.f of 0.5.
 The hydrogen atoms of the solvate molecules were generated by geometrical
  considerations, constrained to idealized geometries, and allowed to ride
  on their carrier atoms with an isotropic displacement parameter related to
  the equivalent displacement parameter of their carrier atoms.
 To improve the hydrogen parameters chemical more reasonable, ultimately
   restrain instructions (DFIX, DANG), were applied in the refinement
;
```

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_publ_section_references
;
 Allen, F.H. (2000). Acta Cryst. B58, 380-388.

 Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

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  Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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  Giacovazzo, C., Polidori, G. &  Spagna, R. (2003).
  SIR2002. A Package for crystal structure solution by direct methods
  and refinement. J. Appl. Cryst. 36, 1103.

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  Volume A, Space-group symmetry, Kluwer Academic Publishers,
  Dordrecht, The Netherlands.

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  University of Groningen, The Netherlands. (unpublished).

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  Refinement. University of G\"ottingen, Germany.

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  University of G\"ottingen, Germany.

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 Wilson, A.J.C. (1992). Ed. International Tables for Crystallography,
  Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.
;


_publ_section_figure_captions
;
   Fig. 1. Perspective PLUTO drawing of the molecule illustrating the
           configuration and the adopted numbering scheme.

   Fig. 2. Molecular packing viewed down unit cell axes.

   Fig. 3. Perspective ORTEP drawing of the title compound.
           Displacement ellipsoids for non-H are represented at the 50%
           probability level.
           The H-atoms have been omitted to improve clarity.
;
```

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#==============================================================================

# 5. CHEMICAL DATA

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;
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
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# 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
'C19 H31 Fe N8 O8 S2'
_chemical_formula_iupac               ?
_chemical_formula_weight                 619.48
_chemical_compound_source            'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
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 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
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 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      '-P 1'
_symmetry_space_group_name_H-M       'P -1'
_symmetry_Int_Tables_number                2

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 -x,-y,-z

_cell_length_a                         10.701(2)
_cell_length_b                         10.846(2)
_cell_length_c                         11.910(2)
_cell_angle_alpha                      83.347(3)
_cell_angle_beta                       83.896(3)
_cell_angle_gamma                      68.914(3)
_cell_volume                          1278.0(4)
```

```
_cell_formula_units_Z                 2
_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      2956
_cell_measurement_theta_min        2.54
_cell_measurement_theta_max       28.53
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   2956 reflections after integration using the SAINTPLUS
   software package (Bruker, 2000).

 The unit cell was identified as triclinic, space group, P-1,
   although reduced cell calculations indicate (pseudo) metric monoclinic
   C-centered lattice symmetry4, but examination of the final atomic
   coordinates of the structure did not support for the extra metric
   symmetry elements (Spek, 1988; Le Page 1987, 1988).
;

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_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.610
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              646
_exptl_absorpt_coefficient_mu     0.815
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min    0.8342
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#===============================================================================

# 7. EXPERIMENTAL DATA

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;
;
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_diffrn_radiation_wavelength           0.71073
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_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-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean     '4096x4096 / 62x62 (binned 512)'
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_diffrn_standards_decay_%            0

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              9700
_diffrn_reflns_av_R_equivalents   0.0412
_diffrn_reflns_av_sigmaI/netI     0.0748
_diffrn_reflns_limit_h_min        -13
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -13
_diffrn_reflns_limit_k_max        12
_diffrn_reflns_limit_l_min        -14
_diffrn_reflns_limit_l_max        14
_diffrn_reflns_theta_min          2.58
_diffrn_reflns_theta_max          26.01
_diffrn_measured_fraction_theta_max    0.971
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.980

_diffrn_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
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_reflns_number_gt                 3702
_reflns_threshold_expression     I>2\s(I)


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_computing_data_reduction           'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
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 SIR2002 (Burla et al., 2003)
;
_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
```

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_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^)+(0.0588P)^2^+3.20P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   difmap
_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         4874
_refine_ls_number_parameters     469
_refine_ls_number_restraints     9
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0801
_refine_ls_R_factor_gt           0.0560
_refine_ls_wR_factor_ref         0.1424
_refine_ls_wR_factor_gt          0.1301
_refine_ls_goodness_of_fit_ref   1.041
_refine_ls_restrained_S_all      1.042
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_refine_diff_density_min        -0.943
_refine_diff_density_rms         0.112

_vrn_publ_code_frame_time_sec      20.0
_vrn_publ_code_meas_time_hour      13.5

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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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S1 S Uani 0.13051(10) 0.89042(10) 0.40686(9) 1.000 0.0144(3) . .
S2 S Uani 0.29420(11) 1.08272(10) 0.37074(8) 1.000 0.0139(3) . .
O1 O Uani 0.5036(3) 0.8603(3) 0.2395(2) 1.000 0.0126(8) . .
O2 O Uani 0.2769(3) 0.8223(3) -0.1354(3) 1.000 0.0190(10) . .
O3 O Uani 0.3629(3) 0.6991(3) 0.2856(2) 1.000 0.0153(9) . .
O4 O Uani 0.8222(3) 0.5841(3) 0.4844(3) 1.000 0.0185(10) . .
N1 N Uani 0.2344(3) 0.9463(3) 0.1865(3) 1.000 0.0124(10) . .
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N4 N Uani -0.0932(4) 1.0411(4) 0.3114(4) 1.000 0.0203(12) . .
N5 N Uani 0.4209(3) 0.8181(3) 0.4576(3) 1.000 0.0111(10) . .
N6 N Uani 0.6366(4) 0.3919(3) 0.2577(3) 1.000 0.0185(11) . .
N7 N Uani 0.3939(3) 0.9013(3) 0.5455(3) 1.000 0.0128(10) . .
N8 N Uani 0.3125(4) 1.1186(4) 0.5849(3) 1.000 0.0143(11) . .
C1 C Uani 0.2873(4) 0.9407(4) 0.0830(3) 1.000 0.0127(12) . .
C2 C Uani 0.4288(4) 0.8752(4) 0.0522(3) 1.000 0.0114(11) . .
C3 C Uani 0.4692(4) 0.8532(4) -0.0628(3) 1.000 0.0136(11) . .
C4 C Uani 0.6025(4) 0.7931(4) -0.0930(4) 1.000 0.0167(12) . .
C5 C Uani 0.6639(4) 0.7703(4) 0.0932(3) 1.000 0.0128(11) . .
C6 C Uani 0.5274(4) 0.8378(4) 0.1318(3) 1.000 0.0126(11) . .
C7 C Uani 0.3700(5) 0.8922(4) -0.1534(3) 1.000 0.0170(12) . .
C8 C Uani 0.7726(5) 0.7153(5) 0.1722(4) 1.000 0.0174(12) . .
C9 C Uani 0.0408(4) 0.9881(4) 0.2967(3) 1.000 0.0147(12) . .
C10 C Uani 0.5094(4) 0.7014(4) 0.4794(3) 1.000 0.0125(12) . .
C11 C Uani 0.5528(4) 0.5986(4) 0.4002(3) 1.000 0.0138(12) . .
C12 C Uani 0.6732(4) 0.4897(4) 0.4158(3) 1.000 0.0143(12) . .
C13 C Uani 0.7102(4) 0.3901(4) 0.3435(4) 1.000 0.0176(12) . .
C14 C Uani 0.5237(4) 0.4937(4) 0.2410(3) 1.000 0.0165(12) . .
C15 C Uani 0.4762(4) 0.6023(4) 0.3099(3) 1.000 0.0139(12) . .
C16 C Uani 0.7652(4) 0.4814(4) 0.5059(4) 1.000 0.0161(12) . .
C17 C Uani 0.4432(5) 0.4943(5) 0.1453(4) 1.000 0.0210(14) . .
C18 C Uani 0.3384(4) 1.0267(4) 0.5087(3) 1.000 0.0141(12) . .
O8A O Uani 0.1572(11) 0.5508(9) -0.0054(10) 0.500 0.071(4) . .
O8B O Uani -0.0044(11) 0.8873(10) 0.0503(7) 0.500 0.053(3) . .
C81A C Uani 0.145(5) 0.681(10) 0.000(2) 0.500 0.45(6) . .
C81B C Uani 0.0599(19) 0.788(2) -0.0156(16) 0.500 0.085(8) . .
O5 O Uani 0.0342(4) 0.4763(4) 0.3194(3) 1.000 0.0286(11) . .
O6 O Uani 0.1226(4) 0.6728(4) 0.2107(4) 1.000 0.0462(14) . .
O7 O Uani 0.0529(5) 0.3032(5) 0.1432(4) 1.000 0.0619(17) . .
H1 H Uiso 0.229(4) 0.981(4) 0.025(4) 1.000 0.011(11) . .
H4 H Uiso 0.636(5) 0.779(5) -0.166(4) 1.000 0.028(14) . .
H7 H Uiso 0.426(4) 0.872(4) -0.229(4) 1.000 0.014(11) . .
H7' H Uiso 0.319(4) 0.989(5) -0.162(4) 1.000 0.016(12) . .
H8 H Uiso 0.752(5) 0.665(5) 0.238(5) 1.000 0.034(15) . .
H8' H Uiso 0.849(5) 0.668(5) 0.134(4) 1.000 0.020(12) . .
H8" H Uiso 0.797(6) 0.773(6) 0.193(5) 1.000 0.042(18) . .
H10 H Uiso 0.552(4) 0.678(4) 0.556(3) 1.000 0.010(10) . .
H13 H Uiso 0.787(5) 0.317(5) 0.353(4) 1.000 0.019(12) . .
H16 H Uiso 0.838(4) 0.390(4) 0.514(4) 1.000 0.012(11) . .
H16' H Uiso 0.717(4) 0.493(4) 0.583(4) 1.000 0.011(11) . .
H17 H Uiso 0.353(4) 0.481(4) 0.173(4) 1.000 0.011(11) . .
H17' H Uiso 0.409(4) 0.577(5) 0.104(4) 1.000 0.014(11) . .
H17" H Uiso 0.500(5) 0.432(5) 0.100(4) 1.000 0.034(15) . .
H22 H Uiso 0.308(5) 0.756(6) -0.166(5) 1.000 0.032(16) . .
H24 H Uiso 0.886(9) 0.580(9) 0.436(8) 1.000 0.12(4) . .
H25 H Uiso 0.774(11) 0.731(11) -0.045(10) 1.000 0.17(5) . .
H26 H Uiso -0.135(5) 1.080(5) 0.252(5) 1.000 0.022(14) . .
H26' H Uiso -0.119(5) 1.025(5) 0.367(4) 1.000 0.013(13) . .
H27 H Uiso 0.284(5) 1.193(5) 0.557(4) 1.000 0.017(13) . .
H27' H Uiso 0.364(5) 1.090(5) 0.642(4) 1.000 0.024(14) . .
```

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H811" H Uiso 0.20959 0.70328 -0.05529 0.500 0.6707 . .
H812' H Uiso -0.00305 0.74701 -0.03312 0.500 0.1247 . .
H812" H Uiso 0.13359 0.72141 0.02440 0.500 0.1247 . .
H81 H Uiso 0.09372 0.54843 -0.03996 0.500 0.1056 . .
H82 H Uiso -0.07426 0.87699 0.08210 0.500 0.0789 . .
H811 H Uiso 0.16279 0.69322 0.07656 0.500 0.6707 . .
H812 H Uiso 0.09602 0.82274 -0.08610 0.500 0.1247 . .
H51 H Uiso 0.061(7) 0.534(6) 0.279(6) 1.000 0.09(3) . .
H51' H Uiso 0.103(6) 0.431(9) 0.357(8) 1.000 0.17(5) . .
H61 H Uiso 0.193(4) 0.685(6) 0.226(5) 1.000 0.05(2) . .
H61' H Uiso 0.089(6) 0.736(5) 0.160(5) 1.000 0.09(3) . .
H71 H Uiso 0.033(8) 0.376(4) 0.093(4) 1.000 0.0741 . .
H71' H Uiso 0.037(7) 0.341(5) 0.206(3) 1.000 0.0741 . .

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 0.0141(3) 0.0089(3) 0.0100(3) -0.0062(2) 0.0002(2) -0.0041(2)
S1 0.0158(5) 0.0144(5) 0.0132(5) -0.0053(4) 0.0007(4) -0.0048(4)
S2 0.0211(5) 0.0103(5) 0.0118(5) -0.0061(4) -0.0017(4) -0.0058(4)
O1 0.0153(15) 0.0135(14) 0.0094(14) -0.0050(11) -0.0001(11) -0.0044(12)
O2 0.0239(17) 0.0150(16) 0.0210(17) -0.0077(14) -0.0057(13) -0.0075(14)
O3 0.0168(15) 0.0161(15) 0.0143(15) -0.0090(12) -0.0006(12) -0.0053(12)
O4 0.0216(17) 0.0161(16) 0.0213(17) -0.0046(13) -0.0032(14) -0.0096(13)
N1 0.0181(18) 0.0072(16) 0.0144(18) -0.0083(14) 0.0015(14) -0.0059(14)
N2 0.020(2) 0.0147(18) 0.0109(18) -0.0067(14) 0.0027(14) -0.0063(15)
N3 0.0125(18) 0.0131(18) 0.0188(19) -0.0066(15) -0.0022(14) -0.0024(14)
N4 0.020(2) 0.026(2) 0.013(2) -0.0042(18) 0.0000(18) -0.0055(17)
N5 0.0123(17) 0.0123(17) 0.0124(17) -0.0075(14) 0.0043(13) -0.0082(14)
N6 0.022(2) 0.0129(18) 0.023(2) -0.0073(15) -0.0005(16) -0.0075(15)
N7 0.0184(18) 0.0115(17) 0.0100(17) -0.0088(14) 0.0001(14) -0.0051(14)
N8 0.021(2) 0.0087(19) 0.0127(19) -0.0045(15) -0.0027(15) -0.0033(16)
C1 0.020(2) 0.009(2) 0.011(2) -0.0026(16) -0.0032(17) -0.0063(17)
C2 0.016(2) 0.0096(19) 0.0090(19) -0.0029(15) -0.0012(16) -0.0041(16)
C3 0.026(2) 0.0079(19) 0.010(2) -0.0022(16) -0.0021(17) -0.0091(17)
C4 0.026(2) 0.016(2) 0.011(2) -0.0075(17) 0.0016(18) -0.0098(19)
C5 0.022(2) 0.0060(19) 0.011(2) -0.0037(15) 0.0012(16) -0.0053(16)
C6 0.022(2) 0.0049(19) 0.014(2) -0.0049(15) 0.0010(17) -0.0077(16)
C7 0.028(2) 0.015(2) 0.010(2) -0.0017(17) -0.0029(18) -0.0092(19)
C8 0.019(2) 0.017(2) 0.016(2) -0.0059(19) 0.0003(18) -0.005(2)
C9 0.017(2) 0.012(2) 0.017(2) -0.0086(17) 0.0004(17) -0.0057(17)
C10 0.014(2) 0.013(2) 0.013(2) -0.0025(16) -0.0025(16) -0.0069(17)
C11 0.017(2) 0.012(2) 0.015(2) -0.0060(16) 0.0023(16) -0.0077(17)
C12 0.018(2) 0.014(2) 0.013(2) -0.0016(16) 0.0009(16) -0.0085(17)
C13 0.018(2) 0.009(2) 0.023(2) -0.0065(18) -0.0010(18) 0.0001(18)
C14 0.024(2) 0.015(2) 0.013(2) -0.0068(17) 0.0035(17) -0.0094(18)
C15 0.021(2) 0.008(2) 0.015(2) -0.0043(16) 0.0008(17) -0.0073(17)
C16 0.019(2) 0.010(2) 0.020(2) -0.0007(17) -0.0029(18) -0.0057(17)
C17 0.026(3) 0.017(2) 0.020(2) -0.010(2) -0.005(2) -0.004(2)
C18 0.014(2) 0.020(2) 0.011(2) -0.0081(17) 0.0030(16) -0.0084(17)

O8A 0.061(7) 0.040(5) 0.105(9) -0.045(6) -0.057(6) 0.015(5)
O8B 0.082(7) 0.071(6) 0.032(5) -0.005(4) -0.010(5) -0.058(6)
C81A 0.26(5) 1.24(18) 0.059(16) 0.10(5) -0.07(3) -0.55(9)
C81B 0.061(11) 0.18(2) 0.051(11) -0.016(12) 0.009(9) -0.090(13)
```

```
O5 0.032(2) 0.032(2) 0.0263(19) -0.0071(16) -0.0035(16) -0.0147(17)
O6 0.040(2) 0.035(2) 0.072(3) -0.005(2) -0.015(2) -0.020(2)
O7 0.054(3) 0.078(3) 0.054(3) -0.037(3) 0.007(2) -0.017(3)

#===============================================================================

# 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       2.2508(14)                    .      .                 yes
 Fe      S2       2.2549(13)                    .      .                 yes
 Fe      O1         1.939(3)                    .      .                 yes
 Fe      O3         1.930(3)                    .      .                 yes
 Fe      N1         1.917(4)                    .      .                 yes
 Fe      N5         1.916(4)                    .      .                 yes
 S1      C9         1.726(4)                    .      .                 yes
 S2      C18        1.738(4)                    .      .                 yes
 O1      C6         1.315(4)                    .      .                 yes
 O2      C7         1.440(6)                    .      .                 yes
 O3      C15        1.321(5)                    .      .                 yes
 O4      C16        1.438(5)                    .      .                 yes
 O2      H22         0.79(6)                    .      .                 no
 O4      H24        0.84(10)                    .      .                 no
 O8A     C81A       1.38(10)                    .      .                 yes
 O8B     C81B        1.34(2)                    .      .                 yes
 O8A     H81          0.8400                    .      .                 no
 O8B     H82          0.8400                    .      .                 no
 O5      H51'        0.86(9)                    .      .                 no
 O5      H51         0.86(7)                    .      .                 no
 O6      H61         0.85(5)                    .      .                 no
 O6      H61'        0.86(5)                    .      .                 no
 O7      H71'        0.87(4)                    .      .                 no
 O7      H71         0.91(4)                    .      .                 no
 N1      N3         1.403(5)                    .      .                 yes
 N1      C1         1.299(5)                    .      .                 yes
 N2      C4         1.341(6)                    .      .                 yes
 N2      C5         1.345(5)                    .      .                 yes
 N3      C9         1.330(5)                    .      .                 yes
 N4      C9         1.339(6)                    .      .                 yes
 N5      C10        1.296(5)                    .      .                 yes
 N5      N7         1.400(5)                    .      .                 yes
 N6      C13        1.349(6)                    .      .                 yes
 N6      C14        1.326(6)                    .      .                 yes
 N7      C18        1.316(5)                    .      .                 yes
 N8      C18        1.361(5)                    .      .                 yes
```

```
 N2      H25        0.82(12)                    .      .                 no
 N4      H26         0.86(6)                    .      .                 no
 N4      H26'        0.72(5)                    .      .                 no
 N8      H27         0.80(5)                    .      .                 no
 N8      H27'        0.88(5)                    .      .                 no
 C1      C2         1.449(6)                    .      .                 no
 C2      C3         1.413(5)                    .      .                 no
 C2      C6         1.412(6)                    .      .                 no
 C3      C7         1.512(6)                    .      .                 no
 C3      C4         1.366(6)                    .      .                 no
 C5      C8         1.482(7)                    .      .                 no
 C5      C6         1.431(6)                    .      .                 no
 C10     C11        1.458(5)                    .      .                 no
 C11     C15        1.409(6)                    .      .                 no
 C11     C12        1.412(6)                    .      .                 no
 C12     C16        1.506(6)                    .      .                 no
 C12     C13        1.379(6)                    .      .                 no
 C14     C15        1.423(6)                    .      .                 no
 C14     C17        1.498(7)                    .      .                 no
 C1      H1          0.94(5)                    .      .                 no
 C4      H4          0.91(5)                    .      .                 no
 C7      H7          1.03(5)                    .      .                 no
 C7      H7'         0.99(5)                    .      .                 no
 C8      H8'         0.90(5)                    .      .                 no
 C8      H8"         0.83(7)                    .      .                 no
 C8      H8          0.96(6)                    .      .                 no
 C10     H10         1.03(4)                    .      .                 no
 C13     H13         0.92(5)                    .      .                 no
 C16     H16'        1.00(5)                    .      .                 no
 C16     H16         1.02(4)                    .      .                 no
 C17     H17"        0.92(5)                    .      .                 no
 C17     H17         1.04(5)                    .      .                 no
 C17     H17'        0.94(5)                    .      .                 no
 C81A    C81B       1.20(10)                    .      .                 no
 C81A    H811'        0.9800                    .      .                 no
 C81A    H811         0.9800                    .      .                 no
 C81A    H811"        0.9800                    .      .                 no
 C81A    H812"        0.5200                    .      .                 no
 C81B    H812         0.9800                    .      .                 no
 C81B    H811'        0.5500                    .      .                 no
 C81B    H812'        0.9800                    .      .                 no
 C81B    H812"        0.9800                    .      .                 no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 S1      Fe      S2          88.38(5)           .      .      .          yes
 S1      Fe      O1        176.83(10)           .      .      .          yes
 S1      Fe      O3         90.02(10)           .      .      .          yes
 S1      Fe      N1         84.99(11)           .      .      .          yes
 S1      Fe      N5         92.91(11)           .      .      .          yes
 S2      Fe      O1         94.46(10)           .      .      .          yes
 S2      Fe      O3         176.64(8)           .      .      .          yes
 S2      Fe      N1         92.56(10)           .      .      .          yes
 S2      Fe      N5         84.70(10)           .      .      .          yes
```

O1	Fe	O3	87.22(13)	.	.	.	yes
O1	Fe	N1	93.47(13)	.	.	.	yes
O1	Fe	N5	88.76(13)	.	.	.	yes
O3	Fe	N1	90.25(13)	.	.	.	yes
O3	Fe	N5	92.43(12)	.	.	.	yes
N1	Fe	N5	176.60(14)	.	.	.	yes
Fe	S1	C9	94.18(15)	.	.	.	yes
Fe	S2	C18	93.86(14)	.	.	.	yes
Fe	O1	C6	121.8(3)	.	.	.	yes
Fe	O3	C15	120.5(3)	.	.	.	yes
C7	O2	H22	109(4)	.	.	.	no
C16	O4	H24	123(6)	.	.	.	no
C81A	O8A	H81	109.00	.	.	.	no
C81B	O8B	H82	110.00	.	.	.	no
H51	O5	H51'	103(7)	.	.	.	no
H61	O6	H61'	104(6)	.	.	.	no
H71	O7	H71'	100(4)	.	.	.	no
Fe	N1	C1	125.4(3)	.	.	.	yes
Fe	N1	N3	120.5(3)	.	.	.	yes
N3	N1	C1	114.0(3)	.	.	.	yes
C4	N2	C5	121.2(4)	.	.	.	yes
N1	N3	C9	111.5(3)	.	.	.	yes
Fe	N5	C10	125.1(3)	.	.	.	yes
N7	N5	C10	113.9(3)	.	.	.	yes
Fe	N5	N7	121.0(2)	.	.	.	yes
C13	N6	C14	119.2(3)	.	.	.	yes
N5	N7	C18	111.4(3)	.	.	.	yes
C5	N2	H25	122(9)	.	.	.	no
C4	N2	H25	115(9)	.	.	.	no
H26	N4	H26'	130(6)	.	.	.	no
C9	N4	H26'	113(5)	.	.	.	no
C9	N4	H26	116(4)	.	.	.	no
C18	N8	H27	113(3)	.	.	.	no
H27	N8	H27'	127(5)	.	.	.	no
C18	N8	H27'	113(3)	.	.	.	no
N1	C1	C2	124.2(4)	.	.	.	yes
C1	C2	C6	122.5(3)	.	.	.	no
C3	C2	C6	119.2(4)	.	.	.	no
C1	C2	C3	118.3(4)	.	.	.	no
C4	C3	C7	118.8(4)	.	.	.	no
C2	C3	C4	118.8(4)	.	.	.	no
C2	C3	C7	122.4(4)	.	.	.	no
N2	C4	C3	122.5(4)	.	.	.	yes
C6	C5	C8	122.0(3)	.	.	.	no
N2	C5	C8	117.8(4)	.	.	.	yes
N2	C5	C6	120.1(4)	.	.	.	yes
O1	C6	C2	125.0(4)	.	.	.	yes
C2	C6	C5	118.0(3)	.	.	.	no
O1	C6	C5	117.1(4)	.	.	.	yes
O2	C7	C3	112.7(3)	.	.	.	yes
S1	C9	N3	124.5(3)	.	.	.	yes
N3	C9	N4	116.3(4)	.	.	.	yes
S1	C9	N4	119.2(3)	.	.	.	yes
N5	C10	C11	123.3(4)	.	.	.	yes
C10	C11	C15	122.0(4)	.	.	.	no
C12	C11	C15	118.6(4)	.	.	.	no
C10	C11	C12	119.4(4)	.	.	.	no
C11	C12	C16	122.2(3)	.	.	.	no
C13	C12	C16	118.9(4)	.	.	.	no
C11	C12	C13	118.9(4)	.	.	.	no
N6	C13	C12	122.9(4)	.	.	.	yes

N6	C14	C17	118.5(4)	.	.	.	yes
C15	C14	C17	118.7(4)	.	.	.	no
N6	C14	C15	122.8(4)	.	.	.	yes
O3	C15	C14	117.9(4)	.	.	.	yes
C11	C15	C14	117.6(4)	.	.	.	no
O3	C15	C11	124.4(4)	.	.	.	yes
O4	C16	C12	111.2(4)	.	.	.	yes
N7	C18	N8	117.3(3)	.	.	.	yes
S2	C18	N7	124.7(3)	.	.	.	yes
S2	C18	N8	117.9(3)	.	.	.	yes
N1	C1	H1	117(3)	.	.	.	no
C2	C1	H1	119(3)	.	.	.	no
C3	C4	H4	124(3)	.	.	.	no
N2	C4	H4	114(3)	.	.	.	no
C3	C7	H7	106(3)	.	.	.	no
C3	C7	H7'	113(3)	.	.	.	no
H7	C7	H7'	105(4)	.	.	.	no
O2	C7	H7'	109(3)	.	.	.	no
O2	C7	H7	111(2)	.	.	.	no
H8'	C8	H8"	100(6)	.	.	.	no
C5	C8	H8"	113(4)	.	.	.	no
H8	C8	H8"	108(5)	.	.	.	no
C5	C8	H8'	109(3)	.	.	.	no
C5	C8	H8	115(4)	.	.	.	no
H8	C8	H8'	112(5)	.	.	.	no
N5	C10	H10	120(2)	.	.	.	no
C11	C10	H10	117(2)	.	.	.	no
N6	C13	H13	116(3)	.	.	.	no
C12	C13	H13	121(3)	.	.	.	no
C12	C16	H16	111(3)	.	.	.	no
C12	C16	H16'	112(3)	.	.	.	no
H16	C16	H16'	104(4)	.	.	.	no
O4	C16	H16'	106(2)	.	.	.	no
O4	C16	H16	111(3)	.	.	.	no
H17'	C17	H17"	111(4)	.	.	.	no
C14	C17	H17"	105(3)	.	.	.	no
H17	C17	H17"	115(4)	.	.	.	no
C14	C17	H17'	114(3)	.	.	.	no
C14	C17	H17	113(3)	.	.	.	no
H17	C17	H17'	99(4)	.	.	.	no
O8A	C81A	C81B	137(5)	.	.	.	yes
O8B	C81B	C81A	134(2)	.	.	.	yes
O8A	C81A	H812"	149.00	.	.	.	no
O8A	C81A	H811"	110.00	.	.	.	no
C81B	C81A	H811"	93.00	.	.	.	no
O8A	C81A	H811	109.00	.	.	.	no
C81B	C81A	H811'	27.00	.	.	.	no
H811'	C81A	H811"	110.00	.	.	.	no
H811'	C81A	H812"	74.00	.	.	.	no
H811'	C81A	H811	109.00	.	.	.	no
H811"	C81A	H812"	97.00	.	.	.	no
H811"	C81A	H811	109.00	.	.	.	no
C81B	C81A	H812"	53.00	.	.	.	no
C81B	C81A	H811	96.00	.	.	.	no
O8A	C81A	H811'	110.00	.	.	.	no
H812"	C81A	H811	44.00	.	.	.	no
O8B	C81B	H812"	109.00	.	.	.	no
O8B	C81B	H812	110.00	.	.	.	no
C81A	C81B	H812'	91.00	.	.	.	no
C81A	C81B	H812"	25.00	.	.	.	no
C81A	C81B	H811'	54.00	.	.	.	no

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 H811'   C81B    H812'         37.00            .      .      .          no
 H811'   C81B    H812"         73.00            .      .      .          no
 H811'   C81B    H812         117.00            .      .      .          no
 H812'   C81B    H812"        109.00            .      .      .          no
 H812'   C81B    H812         109.00            .      .      .          no
 H812"   C81B    H812         110.00            .      .      .          no
 C81A    C81B    H812         101.00            .      .      .          no
 O8B     C81B    H811'        130.00            .      .      .          no
 O8B     C81B    H812'        109.00            .      .      .          no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 S2      Fe      S1      C9        78.94(14)     .      .      .      .   no
 O3      Fe      S1      C9      -104.02(16)     .      .      .      .   no
 N1      Fe      S1      C9       -13.77(17)     .      .      .      .   no
 N5      Fe      S1      C9       163.55(17)     .      .      .      .   no
 S1      Fe      S2      C18       79.39(16)     .      .      .      .   no
 O1      Fe      S2      C18     -102.02(17)     .      .      .      .   no
 N1      Fe      S2      C18      164.30(19)     .      .      .      .   no
 N5      Fe      S2      C18      -13.68(19)     .      .      .      .   no
 S2      Fe      O1      C6        -122.2(3)     .      .      .      .   no
 O3      Fe      O1      C6          60.8(3)     .      .      .      .   no
 N1      Fe      O1      C6         -29.3(3)     .      .      .      .   no
 N5      Fe      O1      C6         153.2(3)     .      .      .      .   no
 S1      Fe      O3      C15       -129.6(3)     .      .      .      .   no
 O1      Fe      O3      C15         52.0(3)     .      .      .      .   no
 N1      Fe      O3      C15        145.4(3)     .      .      .      .   no
 N5      Fe      O3      C15        -36.7(3)     .      .      .      .   no
 S1      Fe      N1      N3          21.2(3)     .      .      .      .   no
 S1      Fe      N1      C1        -162.2(3)     .      .      .      .   no
 S2      Fe      N1      N3         -67.0(3)     .      .      .      .   no
 S2      Fe      N1      C1         109.7(3)     .      .      .      .   no
 O1      Fe      N1      N3        -161.6(3)     .      .      .      .   no
 O1      Fe      N1      C1          15.1(3)     .      .      .      .   no
 O3      Fe      N1      N3         111.1(3)     .      .      .      .   no
 O3      Fe      N1      C1         -72.2(3)     .      .      .      .   no
 S1      Fe      N5      N7         -67.0(3)     .      .      .      .   no
 S1      Fe      N5      C10        113.0(3)     .      .      .      .   no
 S2      Fe      N5      N7          21.1(3)     .      .      .      .   no
 S2      Fe      N5      C10       -158.9(4)     .      .      .      .   no
 O1      Fe      N5      N7         115.7(3)     .      .      .      .   no
 O1      Fe      N5      C10        -64.3(4)     .      .      .      .   no
 O3      Fe      N5      N7        -157.2(3)     .      .      .      .   no
 O3      Fe      N5      C10         22.9(4)     .      .      .      .   no
 Fe      S1      C9      N3           9.3(4)     .      .      .      .   no
 Fe      S1      C9      N4        -171.3(3)     .      .      .      .   no
 Fe      S2      C18     N7           9.5(4)     .      .      .      .   no
 Fe      S2      C18     N8        -169.7(4)     .      .      .      .   no
 Fe      O1      C6      C2          26.9(5)     .      .      .      .   no
 Fe      O1      C6      C5        -153.1(3)     .      .      .      .   no
 Fe      O3      C15     C11         29.6(5)     .      .      .      .   no
 Fe      O3      C15     C14       -151.0(3)     .      .      .      .   no
```

Fe	N1	N3	C9	-19.8(4)	.	.	.	.	no
C1	N1	N3	C9	163.1(4)	.	.	.	.	no
Fe	N1	C1	C2	3.2(6)	.	.	.	.	no
N3	N1	C1	C2	-179.9(4)	.	.	.	.	no
C5	N2	C4	C3	-2.6(6)	.	.	.	.	no
C4	N2	C5	C6	-0.3(6)	.	.	.	.	no
C4	N2	C5	C8	177.4(4)	.	.	.	.	no
N1	N3	C9	S1	4.1(5)	.	.	.	.	no
N1	N3	C9	N4	-175.4(4)	.	.	.	.	no
Fe	N5	N7	C18	-19.6(4)	.	.	.	.	no
C10	N5	N7	C18	160.4(4)	.	.	.	.	no
Fe	N5	C10	C11	-0.1(6)	.	.	.	.	no
N7	N5	C10	C11	179.9(4)	.	.	.	.	no
C14	N6	C13	C12	0.3(7)	.	.	.	.	no
C13	N6	C14	C15	0.1(6)	.	.	.	.	no
C13	N6	C14	C17	179.9(4)	.	.	.	.	no
N5	N7	C18	S2	3.7(5)	.	.	.	.	no
N5	N7	C18	N8	-177.1(4)	.	.	.	.	no
N1	C1	C2	C3	167.5(4)	.	.	.	.	no
N1	C1	C2	C6	-15.1(7)	.	.	.	.	no
C1	C2	C3	C4	179.2(4)	.	.	.	.	no
C1	C2	C3	C7	-1.6(6)	.	.	.	.	no
C6	C2	C3	C4	1.7(6)	.	.	.	.	no
C6	C2	C3	C7	-179.1(4)	.	.	.	.	no
C1	C2	C6	O1	-1.8(7)	.	.	.	.	no
C1	C2	C6	C5	178.3(4)	.	.	.	.	no
C3	C2	C6	O1	175.6(4)	.	.	.	.	no
C3	C2	C6	C5	-4.4(6)	.	.	.	.	no
C2	C3	C4	N2	1.9(6)	.	.	.	.	no
C7	C3	C4	N2	-177.3(4)	.	.	.	.	no
C2	C3	C7	O2	-62.8(5)	.	.	.	.	no
C4	C3	C7	O2	116.5(4)	.	.	.	.	no
N2	C5	C6	O1	-176.2(4)	.	.	.	.	no
N2	C5	C6	C2	3.7(6)	.	.	.	.	no
C8	C5	C6	O1	6.2(6)	.	.	.	.	no
C8	C5	C6	C2	-173.8(4)	.	.	.	.	no
N5	C10	C11	C12	162.7(4)	.	.	.	.	no
N5	C10	C11	C15	-19.2(7)	.	.	.	.	no
C10	C11	C12	C13	177.1(4)	.	.	.	.	no
C10	C11	C12	C16	-5.4(6)	.	.	.	.	no
C15	C11	C12	C13	-1.1(6)	.	.	.	.	no
C15	C11	C12	C16	176.5(4)	.	.	.	.	no
C10	C11	C15	O3	2.7(6)	.	.	.	.	no
C10	C11	C15	C14	-176.7(4)	.	.	.	.	no
C12	C11	C15	O3	-179.2(4)	.	.	.	.	no
C12	C11	C15	C14	1.4(6)	.	.	.	.	no
C11	C12	C13	N6	0.2(7)	.	.	.	.	no
C16	C12	C13	N6	-177.4(4)	.	.	.	.	no
C11	C12	C16	O4	-65.1(5)	.	.	.	.	no
C13	C12	C16	O4	112.5(4)	.	.	.	.	no
N6	C14	C15	O3	179.6(4)	.	.	.	.	no
N6	C14	C15	C11	-1.0(6)	.	.	.	.	no
C17	C14	C15	O3	-0.2(6)	.	.	.	.	no
C17	C14	C15	C11	179.2(4)	.	.	.	.	no
O8A	C81A	C81B	O8B	120(4)	.	.	.	.	no

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loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
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_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 Fe      H61         3.31(5)                 .      .                 no
 Fe      H27'        3.48(6)                 .     2_676              no
 S1      S2       3.1407(17)                 .      .                 no
 S1      O3          2.965(3)                .      .                 no
 S1      N1          2.826(4)                .      .                 no
 S1      N3          2.711(4)                .      .                 no
 S1      N5          3.029(4)                .      .                 no
 S1      N7          3.458(4)                .      .                 no
 S1      C18         3.458(5)                .      .                 no
 S1      S1       3.6744(17)                 .     2_576              no
 S1      N4          3.471(5)                .     2_576              no
 S2      N1          3.024(4)                .      .                 no
 S2      N7          2.712(4)                .      .                 no
 S2      C9          3.450(5)                .      .                 no
 S2      S1       3.1407(17)                 .      .                 no
 S2      O1          3.086(3)                .      .                 no
 S2      N3          3.444(4)                .      .                 no
 S2      N5          2.821(3)                .      .                 no
 S2      C4          3.639(5)                .     2_675              no
 S1      H61          3.13(6)                .      .                 no
 S1      H16          2.99(4)                .     2_666              no
 S1      H26'         2.92(5)                .     2_576              no
 S2      H4           2.89(5)                .     2_675              no
 O1      S2          3.086(3)                .      .                 no
 O1      O3          2.669(5)                .      .                 no
 O1      N1          2.808(5)                .      .                 no
 O1      N5          2.696(4)                .      .                 no
 O1      C1          2.946(5)                .      .                 no
 O1      C10         3.156(4)                .      .                 no
 O1      C11         3.143(5)                .      .                 no
 O1      C15         2.935(5)                .      .                 no
 O1      N8          3.100(5)                .     2_676              no
 O2      C1          3.060(5)                .      .                 no
 O2      C81B         2.71(2)                .      .                 no
 O2      C81A         2.73(7)                .      .                 no
 O2      N6          2.707(5)                .     2_665              no
 O2      N4          2.918(6)                .     2_575              no
 O3      O6          2.926(6)                .      .                 no
 O3      C10         2.932(5)                .      .                 no
 O3      N5          2.776(4)                .      .                 no
 O3      N1          2.726(4)                .      .                 no
 O3      O1          2.669(5)                .      .                 no
 O3      C6          3.049(5)                .      .                 no
 O3      C2          3.346(5)                .      .                 no
 O3      S1          2.965(3)                .      .                 no
 O3      C1          3.282(5)                .      .                 no
 O4      N8          3.074(5)                .     2_676              no
 O4      C10         3.128(6)                .      .                 no
 O4      O5          2.838(5)                .     1_655              no
 O4      O5          2.817(5)                .     2_666              no
 O5      O4          2.838(5)                .     1_455              no
 O5      C16         3.321(6)                .     2_666              no
 O5      O7          2.919(6)                .      .                 no
 O5      O6          2.768(6)                .      .                 no
 O5      O4          2.817(5)                .     2_666              no
 O6      C81B         2.88(2)                .      .                 no
 O6      O3          2.926(6)                .      .                 no
 O6      O5          2.768(6)                .      .                 no
 O6      O8B        2.856(11)                .      .                 no
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O6	C17	3.336(7)	.	.	no
O6	O8A	2.957(12)	.	.	no
O6	C81A	2.49(2)	.	.	no
O7	N2	2.831(7)	.	2_665	no
O7	C81B	2.52(2)	.	2_565	no
O7	N3	2.994(6)	.	1_545	no
O7	C81A	2.80(5)	.	2_565	no
O7	O8A	2.807(13)	.	2_565	no
O7	O5	2.919(6)	.	.	no
O8A	O6	2.957(12)	.	.	no
O8A	O7	2.807(13)	.	2_565	no
O8A	N2	3.070(10)	.	2_665	no
O8B	O6	2.856(11)	.	.	no
O8B	C1	3.382(12)	.	2_575	no
O8B	N3	3.128(9)	.	2_575	no
O8B	N3	2.837(11)	.	.	no
O8B	C9	3.386(10)	.	.	no
O1	H27'	2.33(5)	.	2_676	no
O1	H8	2.74(5)	.	.	no
O2	H26	2.08(6)	.	2_575	no
O2	H1	2.61(4)	.	.	no
O2	H811"	1.8300	.	.	no
O2	H812"	2.7000	.	.	no
O2	H812	1.9600	.	.	no
O3	H61	2.08(5)	.	.	no
O3	H16'	2.79(4)	.	2_666	no
O3	H17'	2.58(5)	.	.	no
O3	H17	2.89(4)	.	.	no
O4	H10	2.77(4)	.	.	no
O4	H51'	2.10(9)	.	2_666	no
O4	H27	2.29(5)	.	2_676	no
O5	H24	2.08(10)	.	1_455	no
O5	H71'	2.10(5)	.	.	no
O6	H51	1.92(7)	.	.	no
O6	H812"	2.2200	.	.	no
O6	H811	1.6200	.	.	no
O6	H82	2.8700	.	.	no
O6	H17	2.63(4)	.	.	no
O6	H811'	2.8200	.	.	no
O7	H25	2.02(12)	.	2_665	no
O7	H812	2.6200	.	2_565	no
O7	H811'	2.1700	.	2_565	no
O7	H81	2.1700	.	2_565	no
O7	H812'	1.6800	.	2_565	no
O8A	H25	2.88(11)	.	2_665	no
O8A	H71	2.23(8)	.	2_565	no
O8A	H61'	2.83(6)	.	.	no
O8A	H71	2.78(7)	.	.	no
O8B	H1	2.51(5)	.	2_575	no
O8B	H61'	2.00(6)	.	.	no
N1	S2	3.024(4)	.	.	no
N1	O3	2.726(4)	.	.	no
N1	C6	2.954(6)	.	.	no
N1	S1	2.826(4)	.	.	no
N1	O1	2.808(5)	.	.	no
N1	C9	2.259(5)	.	.	no
N2	C1	3.410(5)	.	2_675	no
N2	O8A	3.070(10)	.	2_665	no
N2	O7	2.831(7)	.	2_665	no
N3	O7	2.994(6)	.	1_565	no
N3	O8B	3.128(9)	.	2_575	no

N3	O8B	2.837(11)	.	.	no
N3	S2	3.444(4)	.	.	no
N3	C81B	3.01(2)	.	2_575	no
N3	S1	2.711(4)	.	.	no
N4	S1	3.471(5)	.	2_576	no
N4	O2	2.918(6)	.	2_575	no
N4	C18	3.442(6)	.	2_576	no
N5	S1	3.029(4)	.	.	no
N5	O3	2.776(4)	.	.	no
N5	N8	3.145(6)	.	2_676	no
N5	O1	2.696(4)	.	.	no
N5	C18	2.244(5)	.	.	no
N5	C15	2.943(5)	.	.	no
N5	S2	2.821(3)	.	.	no
N6	O2	2.707(5)	.	2_665	no
N7	C18	3.214(6)	.	2_676	no
N7	S1	3.458(4)	.	.	no
N7	S2	2.712(4)	.	.	no
N7	N8	3.299(6)	.	2_676	no
N8	O4	3.074(5)	.	2_676	no
N8	O1	3.100(5)	.	2_676	no
N8	C10	3.170(6)	.	2_676	no
N8	N5	3.145(6)	.	2_676	no
N8	N7	3.299(6)	.	2_676	no
N2	H71	2.82(8)	.	2_665	no
N3	H812	2.5400	.	2_575	no
N4	H13	2.88(5)	.	1_465	no
N4	H812	2.9100	.	2_575	no
N5	H27'	2.92(6)	.	2_676	no
N6	H811"	2.8500	.	2_665	no
N6	H22	1.92(6)	.	2_665	no
N7	H7	2.71(5)	.	1_556	no
N7	H26'	2.87(6)	.	2_576	no
C1	C4	3.507(6)	.	2_675	no
C1	O2	3.060(5)	.	.	no
C1	O8B	3.382(12)	.	2_575	no
C1	N2	3.410(5)	.	2_675	no
C2	O3	3.346(5)	.	.	no
C2	C3	3.509(6)	.	2_675	no
C2	C4	3.577(6)	.	2_675	no
C3	C6	3.369(6)	.	2_675	no
C3	C2	3.509(6)	.	2_675	no
C4	C1	3.507(6)	.	2_675	no
C4	S2	3.639(5)	.	2_675	no
C4	C2	3.577(6)	.	2_675	no
C4	C17	3.458(7)	.	2_665	no
C6	C7	3.521(6)	.	2_675	no
C6	C15	3.291(6)	.	.	no
C6	C3	3.369(6)	.	2_675	no
C7	C6	3.521(6)	.	2_675	no
C9	O8B	3.386(10)	.	.	no
C10	C13	3.331(6)	.	2_666	no
C10	O4	3.128(6)	.	.	no
C10	C12	3.386(6)	.	2_666	no
C10	N8	3.170(6)	.	2_676	no
C11	O1	3.143(5)	.	.	no
C11	C11	3.390(6)	.	2_666	no
C11	C12	3.409(6)	.	2_666	no
C12	C11	3.409(6)	.	2_666	no
C12	C10	3.386(6)	.	2_666	no
C13	C10	3.331(6)	.	2_666	no

C15	C16	3.512(6)	.	2_666	no
C15	C6	3.291(6)	.	.	no
C16	O5	3.321(6)	.	2_666	no
C16	C15	3.512(6)	.	2_666	no
C17	C17	3.548(7)	.	2_665	no
C17	O6	3.336(7)	.	.	no
C17	C4	3.458(7)	.	2_665	no
C18	C18	3.282(6)	.	2_676	no
C18	N4	3.442(6)	.	2_576	no
C18	N7	3.214(6)	.	2_676	no
C81A	O7	2.80(6)	.	2_565	no
C81A	O6	2.49(2)	.	.	no
C81A	O2	2.73(7)	.	.	no
C81B	O6	2.88(2)	.	.	no
C81B	O7	2.52(2)	.	2_565	no
C81B	O2	2.71(2)	.	.	no
C81B	N3	3.01(2)	.	2_575	no
C1	H7'	2.91(5)	.	.	no
C3	H17"	3.07(5)	.	2_665	no
C4	H17	3.08(4)	.	2_665	no
C4	H17"	3.03(5)	.	2_665	no
C5	H7'	2.90(5)	.	2_675	no
C6	H7'	2.98(5)	.	2_675	no
C7	H26	2.79(6)	.	2_575	no
C7	H27'	3.04(5)	.	1_554	no
C7	H1	2.54(5)	.	.	no
C8	H82	2.8600	.	1_655	no
C8	H7'	2.99(5)	.	2_675	no
C10	H27	2.81(6)	.	2_676	no
C10	H16'	2.81(4)	.	.	no
C11	H8	2.95(6)	.	.	no
C12	H8	2.94(6)	.	.	no
C13	H22	2.85(6)	.	2_665	no
C14	H22	2.84(6)	.	2_665	no
C14	H10	3.10(4)	.	2_666	no
C15	H61	3.08(5)	.	.	no
C15	H16'	2.76(5)	.	2_666	no
C16	H10	2.57(4)	.	.	no
C16	H51'	2.72(9)	.	2_666	no
C17	H22	3.05(6)	.	2_665	no
C17	H17"	3.00(5)	.	2_665	no
C17	H61	2.88(6)	.	.	no
C18	H26'	2.83(5)	.	2_576	no
C81A	H61	2.80(7)	.	.	no
C81A	H17'	2.99(8)	.	.	no
C81A	H22	2.74(8)	.	.	no
C81A	H71	2.59(10)	.	2_565	no
C81A	H61'	2.03(7)	.	.	no
C81B	H22	2.97(6)	.	.	no
C81B	H61'	2.13(6)	.	.	no
C81B	H71	2.62(7)	.	2_565	no
H1	O8B	2.51(5)	.	2_575	no
H1	H7'	2.34(7)	.	.	no
H1	O2	2.61(4)	.	.	no
H1	C7	2.54(5)	.	.	no
H1	H82	2.2100	.	2_575	no
H811'	H61'	2.1700	.	.	no
H811'	H71	2.1300	.	2_565	no
H811'	O7	2.1700	.	2_565	no
H811'	O6	2.8200	.	.	no
H811"	H22	1.7700	.	.	no

H811"	O2	1.8300	.	.	no
H811"	N6	2.8500	.	2_665	no
H812'	H61'	2.5700	.	.	no
H812'	H71'	2.4800	.	2_565	no
H812'	H71	1.7200	.	2_565	no
H812'	H25	2.4700	.	1_455	no
H812'	H81	2.0300	.	.	no
H812'	O7	1.6800	.	2_565	no
H4	S2	2.89(5)	.	2_675	no
H4	H7	2.28(7)	.	.	no
H812"	O2	2.7000	.	.	no
H812"	H61'	1.6400	.	.	no
H812"	H61	2.5000	.	.	no
H812"	O6	2.2200	.	.	no
H7	H27'	2.58(7)	.	1_554	no
H7	N7	2.71(5)	.	1_554	no
H7	H4	2.28(7)	.	.	no
H7'	H27'	2.54(7)	.	1_554	no
H7'	C1	2.91(5)	.	.	no
H7'	H1	2.34(7)	.	.	no
H7'	C6	2.98(5)	.	2_675	no
H7'	H8"	2.43(8)	.	2_675	no
H7'	C8	2.99(5)	.	2_675	no
H7'	C5	2.90(5)	.	2_675	no
H8	O1	2.74(5)	.	.	no
H8	C12	2.94(6)	.	.	no
H8	C11	2.95(6)	.	.	no
H8'	H81	2.5600	.	2_665	no
H8'	H25	2.30(13)	.	.	no
H8"	H7'	2.43(8)	.	2_675	no
H8"	H82	2.3000	.	1_655	no
H10	O4	2.77(4)	.	.	no
H10	H16'	2.16(6)	.	.	no
H10	C14	3.10(4)	.	2_666	no
H10	C16	2.57(4)	.	.	no
H13	N4	2.88(5)	.	1_645	no
H13	H16	2.34(7)	.	.	no
H16	S1	2.99(4)	.	2_666	no
H16	H13	2.34(7)	.	.	no
H16'	H51'	2.54(9)	.	2_666	no
H16'	C15	2.76(5)	.	2_666	no
H16'	H10	2.16(6)	.	.	no
H16'	C10	2.81(4)	.	.	no
H16'	O3	2.79(4)	.	2_666	no
H17	C4	3.08(4)	.	2_665	no
H17	O3	2.89(4)	.	.	no
H17	H61	2.37(7)	.	.	no
H17	O6	2.63(4)	.	.	no
H17'	O3	2.58(5)	.	.	no
H17'	H61	2.56(7)	.	.	no
H17'	C81A	2.99(8)	.	.	no
H17'	H811	2.5200	.	.	no
H17'	H17"	2.52(7)	.	2_665	no
H17"	H17'	2.52(7)	.	2_665	no
H17"	C4	3.03(5)	.	2_665	no
H17"	H22	2.44(8)	.	2_665	no
H17"	C3	3.07(5)	.	2_665	no
H17"	C17	3.00(5)	.	2_665	no
H22	C81B	2.97(6)	.	.	no
H22	C81A	2.74(8)	.	.	no
H22	H26	2.29(8)	.	2_575	no

H22	C13	2.85(6)	.	2_665	no
H22	H811"	1.7700	.	.	no
H22	C17	3.05(6)	.	2_665	no
H22	H812	2.2600	.	.	no
H22	C14	2.84(6)	.	2_665	no
H22	H17"	2.44(8)	.	2_665	no
H22	N6	1.92(6)	.	2_665	no
H24	O5	2.08(10)	.	1_655	no
H24	H51	2.46(12)	.	1_655	no
H24	H51'	2.47(13)	.	1_655	no
H24	H51'	2.47(13)	.	2_666	no
H24	H27	2.48(11)	.	2_676	no
H25	O7	2.02(12)	.	2_665	no
H25	H812'	2.4700	.	1_655	no
H25	O8A	2.88(11)	.	2_665	no
H25	H8'	2.30(13)	.	.	no
H25	H71	2.03(14)	.	2_665	no
H26	H22	2.29(8)	.	2_575	no
H26	C7	2.79(6)	.	2_575	no
H26	O2	2.08(6)	.	2_575	no
H26	H812	2.2000	.	2_575	no
H26'	C18	2.83(5)	.	2_576	no
H26'	S1	2.92(5)	.	2_576	no
H26'	N7	2.87(6)	.	2_576	no
H27	O4	2.29(5)	.	2_676	no
H27	H24	2.48(11)	.	2_676	no
H27	C10	2.81(6)	.	2_676	no
H27'	H7'	2.54(7)	.	1_556	no
H27'	Fe	3.48(6)	.	2_676	no
H27'	O1	2.33(5)	.	2_676	no
H27'	H7	2.58(7)	.	1_556	no
H27'	C7	3.04(5)	.	1_556	no
H27'	N5	2.92(6)	.	2_676	no
H51	H61'	2.56(9)	.	.	no
H51	O6	1.92(7)	.	.	no
H51	H71'	2.46(9)	.	.	no
H51	H61	2.51(9)	.	.	no
H51	H24	2.46(12)	.	1_455	no
H51'	H71'	2.42(10)	.	.	no
H51'	H24	2.47(13)	.	2_666	no
H51'	H24	2.47(13)	.	1_455	no
H51'	C16	2.72(8)	.	2_666	no
H51'	H16'	2.54(9)	.	2_666	no
H51'	O4	2.10(9)	.	2_666	no
H61	O3	2.08(5)	.	.	no
H61	C15	3.08(5)	.	.	no
H61	Fe	3.31(5)	.	.	no
H61	S1	3.13(6)	.	.	no
H61	H811	1.8300	.	.	no
H61	H51	2.51(9)	.	.	no
H61	H812"	2.5000	.	.	no
H61	C17	2.88(6)	.	.	no
H61	C81A	2.80(7)	.	.	no
H61	H17	2.37(7)	.	.	no
H61	H17'	2.56(7)	.	.	no
H61'	C81A	2.03(7)	.	.	no
H61'	O8B	2.00(6)	.	.	no
H61'	H811	1.2300	.	.	no
H61'	C81B	2.13(6)	.	.	no
H61'	H811'	2.1700	.	.	no
H61'	H812'	2.5700	.	.	no

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 H61'    H812"        1.6400                    .       .                 no
 H61'    H51         2.56(9)                    .       .                 no
 H61'    H82          2.0800                    .       .                 no
 H61'    O8A         2.83(6)                    .       .                 no
 H71     H81          1.4700                    .     2_565               no
 H71     O8A         2.23(8)                    .     2_565               no
 H71     N2          2.82(8)                    .     2_665               no
 H71     C81A       2.59(10)                    .     2_565               no
 H71     C81B        2.62(7)                    .     2_565               no
 H71     H811'        2.1300                    .     2_565               no
 H71     O8A         2.78(7)                    .       .                 no
 H71     H81          2.5300                    .       .                 no
 H71     H25        2.03(14)                    .     2_665               no
 H71     H812'        1.7200                    .     2_565               no
 H71'    H51'       2.42(10)                    .       .                 no
 H71'    H51         2.46(9)                    .       .                 no
 H71'    O5          2.10(5)                    .       .                 no
 H71'    H812'        2.4800                    .     2_565               no
 H71'    H81          2.4800                    .     2_565               no
 H81     H71'         2.4800                    .     2_565               no
 H81     H812'        2.0300                    .       .                 no
 H81     H71          2.5300                    .       .                 no
 H81     O7           2.1700                    .     2_565               no
 H81     H8'          2.5600                    .     2_665               no
 H81     H71          1.4700                    .     2_565               no
 H82     O6           2.8700                    .       .                 no
 H82     C8           2.8600                    .     1_455               no
 H82     H8"          2.3000                    .     1_455               no
 H82     H61'         2.0800                    .       .                 no
 H82     H1           2.2100                    .     2_575               no
 H811    O6           1.6200                    .       .                 no
 H811    H17'         2.5200                    .       .                 no
 H811    H61          1.8300                    .       .                 no
 H811    H61'         1.2300                    .       .                 no
 H812    O2           1.9600                    .       .                 no
 H812    H22          2.2600                    .       .                 no
 H812    O7           2.6200                    .     2_565               no
 H812    N3           2.5400                    .     2_575               no
 H812    N4           2.9100                    .     2_575               no
 H812    H26          2.2000                    .     2_575               no

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_geom_hbond_angle_DHA
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_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
O2      H22     N6         0.79(6)    1.92(6)   2.707(5)     171(7)   2_665 yes
O4      H24     O5        0.84(10)   2.08(10)   2.838(5)     151(9)   1_655 yes
N2      H25     O7        0.82(12)   2.02(12)   2.831(7)    168(12)   2_665 yes
N4      H26     O2         0.86(6)    2.08(6)   2.918(6)     166(6)   2_575 yes
N8      H27     O4         0.80(5)    2.29(5)   3.074(5)     167(5)   2_676 yes
N8      H27'    O1         0.88(5)    2.33(5)   3.100(5)     146(4)   2_676 yes
O5      H51     O6         0.86(7)    1.92(7)   2.768(6)     171(6)     .   yes
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O5      H51'    O4         0.86(9)    2.10(9)   2.817(5)     141(8)   2_666 yes
O6      H61     O3         0.85(5)    2.08(5)   2.926(6)     172(6)     .   yes
O6      H61'    O8B        0.86(5)    2.00(6)  2.856(11)     175(6)     .   yes
O7      H71     O8A        0.91(4)    2.23(8)  2.807(13)     121(7)   2_565 yes
O7      H71'    O5         0.87(4)    2.10(5)   2.919(6)     158(5)     .   yes
O8A     H81     O7          0.8400     2.1700  2.807(13)     133.00   2_565 yes
C1      H1      O8B        0.94(5)    2.51(5)  3.382(12)     154(4)   2_575 yes
C81A    H811'   O7          0.9800     2.1700    2.80(6)     121.00   2_565 yes
C81A    H811"   O2          0.9800     1.8300    2.73(7)     152.00     .   yes
C81B    H812'   O7          0.9800     1.6800    2.52(2)     141.00   2_565 yes
C81A    H812"   O6          0.5200     2.2200    2.49(2)     115.00     .   yes
C81A    H811    O6          0.9800     1.6200    2.49(2)     145.00     .   yes
C81B    H812    O2          0.9800     1.9600    2.71(2)     132.00     .   yes
C81B    H812    N3          0.9800     2.5400    3.01(2)     110.00   2_575 yes

# Loop Mechanism for Extra Tables(s)

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#_publ_manuscript_incl_extra_item
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#'_geom_extra_tableA_col_2'
#'_geom_extra_tableA_col_3'
#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
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#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'


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#loop_
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#_geom_extra_tableA_col_3
# ? ? ?


#
#loop_
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#_geom_extra_tableB_col_3
# ? ? ?


#
#_geom_table_footnote_A
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# ?
#;


#
#_geom_table_footnote_B
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# ?
#;
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#
#_geom_table_footnote_A
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#;


#
#_geom_table_footnote_B
#;
# ?
#;


#===END of Crystallographic Information File
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