Neutral and cationic paramagnetic amino-amidinate Iron(II) complexes

Sciarone, Timo J. J.; Nijhuis, Christian A.; Meetsma, Auke; Hessen, Bart

Published in:
Organometallics

DOI:
10.1021/om701155b

Publication date:
2008

```
# CIF-file generated for  C21H31FeN3Si                CP502

#==============================================================================
data_global
#==============================================================================

# 0. AUDIT DETAILS

_audit_creation_date                 '2001-08-21  14:12:15'
_audit_creation_method               'PLATON <TABLE ACC> option'
_audit_update_record
;
 ?
;

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

# 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              'Organometallics'
# Publication choise FI FM FO CI CM CO
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2007-09-04    11:05:45

 Consider this CIF submission for deposition of coumpound 4
 X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : CP502)
;

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

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?

_journal_date_to_coeditor            ?
_journal_date_from_coeditor          ?
_journal_date_accepted               ?

_journal_date_printers_first         ?
_journal_date_printers_final         ?
```

```
_journal_date_proofs_out             ?
_journal_date_proofs_in              ?

_journal_coeditor_name               ?
_journal_coeditor_code               ?
_journal_coeditor_notes
; ?
;

_journal_techeditor_code             ?
_journal_techeditor_notes
; ?
;

_journal_coden_ASTM                  ?
_journal_name_full                   ?
_journal_year                        ?
_journal_volume                      ?
_journal_issue                       ?
_journal_page_first                  ?
_journal_page_last                   ?


_journal_suppl_publ_number           ?
_journal_suppl_publ_pages            ?


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

# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
 ?
;
_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.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

   '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
;
 ?
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
 The asymmetric unit consists of an half molecule of the title compound.
The molecule (dimer) has a crystallographic imposed twofold axis.
;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
The structure was solved by Patterson methods and extension of the model was
 accomplished by direct methods applied to difference structure factors using
the program DIRDIF.The positional and anisotropic displacement parameters for
the non-hydrogen atoms were refined.
Refinement was complicated (frustrated) by a disorder problem: from the solution
 it was clear that the benzyl ligand was highly disordered. The electron density
 of the carbon atoms appeared to be spread out, indicating conformational
disorder. A disorder model with two conformations of the benzyl ligand
(refined to s.o.f.?s of .44  and .56, respectively) was introduced with
?variable metric? rigid group restraints in the refinement.
A subsequent difference Fourier synthesis resulted in the location of all the
hydrogen atoms which coordinates and isotropic displacement parameters were
refined, except those belonging to disordered C atoms of the benzyl ligand
(C15--C21). The remaining hydrogen atoms were generated by geometrical
 considerations and refined in the riding mode. The a.d.p. of C15 converged
to non-positive definite displacement parameters when allowed to vary
anisotropically, so ultimately this was reset to an isotropic displacement
 factor.
;

# Insert blank lines between references

_publ_section_references
;
 Beurskens, P.T., Beurskens, G., Gelder, R. de   Garc\'ia-Granda, S.
  Gould, R.O.  Isra\"el, & Smits, J.M.M. (1999).
  The DIRDIF99 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.

 Bruker, (2000). SMART, SAINT, SADABS, XPREP and  SHELXTL/NT.
  Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

 International Tables for Crystallography (1983). Vol. A.
   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
   (Present distributor Kluwer Academic Publishers, Dordrecht).
```

International Tables for Crystallography (1992). Vol. C.
  Edited by A.J.C Wilson, Kluwer Academic Publishers,
  Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2001). Extended version of the program PLUTO.
  Groningen University, The Netherlands. (unpublished).

Sheldrick, G.M. SHELXL97. Program for Crystal Structure
  Refinement. University of G\"ottingen, Germany, 1997.

Sheldrick, G.M. SADABS. Version 2. Multi-Scan Absorption Correction Program.
  University of G\"ottingen, Germany, 2001

Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
;

_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.
;

#==

data_c21h31fe

#==

5. CHEMICAL DATA

_chemical_name_systematic
;
 ?
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety
'C42 H62 Fe2 N6 Si2'
_chemical_formula_structural   ?
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C42 H62 Fe2 N6 Si2'
_chemical_formula_weight   818.86

```
_chemical_compound_source          'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Si  Si    0.0817    0.0704
 '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     '-C 2yc'
_symmetry_space_group_name_H-M      'C 2/c'

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

_cell_length_a                        14.9022(9)
_cell_length_b                        13.1648(8)
_cell_length_c                        22.578(1)
_cell_angle_alpha                     90
_cell_angle_beta                      103.166(1)
_cell_angle_gamma                     90
_cell_volume                         4313.0(4)
_cell_formula_units_Z                 4

_cell_measurement_temperature    125(1)
_cell_measurement_reflns_used      2747
_cell_measurement_theta_min        2.41
_cell_measurement_theta_max       23.13
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   2747 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'parallelepiped'
_exptl_crystal_colour            'orange red-brown'
_exptl_crystal_size_max           0.22
```

```
_exptl_crystal_size_mid           0.19
_exptl_crystal_size_min           0.17
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.261
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1744
_exptl_absorpt_coefficient_mu     0.764

_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min   0.8499
_exptl_absorpt_correction_T_max   0.8811

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

# 7. EXPERIMENTAL DATA



_diffrn_ambient_temperature       125(1)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_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
;
_diffrn_measurement_method           'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature
  unit (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean     66.06

_diffrn_standards_number             ?
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      ?

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             20647
_diffrn_reflns_av_R_equivalents   0.0634
_diffrn_reflns_av_sigmaI/netI     0.0729
_diffrn_reflns_limit_h_min        -19
_diffrn_reflns_limit_h_max        19
_diffrn_reflns_limit_k_min        -17
_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -30
_diffrn_reflns_limit_l_max        30
```

```
_diffrn_reflns_theta_min          2.41
_diffrn_reflns_theta_max          28.28
_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              28.28
_diffrn_measured_fraction_theta_full   0.999

_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
_reflns_number_total              5349
_reflns_number_gt                 3689
_reflns_threshold_expression      >2sigma(I)


_computing_data_collection          'SMART, Bruker Version 5.168, 2000'
_computing_cell_refinement          'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction           'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2001)
 ORTEP (Farrugia, 1997; Johnson et al., 2000)
 PLATON (Spek, 1994)
;
_computing_publication_material
;
 PLATON (Spek, 1990)
 SHELXL (Sheldrick, 1997)
;

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

# 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^ > 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^)+(0.0486P)^2^+2.6612P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
```

```
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          5349
_refine_ls_number_parameters      288
_refine_ls_number_restraints      2
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0837
_refine_ls_R_factor_gt            0.0483
_refine_ls_wR_factor_ref          0.1163
_refine_ls_wR_factor_gt           0.1041
_refine_ls_goodness_of_fit_ref    1.017
_refine_ls_restrained_S_all       1.017
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max    0.455
_refine_diff_density_min   -0.454
_refine_diff_density_rms    0.072
_vrn_publ_code_void_volume             0.000
_vrn_publ_code_meas_time              11.900

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

# 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 0.08870(2) 0.26376(3) 0.29826(2) 1.000 0.0203(1) . .
Si Si Uani 0.00021(5) 0.13623(6) 0.39799(3) 1.000 0.0292(2) . .
N1 N Uani -0.15506(14) 0.40618(16) 0.15890(9) 1.000 0.0252(7) . .
N2 N Uani -0.09858(15) 0.34728(15) 0.27921(9) 1.000 0.0240(7) . .
N3 N Uani -0.01015(14) 0.23698(15) 0.34667(9) 1.000 0.0222(6) . .
C1 C Uani -0.0912(2) 0.4889(2) 0.15339(13) 1.000 0.0332(9) . .
C2 C Uani -0.2161(2) 0.3872(2) 0.09858(14) 1.000 0.0436(10) . .
C3 C Uani -0.21156(19) 0.4356(2) 0.20209(13) 1.000 0.0311(9) . .
C4 C Uani -0.1545(2) 0.4401(2) 0.26652(12) 1.000 0.0319(9) . .
C5 C Uani -0.07703(17) 0.30755(19) 0.33416(11) 1.000 0.0222(8) . .
C6 C Uani -0.12392(19) 0.3412(2) 0.38338(11) 1.000 0.0270(8) . .
C7 C Uani -0.0716(2) 0.3768(2) 0.43831(12) 1.000 0.0385(10) . .
C8 C Uani -0.1141(3) 0.4042(3) 0.48504(14) 1.000 0.0557(13) . .
C9 C Uani -0.2075(3) 0.3945(3) 0.47749(16) 1.000 0.0643(16) . .
C10 C Uani -0.2600(3) 0.3592(3) 0.42349(16) 1.000 0.0571(14) . .
C11 C Uani -0.2184(2) 0.3338(3) 0.37622(13) 1.000 0.0411(10) . .
C12 C Uani 0.1089(2) 0.1498(3) 0.45695(14) 1.000 0.0434(11) . .
C13 C Uani -0.0966(2) 0.1222(3) 0.43755(16) 1.000 0.0465(11) . .
C14 C Uani -0.0003(3) 0.0157(2) 0.35467(15) 1.000 0.0485(13) . .
C152 C Uiso 0.1847(3) 0.1438(4) 0.2867(2) 0.558(5) 0.0312(14) . .
```

```
C162 C Uani 0.28036(19) 0.1605(2) 0.32054(13) 0.558(5) 0.024(2) . .
C172 C Uani 0.3387(2) 0.2185(2) 0.29417(14) 0.558(5) 0.0394(19) . .
C182 C Uani 0.4271(2) 0.2414(3) 0.32702(17) 0.558(5) 0.057(3) . .
C192 C Uani 0.4571(2) 0.2062(3) 0.38625(18) 0.558(5) 0.065(3) . .
C202 C Uani 0.3988(2) 0.1482(3) 0.41264(16) 0.558(5) 0.049(2) . .
C212 C Uani 0.3104(2) 0.1253(2) 0.37975(14) 0.558(5) 0.0380(19) . .
C151 C Uiso 0.1792(4) 0.1408(4) 0.3075(3) 0.442(5) 0.0203(14) . .
C161 C Uani 0.2765(2) 0.1732(3) 0.30986(17) 0.442(5) 0.037(3) . .
C171 C Uani 0.3010(3) 0.1957(3) 0.25458(18) 0.442(5) 0.036(2) . .
C181 C Uani 0.3926(3) 0.2221(4) 0.2545(3) 0.442(5) 0.050(3) . .
C191 C Uani 0.4596(3) 0.2260(4) 0.3096(3) 0.442(5) 0.079(5) . .
C201 C Uani 0.4351(4) 0.2035(5) 0.3649(3) 0.442(5) 0.078(5) . .
C211 C Uani 0.3436(3) 0.1771(4) 0.3650(2) 0.442(5) 0.044(3) . .
H3 H Uiso -0.23737 0.49448 0.19181 1.000 0.017(6) . .
H3' H Uiso -0.26880 0.37888 0.20268 1.000 0.062(10) . .
H4 H Uiso -0.11806 0.49782 0.26943 1.000 0.021(7) . .
H4' H Uiso -0.19381 0.45383 0.29142 1.000 0.037(8) . .
H7 H Uiso -0.00126 0.38014 0.45057 1.000 0.043(9) . .
H8 H Uiso -0.07246 0.42253 0.52305 1.000 0.061(10) . .
H9 H Uiso -0.23790 0.41080 0.50852 1.000 0.067(11) . .
H10 H Uiso -0.33421 0.35143 0.41232 1.000 0.093(14) . .
H11 H Uiso -0.25625 0.30451 0.33713 1.000 0.046(9) . .
H12 H Uiso 0.16509 0.15122 0.43934 1.000 0.052(10) . .
H12' H Uiso 0.12905 0.09721 0.47575 1.000 0.060(11) . .
H12" H Uiso 0.09656 0.19784 0.48812 1.000 0.064(11) . .
H13 H Uiso -0.09450 0.17466 0.46507 1.000 0.050(10) . .
H13' H Uiso -0.08962 0.05400 0.45824 1.000 0.065(11) . .
H13" H Uiso -0.15477 0.11978 0.40608 1.000 0.066(12) . .
H14 H Uiso -0.05343 0.01045 0.32047 1.000 0.118(18) . .
H14' H Uiso 0.00149 -0.04464 0.38108 1.000 0.077(12) . .
H14" H Uiso 0.05681 0.01079 0.33733 1.000 0.063(11) . .
H152 H Uiso 0.16276 0.07855 0.29997 0.558(5) 0.0374 . .
H172 H Uiso 0.31816 0.24257 0.25367 0.558(5) 0.0474 . .
H182 H Uiso 0.46698 0.28108 0.30899 0.558(5) 0.0685 . .
H192 H Uiso 0.51750 0.22188 0.40872 0.558(5) 0.0776 . .
H202 H Uiso 0.41928 0.12414 0.45314 0.558(5) 0.0593 . .
H212 H Uiso 0.27049 0.08561 0.39777 0.558(5) 0.0455 . .
H1 H Uiso -0.05514 0.50095 0.19092 1.000 0.043(9) . .
H1' H Uiso -0.05323 0.46875 0.12688 1.000 0.035(8) . .
H1" H Uiso -0.12620 0.55210 0.13591 1.000 0.047(9) . .
H2 H Uiso -0.25809 0.33217 0.10332 1.000 0.035(8) . .
H2' H Uiso -0.24992 0.43979 0.07450 1.000 0.064(11) . .
H2" H Uiso -0.17983 0.36651 0.07358 1.000 0.047(10) . .
H152'  H Uiso 0.18400 0.13765 0.24288 0.558(5) 0.0374 . .
H151'  H Uiso 0.15858 0.09389 0.27279 0.442(5) 0.0243 . .
H151 H Uiso 0.17726 0.10334 0.34524 0.442(5) 0.0243 . .
H171 H Uiso 0.25577 0.19302 0.21739 0.442(5) 0.0429 . .
H181 H Uiso 0.40913 0.23722 0.21725 0.442(5) 0.0595 . .
H191 H Uiso 0.52139 0.24378 0.30954 0.442(5) 0.0948 . .
H201 H Uiso 0.48035 0.20616 0.40209 0.442(5) 0.0936 . .
H211 H Uiso 0.32706 0.16195 0.40230 0.442(5) 0.0532 . .

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 0.0222(2) 0.0171(2) 0.0226(2) -0.0007(1) 0.0069(1) -0.0004(2)
```

```
Si 0.0335(4) 0.0266(4) 0.0280(4) 0.0087(3) 0.0083(3) -0.0011(3)
N1 0.0275(12) 0.0225(11) 0.0240(11) 0.0028(9) 0.0027(9) 0.0024(9)
N2 0.0308(12) 0.0199(11) 0.0238(11) 0.0022(8) 0.0113(9) 0.0067(9)
N3 0.0239(11) 0.0220(11) 0.0214(10) 0.0038(8) 0.0069(9) -0.0009(9)
C1 0.0398(17) 0.0288(15) 0.0337(16) 0.0084(12) 0.0139(14) 0.0010(13)
C2 0.053(2) 0.0320(17) 0.0360(16) 0.0040(13) -0.0100(16) 0.0057(15)
C3 0.0292(15) 0.0249(14) 0.0409(16) 0.0124(12) 0.0115(13) 0.0138(12)
C4 0.0389(17) 0.0266(15) 0.0356(15) 0.0056(12) 0.0197(13) 0.0150(13)
C5 0.0243(14) 0.0226(13) 0.0210(12) -0.0021(10) 0.0080(10) -0.0041(11)
C6 0.0356(16) 0.0269(14) 0.0204(12) 0.0012(10) 0.0102(11) 0.0019(12)
C7 0.053(2) 0.0393(18) 0.0247(14) -0.0029(12) 0.0122(14) -0.0119(15)
C8 0.087(3) 0.054(2) 0.0299(17) -0.0148(15) 0.0212(19) -0.010(2)
C9 0.090(3) 0.072(3) 0.046(2) -0.0039(19) 0.047(2) 0.011(2)
C10 0.048(2) 0.080(3) 0.053(2) 0.0047(19) 0.0315(18) 0.0142(19)
C11 0.0382(18) 0.058(2) 0.0311(16) -0.0008(14) 0.0165(14) 0.0034(15)
C12 0.045(2) 0.045(2) 0.0377(17) 0.0166(15) 0.0043(15) 0.0049(15)
C13 0.051(2) 0.0367(19) 0.058(2) 0.0175(17) 0.0251(18) -0.0054(15)
C14 0.070(3) 0.0239(16) 0.052(2) 0.0055(14) 0.0145(19) -0.0015(15)
C162 0.029(4) 0.008(3) 0.041(4) 0.007(3) 0.019(3) 0.010(3)
C172 0.043(4) 0.036(3) 0.043(3) 0.014(3) 0.018(3) 0.013(3)
C182 0.025(4) 0.021(3) 0.120(7) -0.003(4) 0.006(4) 0.011(3)
C192 0.037(4) 0.042(5) 0.108(7) -0.020(4) 0.001(5) -0.001(3)
C202 0.051(4) 0.048(4) 0.043(4) -0.009(3) -0.001(3) 0.018(3)
C212 0.049(4) 0.028(3) 0.038(3) -0.002(2) 0.012(3) 0.009(3)
C161 0.061(8) 0.020(5) 0.019(3) 0.003(3) -0.013(4) 0.021(5)
C171 0.035(4) 0.030(4) 0.044(4) -0.002(3) 0.011(3) 0.002(3)
C181 0.036(4) 0.034(4) 0.084(6) 0.006(4) 0.025(4) 0.003(3)
C191 0.019(5) 0.049(6) 0.168(12) 0.003(7) 0.019(6) 0.016(4)
C201 0.040(6) 0.058(9) 0.127(11) -0.016(7) -0.002(8) 0.025(6)
C211 0.032(4) 0.046(5) 0.050(5) -0.006(4) -0.001(4) 0.007(4)

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

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds 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      N3         2.055(2)                    .       .                 yes
 Fe      C152       2.186(5)                    .       .                 yes
 Fe      C151       2.087(6)                    .       .                 yes
 Fe      N1         2.235(2)                    .     2_555               yes
 Fe      N2         2.099(2)                    .     2_555               yes
 Si      N3         1.745(2)                    .       .                 yes
 Si      C12        1.856(3)                    .       .                 yes
 Si      C13        1.871(3)                    .       .                 yes
 Si      C14        1.863(3)                    .       .                 yes
 N1      C1         1.470(4)                    .       .                 yes
```

N1	C2	1.477(4)	.	.	yes
N1	C3	1.478(4)	.	.	yes
N2	C4	1.470(3)	.	.	yes
N2	C5	1.317(3)	.	.	yes
N3	C5	1.345(3)	.	.	yes
C3	C4	1.510(4)	.	.	no
C5	C6	1.508(4)	.	.	no
C6	C7	1.388(4)	.	.	no
C6	C11	1.383(4)	.	.	no
C7	C8	1.396(5)	.	.	no
C8	C9	1.369(6)	.	.	no
C9	C10	1.371(5)	.	.	no
C10	C11	1.391(5)	.	.	no
C1	H1'	0.9503	.	.	no
C1	H1"	1.0131	.	.	no
C1	H1	0.9080	.	.	no
C2	H2	0.9790	.	.	no
C2	H2'	0.9508	.	.	no
C2	H2"	0.9077	.	.	no
C3	H3	0.8729	.	.	no
C3	H3'	1.1360	.	.	no
C4	H4'	0.9176	.	.	no
C4	H4	0.9276	.	.	no
C7	H7	1.0223	.	.	no
C8	H8	0.9681	.	.	no
C9	H9	0.9416	.	.	no
C10	H10	1.0817	.	.	no
C11	H11	1.0100	.	.	no
C12	H12"	0.9940	.	.	no
C12	H12'	0.8316	.	.	no
C12	H12	1.0056	.	.	no
C13	H13'	1.0065	.	.	no
C13	H13"	0.9883	.	.	no
C13	H13	0.9247	.	.	no
C14	H14"	1.0166	.	.	no
C14	H14	0.9744	.	.	no
C14	H14'	0.9900	.	.	no
C151	C161	1.501(7)	.	.	no
C152	C162	1.472(5)	.	.	no
C161	C211	1.409(6)	.	.	no
C161	C171	1.409(5)	.	.	no
C162	C172	1.389(4)	.	.	no
C162	C212	1.389(4)	.	.	no
C171	C181	1.409(7)	.	.	no
C172	C182	1.390(5)	.	.	no
C181	C191	1.408(9)	.	.	no
C182	C192	1.389(5)	.	.	no
C191	C201	1.410(9)	.	.	no
C192	C202	1.389(5)	.	.	no
C201	C211	1.408(8)	.	.	no
C202	C212	1.390(4)	.	.	no
C151	H151'	0.9901	.	.	no
C151	H151	0.9906	.	.	no
C152	H152	0.9895	.	.	no
C152	H152'	0.9904	.	.	no
C171	H171	0.9502	.	.	no
C172	H172	0.9501	.	.	no
C181	H181	0.9497	.	.	no
C182	H182	0.9497	.	.	no
C191	H191	0.9504	.	.	no
C192	H192	0.9498	.	.	no

```
 C201    H201         0.9503                    .      .                 no
 C202    H202         0.9500                    .      .                 no
 C211    H211         0.9510                    .      .                 no
 C212    H212         0.9500                    .      .                 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
 N3      Fe      C152     120.50(14)              .      .      .          yes
 N3      Fe      C151     109.82(18)              .      .      .          yes
 N1      Fe      N3        102.35(8)           2_555     .      .          yes
 N2      Fe      N3        136.71(9)           2_555     .      .          yes
 N1      Fe      C152     114.88(14)           2_555     .      .          yes
 N2      Fe      C152      96.14(13)           2_555     .      .          yes
 N1      Fe      C151     113.29(17)           2_555     .      .          yes
 N2      Fe      C151     108.86(19)           2_555     .      .          yes
 N1      Fe      N2         79.23(8)           2_555     .    2_555        yes
 N3      Si      C12      109.50(14)              .      .      .          yes
 N3      Si      C13      115.52(14)              .      .      .          yes
 N3      Si      C14      108.04(12)              .      .      .          yes
 C12     Si      C13      107.99(15)              .      .      .          yes
 C12     Si      C14      110.92(18)              .      .      .          yes
 C13     Si      C14      104.78(18)              .      .      .          yes
 C1      N1      C2         108.8(2)              .      .      .          yes
 C1      N1      C3         109.8(2)              .      .      .          yes
 Fe      N1      C1       115.28(16)           2_555     .      .          yes
 C2      N1      C3         109.2(2)              .      .      .          yes
 Fe      N1      C2       112.10(15)           2_555     .      .          yes
 Fe      N1      C3       101.35(15)           2_555     .      .          yes
 C4      N2      C5         121.3(2)              .      .      .          yes
 Fe      N2      C4       114.66(15)           2_555     .      .          yes
 Fe      N2      C5       121.91(17)           2_555     .      .          yes
 Fe      N3      Si       121.20(11)              .      .      .          yes
 Fe      N3      C5       110.89(16)              .      .      .          yes
 Si      N3      C5       127.88(18)              .      .      .          yes
 N1      C3      C4         111.4(2)              .      .      .          yes
 N2      C4      C3         109.0(2)              .      .      .          yes
 N2      C5      N3         118.8(2)              .      .      .          yes
 N2      C5      C6         121.5(2)              .      .      .          yes
 N3      C5      C6         119.6(2)              .      .      .          yes
 C5      C6      C7         119.8(3)              .      .      .          no
 C5      C6      C11        121.6(2)              .      .      .          no
 C7      C6      C11        118.5(3)              .      .      .          no
 C6      C7      C8         120.2(3)              .      .      .          no
 C7      C8      C9         120.3(3)              .      .      .          no
 C8      C9      C10        120.0(4)              .      .      .          no
 C9      C10     C11        120.0(4)              .      .      .          no
 C6      C11     C10        120.9(3)              .      .      .          no
 H1      C1      H1"          111.27              .      .      .          no
 H1'     C1      H1"          108.15              .      .      .          no
 N1      C1      H1"          110.83              .      .      .          no
 N1      C1      H1           107.90              .      .      .          no
 N1      C1      H1'          109.65              .      .      .          no
 H1      C1      H1'          109.01              .      .      .          no
 N1      C2      H2           107.41              .      .      .          no
```

H2'	C2	H2"	100.14	.	.	.	no
N1	C2	H2"	107.18	.	.	.	no
H2	C2	H2'	109.43	.	.	.	no
N1	C2	H2'	122.62	.	.	.	no
H2	C2	H2"	109.38	.	.	.	no
C4	C3	H3	109.80	.	.	.	no
C4	C3	H3'	105.91	.	.	.	no
N1	C3	H3'	112.19	.	.	.	no
N1	C3	H3	109.88	.	.	.	no
H3	C3	H3'	107.47	.	.	.	no
H4	C4	H4'	103.91	.	.	.	no
N2	C4	H4'	117.19	.	.	.	no
N2	C4	H4	111.74	.	.	.	no
C3	C4	H4	107.01	.	.	.	no
C3	C4	H4'	107.46	.	.	.	no
C6	C7	H7	126.11	.	.	.	no
C8	C7	H7	113.45	.	.	.	no
C7	C8	H8	115.14	.	.	.	no
C9	C8	H8	124.18	.	.	.	no
C10	C9	H9	117.71	.	.	.	no
C8	C9	H9	122.26	.	.	.	no
C9	C10	H10	125.83	.	.	.	no
C11	C10	H10	114.14	.	.	.	no
C6	C11	H11	118.66	.	.	.	no
C10	C11	H11	120.29	.	.	.	no
H12	C12	H12"	124.97	.	.	.	no
H12'	C12	H12"	105.77	.	.	.	no
H12	C12	H12'	88.91	.	.	.	no
Si	C12	H12	112.79	.	.	.	no
Si	C12	H12'	116.14	.	.	.	no
Si	C12	H12"	107.28	.	.	.	no
H13'	C13	H13"	106.61	.	.	.	no
Si	C13	H13'	107.47	.	.	.	no
Si	C13	H13"	107.78	.	.	.	no
Si	C13	H13	109.59	.	.	.	no
H13	C13	H13"	113.39	.	.	.	no
H13	C13	H13'	111.73	.	.	.	no
H14	C14	H14'	109.02	.	.	.	no
Si	C14	H14"	110.65	.	.	.	no
Si	C14	H14'	111.77	.	.	.	no
Si	C14	H14	112.45	.	.	.	no
H14	C14	H14"	106.90	.	.	.	no
H14'	C14	H14"	105.72	.	.	.	no
Fe	C151	C161	112.4(3)	.	.	.	yes
Fe	C152	C162	114.4(3)	.	.	.	yes
C171	C161	C211	120.0(3)	.	.	.	no
C151	C161	C171	118.1(4)	.	.	.	no
C151	C161	C211	121.8(4)	.	.	.	no
C172	C162	C212	120.0(3)	.	.	.	no
C152	C162	C212	120.7(3)	.	.	.	no
C152	C162	C172	119.1(3)	.	.	.	no
C161	C171	C181	120.0(4)	.	.	.	no
C162	C172	C182	120.0(3)	.	.	.	no
C171	C181	C191	120.0(5)	.	.	.	no
C172	C182	C192	120.0(3)	.	.	.	no
C181	C191	C201	120.0(5)	.	.	.	no
C182	C192	C202	120.0(3)	.	.	.	no
C191	C201	C211	120.0(5)	.	.	.	no
C192	C202	C212	120.0(3)	.	.	.	no
C161	C211	C201	120.0(4)	.	.	.	no
C162	C212	C202	120.0(3)	.	.	.	no

```
 Fe      C151    H151'       109.13              .       .       .          no
 Fe      C151    H151        109.11              .       .       .          no
 C161    C151    H151'       109.18              .       .       .          no
 C161    C151    H151        109.16              .       .       .          no
 H151'   C151    H151        107.80              .       .       .          no
 H152'   C152    H152        107.61              .       .       .          no
 Fe      C152    H152        108.70              .       .       .          no
 C162    C152    H152'       108.62              .       .       .          no
 Fe      C152    H152'       108.67              .       .       .          no
 C162    C152    H152        108.67              .       .       .          no
 C181    C171    H171        120.03              .       .       .          no
 C161    C171    H171        120.01              .       .       .          no
 C182    C172    H172        119.98              .       .       .          no
 C162    C172    H172        120.00              .       .       .          no
 C171    C181    H181        119.97              .       .       .          no
 C191    C181    H181        120.01              .       .       .          no
 C192    C182    H182        120.03              .       .       .          no
 C172    C182    H182        120.01              .       .       .          no
 C201    C191    H191        119.96              .       .       .          no
 C181    C191    H191        120.01              .       .       .          no
 C202    C192    H192        119.98              .       .       .          no
 C182    C192    H192        119.97              .       .       .          no
 C211    C201    H201        120.02              .       .       .          no
 C191    C201    H201        120.00              .       .       .          no
 C212    C202    H202        119.97              .       .       .          no
 C192    C202    H202        120.07              .       .       .          no
 C201    C211    H211        119.98              .       .       .          no
 C161    C211    H211        119.99              .       .       .          no
 C162    C212    H212        119.98              .       .       .          no
 C202    C212    H212        120.01              .       .       .          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
 C152    Fe      N3      Si          19.7(2)     .       .       .       .   no
 C152    Fe      N3      C5        -162.3(2)     .       .       .       .   no
 N1      Fe      N3      Si      -109.29(12)   2_555     .       .       .   no
 N1      Fe      N3      C5        68.71(17)   2_555     .       .       .   no
 N2      Fe      N3      Si       163.38(10)   2_555     .       .       .   no
 N2      Fe      N3      C5         -18.6(2)   2_555     .       .       .   no
 N3      Fe      C152    C162      -109.9(3)     .       .       .       .   no
 N1      Fe      C152    C162        13.3(3)   2_555     .       .       .   no
 N2      Fe      C152    C162        94.2(3)   2_555     .       .       .   no
 N3      Fe      N1      C1       -50.18(18)     .       .     2_555   2_555 no
 N3      Fe      N1      C2        74.99(18)     .       .     2_555   2_555 no
 N3      Fe      N1      C3      -168.67(15)     .       .     2_555   2_555 no
 C152    Fe      N1      C1         177.4(2)     .       .     2_555   2_555 no
 C152    Fe      N1      C2         -57.4(2)     .       .     2_555   2_555 no
 C152    Fe      N1      C3          58.9(2)     .       .     2_555   2_555 no
 N3      Fe      N2      C4         106.6(2)     .       .     2_555   2_555 no
 N3      Fe      N2      C5         -89.8(2)     .       .     2_555   2_555 no
 C152    Fe      N2      C4        -104.2(2)     .       .     2_555   2_555 no
 C152    Fe      N2      C5          59.4(2)     .       .     2_555   2_555 no
```

N2	Fe	C152	H152'	-27.31	2_555	.	.	.	no
N2	Fe	C152	H152	-144.15	2_555	.	.	.	no
N3	Fe	C152	H152	11.76	.	.	.	.	no
N1	Fe	C152	H152'	-108.26	2_555	.	.	.	no
N3	Fe	C152	H152'	128.59	.	.	.	.	no
N1	Fe	C152	H152	134.90	2_555	.	.	.	no
C13	Si	N3	Fe	-179.41(15)	.	.	.	.	no
C13	Si	N3	C5	2.9(3)	.	.	.	.	no
C12	Si	N3	Fe	58.43(17)	.	.	.	.	no
C12	Si	N3	C5	-119.2(2)	.	.	.	.	no
C14	Si	N3	Fe	-62.48(19)	.	.	.	.	no
C14	Si	N3	C5	119.9(2)	.	.	.	.	no
C13	Si	C14	H14'	-52.75	.	.	.	.	no
C12	Si	C14	H14	-173.45	.	.	.	.	no
C12	Si	C14	H14'	63.54	.	.	.	.	no
C12	Si	C14	H14"	-53.99	.	.	.	.	no
C13	Si	C14	H14	70.26	.	.	.	.	no
N3	Si	C12	H12	-58.78	.	.	.	.	no
N3	Si	C12	H12'	-159.34	.	.	.	.	no
N3	Si	C12	H12"	82.64	.	.	.	.	no
C13	Si	C12	H12	174.65	.	.	.	.	no
C13	Si	C12	H12'	74.10	.	.	.	.	no
C13	Si	C12	H12"	-43.92	.	.	.	.	no
C14	Si	C12	H12	60.36	.	.	.	.	no
C14	Si	C12	H12'	-40.19	.	.	.	.	no
C14	Si	C12	H12"	-158.21	.	.	.	.	no
N3	Si	C13	H13	-70.65	.	.	.	.	no
N3	Si	C13	H13'	167.74	.	.	.	.	no
N3	Si	C13	H13"	53.18	.	.	.	.	no
C12	Si	C13	H13	52.31	.	.	.	.	no
C12	Si	C13	H13'	-69.29	.	.	.	.	no
C12	Si	C13	H13"	176.14	.	.	.	.	no
C14	Si	C13	H13	170.60	.	.	.	.	no
C14	Si	C13	H13'	49.00	.	.	.	.	no
C14	Si	C13	H13"	-65.57	.	.	.	.	no
N3	Si	C14	H14	-53.43	.	.	.	.	no
N3	Si	C14	H14'	-176.44	.	.	.	.	no
N3	Si	C14	H14"	66.04	.	.	.	.	no
C13	Si	C14	H14"	-170.28	.	.	.	.	no
C1	N1	C3	C4	-69.6(3)	.	.	.	.	no
Fe	N1	C3	C4	52.7(2)	2_555	.	.	.	no
C2	N1	C3	C4	171.2(2)	.	.	.	.	no
C5	N2	C4	C3	-148.1(2)	.	.	.	.	no
C4	N2	C5	C6	12.9(4)	.	.	.	.	no
Fe	N2	C5	N3	31.9(3)	2_555	.	.	.	no
Fe	N2	C5	C6	-149.6(2)	2_555	.	.	.	no
C4	N2	C5	N3	-165.6(2)	.	.	.	.	no
Fe	N2	C4	C3	15.6(3)	2_555	.	.	.	no
Fe	N3	C5	C6	-146.10(19)	.	.	.	.	no
Fe	N3	C5	N2	32.4(3)	.	.	.	.	no
Si	N3	C5	N2	-149.7(2)	.	.	.	.	no
Si	N3	C5	C6	31.7(3)	.	.	.	.	no
N1	C3	C4	N2	-47.8(3)	.	.	.	.	no
N3	C5	C6	C11	-123.0(3)	.	.	.	.	no
N3	C5	C6	C7	54.4(3)	.	.	.	.	no
N2	C5	C6	C7	-124.1(3)	.	.	.	.	no
N2	C5	C6	C11	58.5(4)	.	.	.	.	no
C5	C6	C7	C8	-177.4(3)	.	.	.	.	no
C5	C6	C11	C10	175.9(3)	.	.	.	.	no
C7	C6	C11	C10	-1.6(5)	.	.	.	.	no
C11	C6	C7	C8	0.1(4)	.	.	.	.	no

```
 C6      C7      C8      C9          1.2(5)     .      .      .      .   no
 C7      C8      C9      C10        -1.0(6)     .      .      .      .   no
 C8      C9      C10     C11        -0.4(6)     .      .      .      .   no
 C9      C10     C11     C6          1.8(6)     .      .      .      .   no
 C192    C202    C212    C162       -0.1(5)     .      .      .      .   no
 H152'   C152    C162    C172         35.60     .      .      .      .   no
 H152'   C152    C162    C212       -149.07     .      .      .      .   no
 H152    C152    C162    C172        152.40     .      .      .      .   no
 H152    C152    C162    C212        -32.28     .      .      .      .   no
 C152    C162    C172    H172         -4.65     .      .      .      .   no
 C212    C162    C172    H172        180.00     .      .      .      .   no
 C152    C162    C212    H212          4.74     .      .      .      .   no
 C172    C162    C212    H212       -179.98     .      .      .      .   no
 C162    C172    C182    H182       -179.98     .      .      .      .   no
 H172    C172    C182    C192        179.98     .      .      .      .   no
 H172    C172    C182    H182         -0.03     .      .      .      .   no
 C172    C182    C192    H192       -179.96     .      .      .      .   no
 H182    C182    C192    C202        179.98     .      .      .      .   no
 H182    C182    C192    H192          0.05     .      .      .      .   no
 C182    C192    C202    H202       -180.00     .      .      .      .   no
 H192    C192    C202    C212        179.98     .      .      .      .   no
 H192    C192    C202    H202         -0.04     .      .      .      .   no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 Fe      H12          3.4620                    .      .                 no
 Fe      H14"         3.5051                    .      .                 no
 Fe      H171         3.5314                    .      .                 no
 Si      C7         3.528(3)                    .      .                 no
 Si      H7           3.4253                    .      .                 no
 Si      H151         3.1621                    .      .                 no
 N2      C1         3.439(4)                    .    2_555               no
 C1      N2         3.439(4)                    .    2_555               no
 C1      C5         3.427(4)                    .    2_555               no
 C2      C211       3.556(6)                    .    2_555               no
 C3      C172       3.441(4)                    .    2_555               no
 C3      C161       3.581(5)                    .    2_555               no
 C4      C11        3.173(4)                    .      .                 no
 C4      C162       3.375(4)                    .    5_455               no
 C4      C161       3.448(5)                    .    5_455               no
 C4      C171       3.428(5)                    .    5_455               no
 C5      C1         3.427(4)                    .    2_555               no
 C6      C13        3.122(5)                    .      .                 no
 C7      C13        3.372(5)                    .      .                 no
 C7      Si         3.528(3)                    .      .                 no
 C8      C202       3.568(5)                    .    7_556               no
 C8      C192       3.596(5)                    .    7_556               no
 C11     C171       3.448(5)                    .    2_555               no
 C11     C4         3.173(4)                    .      .                 no
 C11     C13        3.440(5)                    .      .                 no
 C13     C11        3.440(5)                    .      .                 no
 C13     C7         3.372(5)                    .      .                 no
 C13     C6         3.122(5)                    .      .                 no
 C14     C151       3.507(7)                    .      .                 no
 C1      H4           2.7415                    .      .                 no
 C4      H11          3.0213                    .      .                 no
```

C4	H1	2.6266	.	.	no
C5	@52'	3.0506	.	2_555	no
C5	H1'	2.8753	.	2_555	no
C5	H171	3.0513	.	2_555	no
C6	H13	2.8342	.	.	no
C6	H4'	2.5708	.	.	no
C6	H13"	3.0130	.	.	no
C7	H202	2.9368	.	7_556	no
C7	H1'	2.8878	.	2_555	no
C7	H13	2.7671	.	.	no
C8	H192	3.0013	.	7_556	no
C8	H202	3.0517	.	5_455	no
C8	H202	2.9445	.	7_556	no
C8	H13	3.0790	.	.	no
C9	H212	3.0673	.	5_455	no
C10	H212	3.0900	.	5_455	no
C11	H13"	3.0014	.	.	no
C11	H4'	2.5715	.	.	no
C11	H171	2.7714	.	2_555	no
C12	H151	2.9906	.	.	no
C13	H9	3.0203	.	7_456	no
C14	H152	3.0792	.	.	no
C14	H151	2.9385	.	.	no
C151	C14	3.507(7)	.	.	no
C161	C4	3.448(5)	.	5_545	no
C161	C3	3.581(5)	.	2_555	no
C162	C4	3.375(4)	.	5_545	no
C171	C4	3.428(5)	.	5_545	no
C171	C11	3.448(5)	.	2_555	no
C172	C3	3.441(4)	.	2_555	no
C181	C181	3.253(7)	.	2_655	no
C181	C191	2.898(7)	.	2_655	no
C191	C181	2.898(7)	.	2_655	no
C191	C191	3.189(9)	.	2_655	no
C192	C8	3.596(5)	.	7_556	no
C202	C8	3.568(5)	.	7_556	no
C211	C2	3.556(6)	.	2_555	no
C151	H14"	2.6961	.	.	no
C151	H12	3.0346	.	.	no
C152	H4'	3.0750	.	5_545	no
C152	H14"	2.9996	.	.	no
C161	H3'	2.7222	.	2_555	no
C161	H4	3.0474	.	5_545	no
C161	H4'	2.9654	.	5_545	no
C161	H2	2.9228	.	2_555	no
C162	H4'	2.8458	.	5_545	no
C162	H4	3.0009	.	5_545	no
C162	H2	2.9039	.	2_555	no
C162	H3'	2.9204	.	2_555	no
C171	H11	2.4810	.	2_555	no
C171	H3'	2.6810	.	2_555	no
C171	H4	2.8582	.	5_545	no
C171	H3	2.9973	.	5_545	no
C172	H3'	2.3626	.	2_555	no
C172	H4	3.0547	.	5_545	no
C181	H4	2.9801	.	5_545	no
C181	H11	2.7696	.	2_555	no
C181	H191	2.1585	.	2_655	no
C181	H181	2.8841	.	2_655	no
C181	H3'	3.0677	.	2_555	no
C182	H3'	2.9274	.	2_555	no

C191	H191	2.7781	.	2_655	no
C191	H181	2.1809	.	2_655	no
C192	H8	2.9012	.	7_556	no
C202	H8	2.8215	.	7_556	no
C202	H12"	3.0105	.	7_556	no
C211	H2	2.5920	.	2_555	no
C212	H2	2.8821	.	2_555	no
C212	H4'	3.0033	.	5_545	no
C212	H12	2.8183	.	.	no
H1	C4	2.6266	.	.	no
H1	H4	2.5323	.	2_555	no
H1	H4	2.1864	.	.	no
H1'	C5	2.8753	.	2_555	no
H1'	H2"	2.4052	.	.	no
H1'	C7	2.8878	.	2_555	no
H1'	H7	2.3927	.	2_555	no
H1"	H2'	2.5186	.	.	no
H1"	H3	2.4219	.	.	no
H151'	H171	2.4881	.	.	no
H151'	H14	2.5676	.	2_555	no
H151'	H14"	2.5743	.	.	no
H2	H3'	2.3663	.	.	no
H2	C162	2.9039	.	2_555	no
H2	C212	2.8821	.	2_555	no
H2	C161	2.9228	.	2_555	no
H2	C211	2.5920	.	2_555	no
H2	H211	2.4566	.	2_555	no
H2'	H1"	2.5186	.	.	no
H2'	H9	2.4983	.	4_564	no
H2'	H12'	2.5748	.	8_454	no
H2"	H1'	2.4052	.	.	no
H152'	H172	2.3963	.	.	no
H152'	C5	3.0506	.	2_555	no
H3	H1"	2.4219	.	.	no
H3	C171	2.9973	.	5_455	no
H3'	H2	2.3663	.	.	no
H3'	C162	2.9204	.	2_555	no
H3'	C172	2.3626	.	2_555	no
H3'	C182	2.9274	.	2_555	no
H3'	H172	2.2501	.	2_555	no
H3'	C161	2.7222	.	2_555	no
H3'	C171	2.6810	.	2_555	no
H3'	C181	3.0677	.	2_555	no
H4	C1	2.7415	.	.	no
H4	H1	2.1864	.	.	no
H4	H1	2.5323	.	2_555	no
H4	C162	3.0009	.	5_455	no
H4	C172	3.0547	.	5_455	no
H4	C181	2.9801	.	5_455	no
H4	C161	3.0474	.	5_455	no
H4	C171	2.8582	.	5_455	no
H4'	C152	3.0750	.	5_455	no
H4'	C6	2.5708	.	.	no
H4'	C11	2.5715	.	.	no
H4'	H11	2.4965	.	.	no
H4'	C161	2.9654	.	5_455	no
H4'	C162	2.8458	.	5_455	no
H4'	C212	3.0033	.	5_455	no
H7	H202	2.2388	.	7_556	no
H7	Si	3.4253	.	.	no
H7	H1'	2.3927	.	2_555	no

H8	C202	2.8215	.	7_556	no
H8	C192	2.9012	.	7_556	no
H8	H201	2.5601	.	7_556	no
H8	H192	2.4665	.	7_556	no
H8	H202	2.3061	.	7_556	no
H9	H2'	2.4983	.	4_565	no
H9	C13	3.0203	.	7_456	no
H11	H4'	2.4965	.	.	no
H11	C4	3.0213	.	.	no
H11	C181	2.7696	.	2_555	no
H11	H172	2.2039	.	2_555	no
H11	C171	2.4810	.	2_555	no
H11	H171	1.9167	.	2_555	no
H11	H181	2.4917	.	2_555	no
H12	H151	2.2627	.	.	no
H12	Fe	3.4620	.	.	no
H12	C212	2.8183	.	.	no
H12	H212	2.1830	.	.	no
H12	C151	3.0346	.	.	no
H12'	H2'	2.5748	.	8_555	no
H12"	C202	3.0104	.	7_556	no
H13	C6	2.8342	.	.	no
H13	C7	2.7671	.	.	no
H13	C8	3.0790	.	.	no
H13"	C6	3.0130	.	.	no
H13"	C11	3.0014	.	.	no
H14	@51'	2.5676	.	2_555	no
H14"	Fe	3.5051	.	.	no
H14"	C152	2.9996	.	.	no
H14"	H152	2.1464	.	.	no
H14"	C151	2.6961	.	.	no
H14"	H151'	2.5743	.	.	no
H14"	H151	2.1430	.	.	no
H151	H211	2.4348	.	.	no
H151	C14	2.9385	.	.	no
H151	Si	3.1621	.	.	no
H151	C12	2.9906	.	.	no
H151	H12	2.2627	.	.	no
H151	H14"	2.1430	.	.	no
H152	H14"	2.1464	.	.	no
H152	C14	3.0792	.	.	no
H152	H212	2.4180	.	.	no
H171	Fe	3.5314	.	.	no
H171	H151'	2.4881	.	.	no
H171	C11	2.7714	.	2_555	no
H171	H11	1.9167	.	2_555	no
H171	C5	3.0513	.	2_555	no
H172	H11	2.2039	.	2_555	no
H172	H152'	2.3963	.	.	no
H172	H3'	2.2501	.	2_555	no
H181	C181	2.8841	.	2_655	no
H181	C191	2.1809	.	2_655	no
H181	H191	1.3156	.	2_655	no
H181	H11	2.4917	.	2_555	no
H191	H181	1.3156	.	2_655	no
H191	C181	2.1585	.	2_655	no
H191	C191	2.7781	.	2_655	no
H192	C8	3.0013	.	7_556	no
H192	H8	2.4665	.	7_556	no
H201	H8	2.5601	.	7_556	no
H202	C8	3.0517	.	5_545	no

```
 H202    C7          2.9368                    .     7_556                no
 H202    C8          2.9445                    .     7_556                no
 H202    H7          2.2388                    .     7_556                no
 H202    H8          2.3061                    .     7_556                no
 H211    H151        2.4348                    .       .                  no
 H211    H2          2.4566                    .     2_555                no
 H212    C10         3.0900                    .     5_545                no
 H212    H12         2.1830                    .       .                  no
 H212    H152        2.4180                    .       .                  no
 H212    C9          3.0673                    .     5_545                no

# End of Crystallographic Information File
```