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  C14H24ClFeN3Si               CP471

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

# 0. AUDIT DETAILS

_audit_creation_date                1999-02-11
_audit_creation_method              'PLATON <TABLE ACC> option'
_audit_update_record
;
 ?
;

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

# 1. SUBMISSION DETAILS

# Name and address of author for correspondence
_publ_contact_author_name
;
   Drs. A. Meetsma
;
_publ_contact_author_address
;
  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 AD
_publ_requested_category            ?
_publ_requested_coeditor_name       ?

_publ_contact_letter               # Include date of submission
;
 Date of submission :  2007-09-04    10:33:27

 Consider this CIF submission for depostion of compound 1b
 Xray-structure of a manuscript to be submitted to : organometallics
  (Our Code : CP471
;

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

# 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_address

  'Meetsma, Auke'

;
  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,
 which 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 by a disorder problem: from the solution it was
 clear that the trimethyl-Silicon fragment  and the C1, C2 and C3 positions
 were disordered. A disorder model  with site occupancy factor refinement
was applied. In the subsequent refinement bond restrains for the Si-C
distances were applied.
A subsequent difference Fourier synthesis resulted in the location of
 the hydrogen atoms, of the phenyl ligand, which coordinates and isotropic
 displacement parameters were refined.  The remainder hydrogen atoms were
included in the final refinement riding on their carrier atoms with their
 positions calculated by using sp3 hybridization at the C-atom as appropriate
with Uiso = c x Uequiv of their parent atom, where c = 1.2 for the  non-methyl
 hydrogen atoms and c = 1.5 for the methyl hydrogen atoms and where values
Uequiv are related to the atoms to which the H atoms are bonded.
The methyl-groups were refined as rigid groups, which were allowed to
rotate freely.
;

# Insert blank lines between references

_publ_section_references
;

 Beurskens, P.T., Beurskens, G., Bosman, W.P., Gelder, R. de
   Garc\'ia-Granda, S., Gould, R.O., Isra\"el, R. & Smits, J.M.M. &
   (1997) The DIRDIF97 program system,
   Technical Report of the Crystallography Laboratory,
   University of Nijmegen, The Netherlands.

 Boer, J.L. de & Duisenberg, A.J.M. (1984). Acta Cryst. A40, C-410.


 Bolhuis, F. van (1971). J. Appl. Cryst. 4, 263-264.
```

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

Burnett, M.N. & Johnson, C.K. (1996). ORTEP. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee.

Duisenberg, A.J.M. (1992). J. Appl. Cryst. 25, 92-96.

Enraf-Nonius (1994). CAD4-UNIX Software. Version 5.1
Utrecht modified version October 1994.
Enraf-Nonius, Delft, The Netherlands.

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. (1996). Extended version of the program PLUTO.
Groningen University, The Netherlands. (unpublished).

Sheldrick, G.M. (1997). SHELXL-97. Program for the Refinement
of Crystal Structures, University of G\\"ottingen, Germany.

Snow, M.R. & Tiekink, E.R.T. (1988). Acta Cryst. B44, 676-677.

Spek, A.L. (1987). Acta Cryst. C43, 1233-1235.

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

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

Spek, A.L. (1997). HELENA, Program for Data Reduction, Utrecht
University, The Netherlands.

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

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

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

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

Fig. 3. Perspective ORTEP drawing of the title compound.
All non-hydrogen atoms are represented by thermal vibrational
ellipsoids drawn to encompass 50% of the electron density.
The hydrogen atoms are omitted for sake of clarity.

;

```
_publ_section_acknowledgements
;
 ?
;

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

data_c14h24cl

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

# 5. CHEMICAL DATA

_chemical_name_systematic
;
 ?
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
'(C14 H24 Cl Fe N3 Si)2'
_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
'C28 H48 Cl2 Fe2 N6 Si2'
_chemical_formula_weight                707.50
_chemical_compound_source            'by syntheses'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Si  Si     .0817     .0704
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N     .0061     .0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe  Fe     .3463     .8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl  Cl     .1484     .1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H     .0000     .0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C     .0033     .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      '-I 2ya'
_symmetry_space_group_name_H-M       'I 2/a'

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

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

_cell_length_a                          18.514(1)
_cell_length_b                           8.132(1)
_cell_length_c                          23.124(6)
_cell_angle_alpha                       90
_cell_angle_beta                        91.58(1)
_cell_angle_gamma                       90
_cell_volume                          3480.1(10)
_cell_formula_units_Z                       4
_cell_measurement_temperature         130
_cell_measurement_reflns_used         22
_cell_measurement_theta_min           16.48
_cell_measurement_theta_max           20.38
_cell_special_details
;
 Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined
 from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting.
 Reduced cell calculations did not indicate any higher metric lattice symmetry
 and examination of the final atomic coordinates of the structure did not yield
 extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description            plate
_exptl_crystal_colour                 'orange transparent'
_exptl_crystal_size_max           0.24
_exptl_crystal_size_mid           0.20
_exptl_crystal_size_min           0.10
_exptl_crystal_size_rad               ?
_exptl_crystal_density_meas         ?
_exptl_crystal_density_diffrn             1.350
_exptl_crystal_density_method         ?
_exptl_crystal_F_000                       1488
_exptl_absorpt_coefficient_mu              1.08
_exptl_crystal_density_meas_temp      ?
_exptl_absorpt_correction_type        ?
_exptl_absorpt_process_details       ?
_exptl_absorpt_correction_T_min      ?
_exptl_absorpt_correction_T_max      ?

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

# 7. EXPERIMENTAL DATA

_exptl_special_details
;
 ?
;
_diffrn_ambient_temperature           130
_diffrn_radiation_wavelength             .71073
_diffrn_radiation_type                'Mo K\a'
_diffrn_radiation_source              'fine focus sealed Philips Mo tube '
_diffrn_radiation_monochromator       'perpendicular mounted graphite'
_diffrn_radiation_detector
;
     scintillation NaI crystal with photomultiplier
;
_diffrn_measurement_device_type
```

```
;
     Enraf Nonius CAD-4F diffractometer
;

_diffrn_measurement_method          '\w/2\q'

_diffrn_special_details
;
 Crystal into the cold nitrogen stream  of the low-temperature unit
   (Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
   Graphite-monochromated Mo K\a radiation,
   \w/2\q scan, \D\w = (0.90 + 0.34 tg \q)\%.
;
_diffrn_detector_area_resol_mean    ?

_diffrn_standards_number            3
_diffrn_standards_interval_count    ?
_diffrn_standards_interval_time     180
_diffrn_standards_decay_%           1.2

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
  4  0  4
  0  2  0
  4  0 -4

# number of measured reflections (redundant set)
_diffrn_reflns_number             7598
_diffrn_reflns_av_R_equivalents   0.0519
_diffrn_reflns_av_sigmaI/netI     0.0497
_diffrn_reflns_limit_h_min        -23
_diffrn_reflns_limit_h_max        18
_diffrn_reflns_limit_k_min        -10
_diffrn_reflns_limit_k_max        10
_diffrn_reflns_limit_l_min        -19
_diffrn_reflns_limit_l_max        29
_diffrn_reflns_theta_min          1.76
_diffrn_reflns_theta_max          26.99

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization  effects, scale
 variation, but not for absorption and reduced to F~o~^2^
;

# number of unique reflections
_reflns_number_total              3751
_reflns_number_gt                 2995
_reflns_threshold_expression      I>2sigma(I)


_computing_data_collection          'CAD4-UNIX Software Version 5.1, 1994'
_computing_cell_refinement          'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction           'HELENA (Spek, 1993)'
_computing_structure_solution
;
 DIRDIF-97 (Beurskens et al., 1997)
;
_computing_structure_refinement     'SHELXL-97 (Sheldrick, 1997)'
```

```
_computing_molecular_graphics
;
 PLUTO (Meetsma, 1997)
 ORTEP (Burnett et al., 1996)
 PLATON (Spek, 1994, 1996)
;
_computing_publication_material      'PLATON (Spek, 1990)'

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

# 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 w=1/[\s^2^(Fo^2^)+(0.0252P)^2^+13.5755P] 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     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          3751
_refine_ls_number_parameters      267
_refine_ls_number_restraints      6
_refine_ls_R_factor_all           0.0690
_refine_ls_R_factor_gt            0.0514
_refine_ls_wR_factor_ref          0.1128
_refine_ls_wR_factor_gt           0.1070
_refine_ls_goodness_of_fit_ref    1.073
_refine_ls_restrained_S_all       1.094
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max           .807
_refine_diff_density_min          -.827
_refine_diff_density_rms           .073

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

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_
_atom_site_label
_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
```

Fe	Uani	.31142(2)	.11967(6)	-.04355(2)	1.000	.0290(1)
Cl	Uani	.38601(6)	-.09901(15)	-.02570(5)	1.000	.0656(4)
Si	Uani	.28792(6)	-.05229(15)	.14587(5)	1.000	.0493(4)
N1	Uani	.37921(16)	.3044(5)	-.08488(13)	1.000	.0456(10)
N2	Uani	.33353(18)	.2675(4)	.02712(12)	1.000	.0416(10)
N3	Uani	.27973(13)	.1007(3)	.09343(11)	1.000	.0273(7)
C1B	Uani	.3475(5)	.3531(13)	-.1450(4)	.567(12)	.062(3)
C2B	Uani	.4516(9)	.244(2)	-.0951(6)	.567(12)	.064(4)
C3B	Uani	.3763(6)	.4432(9)	-.0489(3)	.567(12)	.047(3)
C4	Uani	.3824(3)	.4050(6)	.01396(18)	1.000	.077(2)
C5	Uani	.33120(17)	.2089(4)	.07989(13)	1.000	.0278(9)
C6	Uani	.38709(18)	.2609(4)	.12426(14)	1.000	.0315(9)
C7	Uani	.4580(2)	.2110(6)	.1192(2)	1.000	.0489(14)
C8	Uani	.5101(3)	.2521(7)	.1594(3)	1.000	.072(2)
C9	Uani	.4924(3)	.3474(8)	.2048(3)	1.000	.082(2)
C10	Uani	.4234(4)	.4048(8)	.2107(2)	1.000	.086(2)
C11	Uani	.3691(3)	.3589(6)	.17040(19)	1.000	.0588(16)
C1A	Uani	.3348(6)	.4331(19)	-.1117(6)	.433(12)	.068(5)
C2A	Uani	.4359(13)	.241(4)	-.1202(8)	.433(12)	.095(8)
C3A	Uani	.4186(7)	.3922(15)	-.0309(4)	.433(12)	.050(3)
C12C	Uani	.2950(7)	-.1506(19)	-.1597(8)	.521(8)	.097(7)
C13C	Uani	.1899(7)	.0486(12)	-.2239(3)	.521(8)	.079(4)
C14C	Uani	.1339(6)	-.1851(12)	-.1378(5)	.521(8)	.080(4)
C12D	Uani	.2923(8)	-.047(2)	-.1889(8)	.479(8)	.116(9)
C13D	Uani	.1316(5)	-.0838(12)	-.1850(5)	.479(8)	.060(3)
C14D	Uani	.2232(10)	-.2502(10)	-.0975(6)	.479(8)	.123(7)
H2D	Uiso	.44894	.14909	-.12100	.567(12)	.0956
H2E	Uiso	.47489	.21221	-.05825	.567(12)	.0956
H2F	Uiso	.47998	.33159	-.11300	.567(12)	.0956
H3C	Uiso	.33008	.50128	-.05674	.567(12)	.0561
H3D	Uiso	.41594	.51897	-.05884	.567(12)	.0561
H4A	Uiso	.35309	.50654	.01072	1.000	.0916
H4B	Uiso	.41649	.41930	.04731	1.000	.0916
H7	Uiso	.472(2)	.158(6)	.0903(18)	1.000	.054(13)
H8	Uiso	.564(3)	.209(8)	.154(2)	1.000	.099(19)
H9	Uiso	.528(3)	.366(6)	.229(2)	1.000	.075(15)
H10	Uiso	.408(3)	.467(7)	.237(2)	1.000	.072(16)
H11	Uiso	.324(2)	.384(5)	.1748(18)	1.000	.051(12)
H1D	Uiso	.29607	.37908	-.14174	.567(12)	.0931
H1E	Uiso	.35313	.26134	-.17194	.567(12)	.0931
H1F	Uiso	.37313	.44962	-.15927	.567(12)	.0931
H1A	Uiso	.29609	.46355	-.08565	.433(12)	.1029
H1B	Uiso	.31356	.39253	-.14828	.433(12)	.1029
H1C	Uiso	.36479	.52963	-.11915	.433(12)	.1029
H2A	Uiso	.47106	.32880	-.12714	.433(12)	.1423
H2B	Uiso	.41509	.20318	-.15721	.433(12)	.1423
H2C	Uiso	.46003	.14961	-.10017	.433(12)	.1423
H3A	Uiso	.46326	.33026	-.02101	.433(12)	.0594
H3B	Uiso	.43321	.50395	-.04291	.433(12)	.0594
H12A	Uiso	.33448	-.07071	-.15593	.521(8)	.1465
H12B	Uiso	.29344	-.19567	-.19902	.521(8)	.1465
H12C	Uiso	.30306	-.23993	-.13181	.521(8)	.1465
H13A	Uiso	.22029	.14596	-.22896	.521(8)	.1191
H13B	Uiso	.13890	.08072	-.22634	.521(8)	.1191
H13C	Uiso	.19975	-.03167	-.25425	.521(8)	.1191
H14A	Uiso	.13628	-.27645	-.16529	.521(8)	.1198
H14B	Uiso	.08964	-.12175	-.14542	.521(8)	.1198
H14C	Uiso	.13373	-.22852	-.09825	.521(8)	.1198
H12D	Uiso	.28617	.03449	-.21971	.479(8)	.1731
H12E	Uiso	.30006	-.15600	-.20602	.479(8)	.1731
H12F	Uiso	.33424	-.01810	-.16417	.479(8)	.1731

```
 H13D    Uiso        .12160       .01169      -.20979   .479(8)       .0900
 H13E    Uiso        .09205      -.09840      -.15817   .479(8)       .0900
 H13F    Uiso        .13593      -.18238      -.20901   .479(8)       .0900
 H14D    Uiso        .22899      -.34674      -.12230   .479(8)       .1853
 H14E    Uiso        .18025      -.26413      -.07415   .479(8)       .1853
 H14F    Uiso        .26597      -.23838      -.07187   .479(8)       .1853

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        .0300(2)   .0308(2)   .0265(2)   -.0008(2)    .0050(2)   -.0024(2)
  Cl        .0682(7)   .0663(7)   .0622(6)   -.0073(6)    .0021(5)    .0361(6)
  Si        .0450(6)   .0454(6)   .0581(7)    .0300(5)    .0127(5)    .0106(5)
  N1       .0420(17)    .058(2)  .0370(16)   .0094(15)   .0059(13)  -.0161(15)
  N2         .067(2)  .0313(15)  .0265(14)   .0021(12)   .0007(13)  -.0198(15)
  N3       .0296(13)  .0232(13)  .0294(12)   .0036(11)   .0059(10)   .0031(11)
  C1B        .078(6)    .071(6)    .036(4)     .015(4)    -.002(4)    -.034(5)
  C2B        .050(6)    .066(6)    .077(9)    -.015(7)     .024(6)    -.024(5)
  C3B        .071(6)    .034(4)    .035(4)     .008(3)     .008(4)    -.016(4)
  C4         .135(5)    .056(3)    .038(2)     .011(2)    -.012(3)    -.063(3)
  C5       .0353(16)  .0199(15)  .0282(15)  -.0032(12)   .0029(13)   .0037(12)
  C6       .0373(17)  .0260(16)  .0310(16)   .0019(13)  -.0001(13)  -.0014(13)
  C7         .039(2)    .050(2)    .058(3)     .008(2)   .0054(19)  -.0010(18)
  C8         .044(2)    .078(4)    .092(4)     .025(3)    -.017(3)    -.013(3)
  C9         .079(4)    .088(4)    .078(4)     .032(3)    -.043(3)    -.039(3)
  C10        .122(5)    .083(4)    .052(3)    -.025(3)    -.019(3)    -.015(4)
  C11        .066(3)    .061(3)    .049(2)    -.022(2)    -.005(2)     .010(2)
  C1A        .063(7)   .088(10)    .053(8)     .042(7)    -.021(6)    -.037(7)
  C2A       .071(14)   .137(16)   .080(13)   -.023(15)    .057(11)   -.038(12)
  C3A        .056(6)    .058(6)    .035(5)     .020(5)    -.007(4)    -.034(5)
  C12C       .067(7)   .100(12)   .125(14)   -.083(10)    -.002(8)     .024(8)
  C13C      .147(10)    .056(6)    .035(4)    -.022(4)     .015(5)    -.024(6)
  C14C       .106(8)    .056(6)    .079(7)    -.035(5)     .039(6)    -.058(6)
  C12D       .070(9)   .143(17)   .136(17)   -.107(14)    .041(10)   -.007(11)
  C13D       .054(5)    .053(6)    .071(6)    -.031(5)    -.025(5)     .010(4)
  C14D      .231(18)    .015(4)   .118(11)    -.018(5)   -.103(12)     .009(7)

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

# 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	Cl	2.2822(14)	.	.	yes
Fe	N1	2.193(4)	.	.	yes
Fe	N2	2.061(3)	.	.	yes
Fe	N3	2.024(3)	.	2_555	yes
Si	N3	1.741(3)	.	.	yes
N1	C1B	1.546(10)	.	.	yes
N1	C2B	1.453(17)	.	.	yes
N1	C3B	1.404(8)	.	.	yes
N1	C1A	1.459(14)	.	.	yes
N1	C2A	1.44(2)	.	.	yes
N1	C3A	1.597(11)	.	.	yes
N2	C4	1.475(6)	.	.	yes
N2	C5	1.312(4)	.	.	yes
N3	C5	1.340(4)	.	.	yes
C3A	C4	1.255(12)	.	.	no
C3B	C4	1.488(8)	.	.	no
C5	C6	1.498(5)	.	.	no
C6	C11	1.380(6)	.	.	no
C6	C7	1.382(5)	.	.	no
C7	C8	1.363(8)	.	.	no
C8	C9	1.352(9)	.	.	no
C9	C10	1.370(9)	.	.	no
C10	C11	1.402(8)	.	.	no
C1A	H1A	.9806	.	.	no
C1A	H1B	.9801	.	.	no
C1A	H1C	.9795	.	.	no
C1B	H1F	.9792	.	.	no
C1B	H1D	.9803	.	.	no
C1B	H1E	.9795	.	.	no
C2A	H2B	.9784	.	.	no
C2A	H2A	.9824	.	.	no
C2A	H2C	.9773	.	.	no
C2B	H2F	.9832	.	.	no
C2B	H2D	.9773	.	.	no
C2B	H2E	.9791	.	.	no
C3A	H3B	.9901	.	.	no
C3A	H3A	.9896	.	.	no
C3B	H3C	.9898	.	.	no
C3B	H3D	.9901	.	.	no
C4	H4B	.9898	.	.	no
C4	H4A	.9898	.	.	no
C7	H7	.84(4)	.	.	no
C8	H8	1.07(6)	.	.	no
C9	H9	.87(5)	.	.	no
C10	H10	.85(5)	.	.	no
C11	H11	.87(4)	.	.	no
C12C	H12A	.9800	.	.	no
C12C	H12B	.9800	.	.	no
C12C	H12C	.9801	.	.	no
C13C	H13A	.9802	.	.	no
C13C	H13B	.9798	.	.	no
C13C	H13C	.9793	.	.	no
C14C	H14A	.9795	.	.	no
C14C	H14B	.9798	.	.	no
C14C	H14C	.9804	.	.	no
C12D	H12D	.9773	.	.	no
C12D	H12E	.9829	.	.	no
C12D	H12F	.9801	.	.	no
C13D	H13D	.9798	.	.	no
C13D	H13E	.9799	.	.	no

```
 C13D    H13F          .9797                    .       .                 no
 C14D    H14D          .9798                    .       .                 no
 C14D    H14E          .9800                    .       .                 no
 C14D    H14F          .9806                    .       .                 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
 Cl      Fe      N1       105.18(10)             .       .       .          yes
 Cl      Fe      N2       101.84(10)             .       .       .          yes
 Cl      Fe      N3        122.32(8)             .       .     2_555        yes
 N1      Fe      N2        80.94(12)             .       .       .          yes
 N1      Fe      N3       106.38(11)             .       .     2_555        yes
 N2      Fe      N3       129.85(12)             .       .     2_555        yes
 Fe      N1      C1B        111.1(4)             .       .       .          yes
 Fe      N1      C2B        112.4(7)             .       .       .          yes
 Fe      N1      C3B        105.1(4)             .       .       .          yes
 Fe      N1      C1A        110.7(5)             .       .       .          yes
 Fe      N1      C2A       115.8(13)             .       .       .          yes
 Fe      N1      C3A        102.7(4)             .       .       .          yes
 C1B     N1      C2B        105.6(7)             .       .       .          yes
 C1B     N1      C3B        107.9(6)             .       .       .          yes
 C2B     N1      C3B        114.8(8)             .       .       .          yes
 C1A     N1      C2A       115.2(11)             .       .       .          yes
 C1A     N1      C3A        104.6(8)             .       .       .          yes
 C2A     N1      C3A       106.2(10)             .       .       .          yes
 Fe      N2      C4         112.8(2)             .       .       .          yes
 Fe      N2      C5         121.0(2)             .       .       .          yes
 C4      N2      C5         120.2(3)             .       .       .          yes
 Si      N3      C5         125.7(2)             .       .       .          yes
 Fe      N3      Si        120.45(13)          2_555     .       .          yes
 Fe      N3      C5         113.8(2)          2_555     .       .          yes
 N1      C3A     C4         116.1(9)            .       .       .          yes
 N1      C3B     C4         114.1(5)            .       .       .          yes
 N2      C4      C3A        116.9(7)            .       .       .          yes
 N2      C4      C3B        109.2(5)            .       .       .          yes
 N2      C5      N3         119.8(3)            .       .       .          yes
 N3      C5      C6         120.5(3)            .       .       .          yes
 N2      C5      C6         119.7(3)            .       .       .          yes
 C5      C6      C7         119.9(3)            .       .       .          no
 C7      C6      C11        119.0(4)            .       .       .          no
 C5      C6      C11        121.0(3)            .       .       .          no
 C6      C7      C8         121.8(4)            .       .       .          no
 C7      C8      C9         119.2(5)            .       .       .          no
 C8      C9      C10        121.3(6)            .       .       .          no
 C9      C10     C11        119.8(5)            .       .       .          no
 C6      C11     C10        118.9(5)            .       .       .          no
 H1A     C1A     H1C          109.46            .       .       .          no
 H1B     C1A     H1C          109.50            .       .       .          no
 N1      C1A     H1C          109.52            .       .       .          no
 N1      C1A     H1A          109.45            .       .       .          no
 N1      C1A     H1B          109.48            .       .       .          no
 H1A     C1A     H1B          109.42            .       .       .          no
 N1      C1B     H1F          109.45            .       .       .          no
 N1      C1B     H1D          109.37            .       .       .          no
```

N1	C1B	H1E	109.42	.	.	.	no
H1D	C1B	H1E	109.50	.	.	.	no
H1D	C1B	H1F	109.51	.	.	.	no
H1E	C1B	H1F	109.59	.	.	.	no
N1	C2A	H2A	109.17	.	.	.	no
N1	C2A	H2B	109.42	.	.	.	no
N1	C2A	H2C	109.49	.	.	.	no
H2B	C2A	H2C	109.84	.	.	.	no
H2A	C2A	H2B	109.41	.	.	.	no
H2A	C2A	H2C	109.50	.	.	.	no
N1	C2B	H2D	109.61	.	.	.	no
N1	C2B	H2E	109.50	.	.	.	no
N1	C2B	H2F	109.25	.	.	.	no
H2D	C2B	H2E	109.78	.	.	.	no
H2D	C2B	H2F	109.43	.	.	.	no
H2E	C2B	H2F	109.27	.	.	.	no
N1	C3A	H3A	108.29	.	.	.	no
C4	C3A	H3B	108.18	.	.	.	no
N1	C3A	H3B	108.27	.	.	.	no
C4	C3A	H3A	108.25	.	.	.	no
H3A	C3A	H3B	107.40	.	.	.	no
N1	C3B	H3D	108.78	.	.	.	no
C4	C3B	H3C	108.70	.	.	.	no
N1	C3B	H3C	108.79	.	.	.	no
H3C	C3B	H3D	107.65	.	.	.	no
C4	C3B	H3D	108.66	.	.	.	no
N2	C4	H4A	108.05	.	.	.	no
C3B	C4	H4B	140.03	.	.	.	no
H4A	C4	H4B	107.30	.	.	.	no
C3A	C4	H4A	108.11	.	.	.	no
C3A	C4	H4B	108.07	.	.	.	no
N2	C4	H4B	108.05	.	.	.	no
C3B	C4	H4A	74.05	.	.	.	no
C6	C7	H7	122(3)	.	.	.	no
C8	C7	H7	116(3)	.	.	.	no
C7	C8	H8	119(3)	.	.	.	no
C9	C8	H8	122(3)	.	.	.	no
C10	C9	H9	125(3)	.	.	.	no
C8	C9	H9	114(3)	.	.	.	no
C9	C10	H10	127(4)	.	.	.	no
C11	C10	H10	113(4)	.	.	.	no
C10	C11	H11	122(3)	.	.	.	no
C6	C11	H11	119(3)	.	.	.	no
H12A	C12C	H12B	109.47	.	.	.	no
H12A	C12C	H12C	109.46	.	.	.	no
Si	C12C	H12A	109.48	2_555	.	.	no
H12B	C12C	H12C	109.47	.	.	.	no
Si	C12C	H12B	109.48	2_555	.	.	no
Si	C12C	H12C	109.47	2_555	.	.	no
H13A	C13C	H13B	109.46	.	.	.	no
H13A	C13C	H13C	109.51	.	.	.	no
Si	C13C	H13A	109.42	2_555	.	.	no
H13B	C13C	H13C	109.55	.	.	.	no
Si	C13C	H13B	109.42	2_555	.	.	no
Si	C13C	H13C	109.46	2_555	.	.	no
H14A	C14C	H14B	109.54	.	.	.	no
H14A	C14C	H14C	109.49	.	.	.	no
Si	C14C	H14A	109.48	2_555	.	.	no
H14B	C14C	H14C	109.45	.	.	.	no
Si	C14C	H14B	109.46	2_555	.	.	no
Si	C14C	H14C	109.42	2_555	.	.	no

```
 H12D    C12D    H12E         109.46             .      .      .          no
 H12D    C12D    H12F         109.69             .      .      .          no
 Si      C12D    H12D         109.64           2_555    .      .          no
 H12E    C12D    H12F         109.21             .      .      .          no
 Si      C12D    H12E         109.33           2_555    .      .          no
 Si      C12D    H12F         109.49           2_555    .      .          no
 H13D    C13D    H13E         109.51             .      .      .          no
 H13D    C13D    H13F         109.51             .      .      .          no
 Si      C13D    H13D         109.43           2_555    .      .          no
 H13E    C13D    H13F         109.51             .      .      .          no
 Si      C13D    H13E         109.42           2_555    .      .          no
 Si      C13D    H13F         109.44           2_555    .      .          no
 H14D    C14D    H14E         109.47             .      .      .          no
 H14D    C14D    H14F         109.43             .      .      .          no
 Si      C14D    H14D         109.52           2_555    .      .          no
 H14E    C14D    H14F         109.41             .      .      .          no
 Si      C14D    H14E         109.51           2_555    .      .          no
 Si      C14D    H14F         109.48           2_555    .      .          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
 Cl      Fe      N1      C1B        122.3(4)     .      .      .      .   no
 Cl      Fe      N1      C2B          4.2(6)     .      .      .      .   no
 Cl      Fe      N1      C3B       -121.3(4)     .      .      .      .   no
 N2      Fe      N1      C1B       -137.8(4)     .      .      .      .   no
 N2      Fe      N1      C2B        104.1(6)     .      .      .      .   no
 N2      Fe      N1      C3B        -21.4(4)     .      .      .      .   no
 N3      Fe      N1      C1B         -8.8(5)   2_555    .      .      .   no
 N3      Fe      N1      C2B       -126.9(6)   2_555    .      .      .   no
 N3      Fe      N1      C3B        107.6(4)   2_555    .      .      .   no
 Cl      Fe      N2      C4         101.3(3)     .      .      .      .   no
 Cl      Fe      N2      C5         -51.6(3)     .      .      .      .   no
 N1      Fe      N2      C4          -2.4(3)     .      .      .      .   no
 N1      Fe      N2      C5        -155.3(3)     .      .      .      .   no
 N3      Fe      N2      C4        -106.3(3)   2_555    .      .      .   no
 N3      Fe      N2      C5         100.9(3)   2_555    .      .      .   no
 Cl      Fe      N3      Si       -24.84(19)     .      .    2_555  2_555 no
 Cl      Fe      N3      C5       152.20(19)     .      .    2_555  2_555 no
 N1      Fe      N3      Si        95.75(17)     .      .    2_555  2_555 no
 N1      Fe      N3      C5         -87.2(2)     .      .    2_555  2_555 no
 N2      Fe      N3      Si      -172.44(15)     .      .    2_555  2_555 no
 N2      Fe      N3      C5           4.6(3)     .      .    2_555  2_555 no
 Fe      N1      C3B     C4          42.9(8)     .      .      .      .   no
 C1B     N1      C3B     C4         161.5(7)     .      .      .      .   no
 C2B     N1      C3B     C4        -81.1(10)     .      .      .      .   no
 Fe      N2      C4      C3B         25.0(6)     .      .      .      .   no
 C5      N2      C4      C3B        178.0(5)     .      .      .      .   no
 Fe      N2      C5      N3         -38.6(4)     .      .      .      .   no
 Fe      N2      C5      C6         140.1(3)     .      .      .      .   no
 C4      N2      C5      N3         170.5(3)     .      .      .      .   no
 C4      N2      C5      C6         -10.8(5)     .      .      .      .   no
 Si      N3      C5      N2         150.4(3)     .      .      .      .   no
```

Si	N3	C5	C6	-28.3(4)	.	.	.	.	no
Fe	N3	C5	N2	-26.4(4)	2_555	.	.	.	no
Fe	N3	C5	C6	154.8(2)	2_555	.	.	.	no
N1	C3B	C4	N2	-47.0(9)	.	.	.	.	no
N2	C5	C6	C11	111.2(4)	.	.	.	.	no
N3	C5	C6	C7	110.1(4)	.	.	.	.	no
N2	C5	C6	C7	-68.6(5)	.	.	.	.	no
N3	C5	C6	C11	-70.1(5)	.	.	.	.	no
C5	C6	C7	C8	-178.3(4)	.	.	.	.	no
C11	C6	C7	C8	1.9(7)	.	.	.	.	no
C7	C6	C11	C10	.0(6)	.	.	.	.	no
C5	C6	C11	C10	-179.8(4)	.	.	.	.	no
C6	C7	C8	C9	-1.5(8)	.	.	.	.	no
C7	C8	C9	C10	-.8(9)	.	.	.	.	no
C8	C9	C10	C11	2.7(10)	.	.	.	.	no
C9	C10	C11	C6	-2.3(8)	.	.	.	.	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	C12C	3.477(17)	.	.	no
Fe	C12D	3.632(18)	.	.	no
Fe	C14D	3.627(12)	.	.	no
Fe	H12A	3.0649	.	.	no
Fe	H12F	3.0460	.	.	no
Fe	H14F	3.0959	.	.	no
Cl	C12C	3.511(18)	.	.	no
Cl	C14D	3.616(17)	.	.	no
Cl	H12A	3.1422	.	.	no
Cl	H12C	3.0797	.	.	no
Cl	H2E	3.1221	.	.	no
Cl	H2C	3.0102	.	.	no
Cl	H14F	2.6894	.	.	no
Cl	H14C	3.0848	.	2_555	no
Cl	H14E	2.9657	.	2_555	no
Cl	H7	3.10(4)	.	3_655	no
Si	C7	3.871(4)	.	.	no
Si	C11	3.703(5)	.	.	no
Si	C12C	1.768(14)	.	2_555	no
Si	C13C	2.014(8)	.	2_555	no
Si	C14C	1.820(11)	.	2_555	no
Si	C13D	1.741(10)	.	2_555	no
Si	C14D	1.967(11)	.	2_555	no
Si	C12D	1.811(16)	.	2_555	no
Si	H12A	2.2893	.	2_555	no
Si	H12B	2.2893	.	2_555	no
Si	H13C	2.5159	.	2_555	no
Si	H14A	2.3365	.	2_555	no
Si	H14B	2.3365	.	2_555	no
Si	H14C	2.3364	.	2_555	no
Si	H12C	2.2893	.	2_555	no
Si	H13A	2.5159	.	2_555	no
Si	H13B	2.5158	.	2_555	no
Si	H12D	2.3290	.	2_555	no
Si	H12E	2.3290	.	2_555	no
Si	H12F	2.3290	.	2_555	no
Si	H13D	2.2638	.	2_555	no

Si	H13E	2.2638	.	2_555	no
Si	H13F	2.2639	.	2_555	no
Si	H14D	2.4737	.	2_555	no
Si	H14E	2.4737	.	2_555	no
Si	H14F	2.4738	.	2_555	no
N3	C12C	2.925(16)	.	2_555	no
N3	C13C	3.083(8)	.	2_555	no
N3	C14C	2.987(11)	.	2_555	no
N3	C13D	3.039(11)	.	2_555	no
N3	C14D	2.856(9)	.	2_555	no
N3	C12D	2.874(17)	.	2_555	no
N3	H1D	2.9032	.	2_555	no
N3	H12A	2.9447	.	2_555	no
N3	H12F	2.8726	.	2_555	no
N3	H14F	2.9231	.	2_555	no
C4	C7	3.191(7)	.	.	no
C5	C13D	3.458(11)	.	2_555	no
C5	C14C	3.525(11)	.	2_555	no
C6	C13D	3.159(11)	.	2_555	no
C6	C13C	3.241(10)	.	2_555	no
C7	C4	3.191(7)	.	.	no
C7	C13D	3.310(11)	.	2_555	no
C7	Si	3.871(4)	.	.	no
C10	C12D	3.596(18)	.	8_555	no
C10	C13C	3.594(13)	.	2_555	no
C11	C13C	3.027(11)	.	2_555	no
C11	Si	3.703(5)	.	.	no
C12C	Fe	3.477(17)	.	.	no
C12C	C13C	2.908(19)	.	.	no
C12C	N3	2.925(16)	.	2_555	no
C12C	Cl	3.511(18)	.	.	no
C12C	Si	1.768(14)	.	2_555	no
C12C	C14C	3.052(17)	.	.	no
C12D	Fe	3.632(18)	.	.	no
C12D	C13D	2.994(18)	.	.	no
C12D	N3	2.874(18)	.	2_555	no
C12D	C14D	3.00(2)	.	.	no
C12D	C10	3.596(18)	.	8_554	no
C12D	Si	1.811(16)	.	2_555	no
C13C	Si	2.014(8)	.	2_555	no
C13C	C11	3.027(11)	.	2_555	no
C13C	C12C	2.908(19)	.	.	no
C13C	N3	3.083(8)	.	2_555	no
C13C	C14C	2.960(14)	.	.	no
C13C	C6	3.241(10)	.	2_555	no
C13C	C10	3.594(13)	.	2_555	no
C13D	C7	3.310(11)	.	2_555	no
C13D	N3	3.039(11)	.	2_555	no
C13D	C5	3.458(11)	.	2_555	no
C13D	C12D	2.994(18)	.	.	no
C13D	C6	3.159(11)	.	2_555	no
C13D	Si	1.741(10)	.	2_555	no
C13D	C14D	2.935(18)	.	.	no
C14C	C5	3.525(11)	.	2_555	no
C14C	N3	2.987(11)	.	2_555	no
C14C	C13C	2.960(14)	.	.	no
C14C	Si	1.820(11)	.	2_555	no
C14C	C12C	3.052(17)	.	.	no
C14D	N3	2.856(9)	.	2_555	no
C14D	C12D	3.00(2)	.	.	no
C14D	Si	1.967(11)	.	2_555	no

C14D	C13D	2.935(18)	.	.	no
C14D	Fe	3.627(12)	.	.	no
C14D	Cl	3.616(17)	.	.	no
C1A	H4A	2.9038	.	.	no
C4	H2E	2.8872	.	.	no
C4	H1A	2.8076	.	.	no
C6	H4B	2.2749	.	.	no
C6	H13B	2.8307	.	2_555	no
C6	H13E	3.0470	.	2_555	no
C6	H13D	2.8394	.	2_555	no
C7	H13E	2.8368	.	2_555	no
C7	H4B	2.4805	.	.	no
C7	H14B	2.9150	.	2_555	no
C7	H13D	3.0590	.	2_555	no
C8	H1C	3.0823	.	3_665	no
C10	H14A	2.9964	.	2_565	no
C10	H13B	2.9034	.	2_555	no
C10	H12D	3.0844	.	8_555	no
C11	H14A	2.9692	.	2_565	no
C11	H13B	2.6121	.	2_555	no
C11	H13D	2.9703	.	2_555	no
C11	H4B	3.0414	.	.	no
C11	H13A	2.7739	.	2_555	no
C12C	H13C	2.9347	.	.	no
C12C	H8	2.65(6)	.	3_655	no
C12D	H8	3.06(6)	.	3_655	no
C12D	H10	2.85(5)	.	8_554	no
C13C	H14B	2.9738	.	.	no
C13C	H11	2.97(4)	.	2_555	no
C13C	H12B	2.8090	.	.	no
C13D	H14E	3.0667	.	.	no
C13D	H9	2.75(5)	.	5_444	no
C14C	H13B	2.9805	.	.	no
C14D	H13E	3.0331	.	.	no
C14D	H13F	3.0551	.	.	no
C14D	H12E	3.0176	.	.	no
H1A	C4	2.8076	.	.	no
H1A	H4A	2.4642	.	.	no
H1B	H2B	2.4430	.	.	no
H1C	H3B	2.1525	.	.	no
H1C	H2A	2.5676	.	.	no
H1C	C8	3.0823	.	3_665	no
H1D	H3C	2.2758	.	.	no
H1D	N3	2.9032	.	2_555	no
H1D	H11	2.3311	.	2_555	no
H1E	H2D	2.2917	.	.	no
H1F	H2F	2.4213	.	.	no
H1F	H3D	2.4976	.	.	no
H1F	H3C	2.5568	.	.	no
H2A	H3B	2.5276	.	.	no
H2A	H3A	2.4624	.	.	no
H2A	H1C	2.5676	.	.	no
H2B	H1B	2.4430	.	.	no
H2C	H3A	2.3466	.	.	no
H2C	Cl	3.0102	.	.	no
H2D	H1E	2.2917	.	.	no
H2E	Cl	3.1221	.	.	no
H2E	C4	2.8872	.	.	no
H2F	H3D	2.3191	.	.	no
H2F	H1F	2.4213	.	.	no
H3A	H2C	2.3466	.	.	no

H3A	H2A	2.4624	.	.	no
H3B	H2A	2.5276	.	.	no
H3B	H1C	2.1525	.	.	no
H3C	H1F	2.5568	.	.	no
H3C	H1D	2.2758	.	.	no
H3D	H2F	2.3191	.	.	no
H3D	H1F	2.4976	.	.	no
H4A	C1A	2.9038	.	.	no
H4A	H1A	2.4642	.	.	no
H4A	H14E	2.4617	.	2_565	no
H4B	H7	2.5501	.	.	no
H4B	C7	2.4805	.	.	no
H4B	C6	2.2749	.	.	no
H4B	C11	3.0414	.	.	no
H7	H4B	2.5501	.	.	no
H7	Cl	3.10(4)	.	3_655	no
H8	C12D	3.06(6)	.	3_655	no
H8	H12F	2.4475	.	3_655	no
H8	H12C	2.5405	.	3_655	no
H8	C12C	2.65(6)	.	3_655	no
H8	H12A	2.1897	.	3_655	no
H9	H13D	2.5049	.	5_555	no
H9	C13D	2.75(5)	.	5_555	no
H9	H13F	2.4586	.	5_555	no
H10	C12D	2.85(6)	.	8_555	no
H10	H12D	2.4928	.	8_555	no
H11	H13A	2.4586	.	2_555	no
H11	C13C	2.97(4)	.	2_555	no
H11	H1D	2.3311	.	2_555	no
H12A	Cl	3.1422	.	.	no
H12A	H8	2.1897	.	3_655	no
H12A	Si	2.2893	.	2_555	no
H12A	Fe	3.0649	.	.	no
H12A	N3	2.9447	.	2_555	no
H12B	C13C	2.8090	.	.	no
H12B	H13C	2.4713	.	7_544	no
H12B	H13C	2.5092	.	.	no
H12B	Si	2.2893	.	2_555	no
H12C	H8	2.5405	.	3_655	no
H12C	Cl	3.0797	.	.	no
H12C	Si	2.2893	.	2_555	no
H12D	H10	2.4928	.	8_554	no
H12D	C10	3.0844	.	8_554	no
H12D	Si	2.3290	.	2_555	no
H12E	C14D	3.0176	.	.	no
H12E	Si	2.3290	.	2_555	no
H12F	N3	2.8726	.	2_555	no
H12F	Fe	3.0460	.	.	no
H12F	Si	2.3290	.	2_555	no
H12F	H8	2.4475	.	3_655	no
H13A	C11	2.7728	.	2_555	no
H13A	Si	2.5159	.	2_555	no
H13A	H11	2.4586	.	2_555	no
H13A	H13A	2.2537	.	7_554	no
H13B	Si	2.5158	.	2_555	no
H13B	C6	2.8307	.	2_555	no
H13B	C10	2.9034	.	2_555	no
H13B	C11	2.6120	.	2_555	no
H13B	C14C	2.9805	.	.	no
H13C	Si	2.5159	.	2_555	no
H13C	H12B	2.4713	.	7_544	no

```
 H13C    H12B        2.5092                    .       .                 no
 H13C    C12C        2.9347                    .       .                 no
 H13D    C6          2.8394                    .     2_555               no
 H13D    Si          2.2638                    .     2_555               no
 H13D    H9          2.5049                    .     5_444               no
 H13D    C7          3.0590                    .     2_555               no
 H13D    C11         2.9704                    .     2_555               no
 H13E    Si          2.2638                    .     2_555               no
 H13E    C6          3.0470                    .     2_555               no
 H13E    C7          2.8368                    .     2_555               no
 H13E    C14D        3.0331                    .       .                 no
 H13F    C14D        3.0551                    .       .                 no
 H13F    H9          2.4586                    .     5_444               no
 H13F    Si          2.2639                    .     2_555               no
 H14A    Si          2.3365                    .     2_555               no
 H14A    C11         2.9692                    .     2_545               no
 H14A    C10         2.9964                    .     2_545               no
 H14B    C13C        2.9738                    .       .                 no
 H14B    Si          2.3365                    .     2_555               no
 H14B    C7          2.9150                    .     2_555               no
 H14C    Cl          3.0848                    .     2_555               no
 H14C    Si          2.3364                    .     2_555               no
 H14D    Si          2.4737                    .     2_555               no
 H14E    C13D        3.0667                    .       .                 no
 H14E    Cl          2.9657                    .     2_555               no
 H14E    Si          2.4737                    .     2_555               no
 H14E    H4A         2.4617                    .     2_545               no
 H14F    Fe          3.0959                    .       .                 no
 H14F    Cl          2.6894                    .       .                 no
 H14F    Si          2.4738                    .     2_555               no
 H14F    N3          2.9231                    .     2_555               no

# End of Crystallographic Information File
```