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

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

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CIF-file generated for C14H24ClFeN3Si

CP471

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0. AUDIT DETAILS

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1. SUBMISSION DETAILS

Name and address of author for correspondence

_publ_contact_author_name

;

Drs. A. Meetsma

;

_publ_contact_author_address

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Zernike Institute for Advanced Materials,
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NL-9747 AG Groningen, The Netherlands.

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_publ_contact_author_fax '+31 50 3634441'
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Consider this CIF submission for deposition of compound 1b

Xray-structure of a manuscript to be submitted to : organometallics

(Our Code : CP471

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2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_accepted ?

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; ?
;

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

_journal_suppl_publ_number       ?
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# 3. TITLE AND AUTHOR LIST

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_publ_section_title_footnote
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# 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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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.
;

```

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#=====

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4. TEXT

_publ_section_synopsis

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;

_publ_section_abstract

;

?

;

Insert blank lines between paragraphs

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;

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 restraints 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.

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 Utrecht modified version October 1994.
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 Dordrecht, The Netherlands.

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 University, The Netherlands.

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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. 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.

;

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_publ_section_acknowledgements
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data_c14h24cl

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# 5. CHEMICAL DATA

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;
?
;
_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_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_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_diffn   1.350
_exptl_crystal_density_method  ?
_exptl_crystal_F_000           1488
_exptl_absorpt_coefficient_mu   1.08
_exptl_crystal_density_meas_temp ?
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_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?

#=====

# 7. EXPERIMENTAL DATA

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;
?
;
_diffn_ambient_temperature      130
_diffn_radiation_wavelength     .71073
_diffn_radiation_type           'Mo K\alpha'
_diffn_radiation_source         'fine focus sealed Philips Mo tube '
_diffn_radiation_monochromator  'perpendicular mounted graphite'
_diffn_radiation_detector

;
    scintillation NaI crystal with photomultiplier
;
_diffn_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\alpha 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_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_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         $I > 2\sigma(I)$ 

_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'
_refine_ls_solution_primary       direct
_refine_ls_solution_secondary     difmap
_refine_ls_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

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  _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

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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Fe      .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)

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10. MOLECULAR GEOMETRY

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_geom_special_details
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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All 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

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_geom_bond_atom_site_label_1
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_geom_bond_atom_site_label_2
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_geom_bond_distance
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_geom_bond_site_symmetry_1
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_geom_bond_site_symmetry_2
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_geom_bond_publ_flag

Fe	C1	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

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_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

C1	Fe	N1	105.18 (10)	.	.	.	yes
C1	Fe	N2	101.84 (10)	.	.	.	yes
C1	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

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_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag

C1	Fe	N1	C1B	122.3 (4)	.	.	.	.	no
C1	Fe	N1	C2B	4.2 (6)	.	.	.	.	no
C1	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
C1	Fe	N2	C4	101.3 (3)	.	.	.	.	no
C1	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
C1	Fe	N3	Si	-24.84 (19)	.	.	2_555	2_555	no
C1	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

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_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
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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	C1	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	C1	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	C1	3.0102	.	.	no
H2D	H1E	2.2917	.	.	no
H2E	C1	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	C1	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	C1	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	C1	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

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