A highly efficient titanium-based olefin polymerisation catalyst with a monoanionic iminoimidazolidide pi-donor ancillary ligand

Kretschmer, Winfried P.; Dijkhuis, C.; Meetsma, A.; Hessen, B.; Teuben, J.H

Published in:
Chemical Communications

DOI:
10.1039/b111343g

Publication date:
2002

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?
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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
Dr Winfried P Kretschmer
;
_publ_contact_author_address        # Address of author for correspondence
;
Dutch Polymer Institute
University of Groningen
Stratingh Institute of Chemistry &
Chemical Engineering
Nijenborgh 4
Groningen
9747 AG
NETHERLANDS
;
_publ_contact_author_email           KRETSCHMER@CHEM.RUG.NL

_publ_requested_journal              'Chemcomm'
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
Date of submission :  2001-08-14
Again    at          2001-12-17
Communication Ref.: B111343G

Consider this CIF submission for depostion of the
X-ray structure of a manuscript to be submitted to : Chemical Communications
(Our Compound_Identification_Code : CP540)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor          ?
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_journal_date_printers_final         ?
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# 3. TITLE AND AUTHOR LIST

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A highly efficient titanium-based olefin polymerisation catalyst with
a monoanionic imino-imidazolidide \p-donor ancillary ligand
;
_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
'Winfried Kretschmer'
;
Dutch Polymer Institute,
Centre for Catalytic Olefin Polymerisation,
Stratingh Institute of Chemistry and Chemical Engineering,
University of Groningen ,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
;
'Chris Dijksterhuis'
;
Dutch Polymer Institute,
Centre for Catalytic Olefin Polymerisation,
Stratingh Institute of Chemistry and Chemical Engineering,
University of Groningen ,
Nijenborgh 4,
```

NL-9747 AG Groningen,
The Netherlands.
;
'Auke Meetsma'
;
Dutch Polymer Institute,
Centre for Catalytic Olefin Polymerisation,
Stratingh Institute of Chemistry and Chemical Engineering,
University of Groningen ,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
;
'Bart Hessen'
;
Dutch Polymer Institute,
Centre for Catalytic Olefin Polymerisation,
Stratingh Institute of Chemistry and Chemical Engineering,
University of Groningen ,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
;
'Jan H. Teuben'
;
Dutch Polymer Institute,
Centre for Catalytic Olefin Polymerisation,
Stratingh Institute of Chemistry and Chemical Engineering,
University of Groningen ,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
;

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4. TEXT

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;
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.
A subsequent difference Fourier synthesis resulted in the location

of all the hydrogen atoms, which coordinates and isotropic displacement parameters were refined.
The absolute structure was determined by Flack's x-, resulting in a value ca. 0.5.
Twinning causes this result and therefore x was fixed at 0.5.

;

Insert blank lines between references

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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.

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

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Utrecht modified version October 1994.
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(Present distributor Kluwer Academic Publishers, Dordrecht).

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Edited by A.J.C Wilson, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

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

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Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. PLUTO drawing of the molecule illustrating the puckering
and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. 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 drawn with an arbitrary radius.
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;

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# 5. CHEMICAL DATA

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;
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_chemical_melting_point              ?
_chemical_formula_moiety
'C20 H19 Cl2 N3 Ti'
_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
'C20 H19 Cl2 N3 Ti'
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_chemical_compound_source           'synthesized by the authors / see text'

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Ti  Ti    0.2776    0.4457
'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'
Cl  Cl    0.1484    0.1585
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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C   C    0.0033    0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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_symmetry_space_group_name_H-M       'P 21 21 21'

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

_cell_length_a                         9.868(1)
_cell_length_b                        10.320(1)
_cell_length_c                        18.840(1)
_cell_angle_alpha                            90
_cell_angle_beta                             90
_cell_angle_gamma                            90
_cell_volume                         1918.6(3)
_cell_formula_units_Z                 4
_cell_measurement_temperature        180
_cell_measurement_reflns_used         22
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_cell_measurement_theta_max          20.46
_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)
;

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_exptl_crystal_density_method        'Not Measured'
_exptl_crystal_F_000                 864
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_diffrn_radiation_type               MoK\a
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_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 = (1.00 + 0.34 tg \q)\%.
;
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_diffrn_standards_number             3
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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
2 -2 -2
-2  2 -2
2  2  2

# number of measured reflections (redundant set)
_diffrn_reflns_number              4788
_diffrn_reflns_av_R_equivalents    0.0134
_diffrn_reflns_av_sigmaI/netI      0.0232
_diffrn_reflns_limit_h_min         -12
_diffrn_reflns_limit_h_max         12
_diffrn_reflns_limit_k_min         0
_diffrn_reflns_limit_k_max         13
_diffrn_reflns_limit_l_min         0
_diffrn_reflns_limit_l_max         24
_diffrn_reflns_theta_min           2.16
_diffrn_reflns_theta_max           27.47

_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
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_reflns_number_gt                  4018
_reflns_threshold_expression       >2sigma(I)


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_computing_cell_refinement           'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction            'HELENA (Spek, 1997)'
_computing_structure_solution
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;
DIRDIF-99 (Beurskens et al., 1999)
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_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 1997)
PLATON (Spek, 1994, 1996)
;
_computing_publication_material      'PLATON (Spek, 1990)'

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# 8. REFINEMENT DATA


_refine_special_details
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Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement.  R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2^)+(0.0434P)^2^+0.3772P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      Patterson
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_refine_ls_abs_structure_Flack    0.5
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_refine_ls_number_parameters      311
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_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0374
_refine_ls_R_factor_gt            0.0316
_refine_ls_wR_factor_ref          0.0764
_refine_ls_wR_factor_gt           0.0735
_refine_ls_goodness_of_fit_ref    1.062
_refine_ls_restrained_S_all       1.062
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.517
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Ti     Ti Uani    0.24172(3)   0.63439(3)   0.24863(2)     1.000    0.0191(1)
Cl1    Cl Uani    0.35330(6)   0.56072(6)   0.14904(3)     1.000    0.0334(2)
Cl2    Cl Uani    0.30955(7)   0.48457(6)   0.33097(3)     1.000    0.0370(2)
N1     N  Uani   0.06634(17)  0.60076(17)   0.23227(9)     1.000    0.0204(5)
N2     N  Uani  -0.14722(18)  0.64025(19)  0.17745(10)     1.000    0.0229(5)
N3     N  Uani  -0.13416(19)  0.65379(19)  0.29433(10)     1.000    0.0243(5)
C1     C  Uani     0.2505(3)    0.8531(2)  0.21813(14)     1.000    0.0312(7)
C2     C  Uani     0.1628(2)    0.8427(2)  0.27647(14)     1.000    0.0288(7)
C3     C  Uani     0.2383(3)    0.8000(2)  0.33501(14)     1.000    0.0317(7)
C4     C  Uani     0.3740(3)    0.7876(3)  0.31309(15)     1.000    0.0344(8)
C5     C  Uani     0.3827(2)    0.8204(2)  0.24183(15)     1.000    0.0327(7)
C6     C  Uani    -0.0623(2)    0.6300(2)  0.23398(11)     1.000    0.0211(6)
C7     C  Uani    -0.2883(2)    0.6516(2)  0.20084(13)     1.000    0.0257(6)
C8     C  Uani    -0.2738(3)    0.6923(3)  0.27782(14)     1.000    0.0294(7)
C9     C  Uani    -0.0822(2)    0.6536(2)  0.36423(12)     1.000    0.0261(6)
C10    C  Uani    -0.1117(3)    0.7579(3)  0.40904(14)     1.000    0.0352(8)
C11    C  Uani    -0.0630(3)    0.7559(3)  0.47814(16)     1.000   0.0479(10)
C12    C  Uani     0.0152(3)    0.6545(4)  0.50214(15)     1.000   0.0471(10)
C13    C  Uani     0.0443(3)    0.5516(3)  0.45790(14)     1.000    0.0387(8)
C14    C  Uani    -0.0056(2)    0.5501(3)  0.38875(13)     1.000    0.0291(7)
C15    C  Uani    -0.1153(2)    0.6209(2)  0.10468(12)     1.000    0.0253(6)
C16    C  Uani     0.0115(3)    0.6495(3)  0.07708(14)     1.000    0.0376(8)
C17    C  Uani     0.0361(3)    0.6316(4)  0.00548(15)     1.000    0.0478(9)
C18    C  Uani    -0.0636(3)    0.5860(4) -0.03877(15)     1.000   0.0517(12)
C19    C  Uani    -0.1890(3)    0.5581(4) -0.01169(15)     1.000    0.0496(9)
C20    C  Uani    -0.2166(2)    0.5753(3)  0.05981(14)     1.000    0.0357(8)
H1     H  Uiso      0.224(3)     0.876(3)   0.1731(15)     1.000     0.034(7)
H2     H  Uiso      0.066(3)     0.860(3)   0.2733(13)     1.000     0.029(7)
H3     H  Uiso      0.202(3)     0.785(3)   0.3777(15)     1.000     0.033(7)
H4     H  Uiso      0.436(3)     0.757(3)   0.3384(16)     1.000     0.045(9)
H5     H  Uiso      0.460(3)     0.813(3)   0.2168(15)     1.000     0.041(8)
H7     H  Uiso     -0.335(2)     0.565(2)   0.1959(12)     1.000     0.016(5)
H7'    H  Uiso     -0.335(3)     0.718(3)   0.1743(15)     1.000     0.033(7)
H8     H  Uiso     -0.282(3)     0.780(3)   0.2841(15)     1.000     0.036(8)
H8'    H  Uiso     -0.329(3)     0.652(3)   0.3069(14)     1.000     0.028(7)
H10    H  Uiso     -0.161(3)     0.829(3)   0.3906(14)     1.000     0.031(7)
H11    H  Uiso     -0.084(4)     0.839(4)     0.508(2)     1.000    0.074(12)
H12    H  Uiso      0.054(3)     0.646(3)   0.5460(18)     1.000     0.051(9)
H13    H  Uiso      0.101(3)     0.477(4)   0.4746(18)     1.000    0.057(10)
H14    H  Uiso      0.010(3)     0.484(3)   0.3583(14)     1.000     0.028(7)
H16    H  Uiso      0.081(3)     0.677(3)   0.1072(15)     1.000     0.036(8)
H17    H  Uiso      0.121(3)     0.650(3)  -0.0097(14)     1.000     0.030(7)
H18    H  Uiso     -0.043(4)     0.585(4)    -0.087(2)     1.000    0.081(13)
H19    H  Uiso     -0.264(3)     0.527(3)  -0.0416(17)     1.000    0.061(10)
H20    H  Uiso     -0.307(3)     0.564(3)   0.0764(16)     1.000     0.046(8)

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_atom_site_aniso_U_13
_atom_site_aniso_U_12
Ti       0.0165(2)  0.0171(2)  0.0237(2)  -0.0026(2)  -0.0006(2)   0.0023(1)
Cl1      0.0283(3)  0.0385(3)  0.0334(3)  -0.0108(3)   0.0066(2)   0.0021(2)
Cl2      0.0425(3)  0.0337(3)  0.0347(3)   0.0042(3)  -0.0021(3)   0.0187(3)
N1       0.0189(8)  0.0198(9)  0.0224(9)  -0.0021(6)  -0.0007(7)  -0.0021(6)
```

```
N2       0.0193(8)  0.0227(8)  0.0268(9)   0.0013(8)  -0.0025(7)   0.0011(8)
N3       0.0222(9) 0.0262(10)  0.0245(9)  -0.0001(8)   0.0015(7)   0.0042(8)
C1      0.0316(11) 0.0186(10) 0.0435(13)  0.0002(10)  0.0020(12) -0.0016(10)
C2      0.0231(11) 0.0135(10) 0.0499(14)  -0.0061(9)  0.0051(10)   0.0003(8)
C3      0.0377(13) 0.0248(11) 0.0326(12) -0.0131(10)  0.0069(12) -0.0042(10)
C4      0.0267(12) 0.0303(13) 0.0461(16) -0.0126(11) -0.0077(11) -0.0019(10)
C5      0.0234(10) 0.0270(11) 0.0478(15) -0.0098(11)  0.0072(11)  -0.0060(8)
C6       0.0248(9)  0.0131(9) 0.0254(11)   0.0004(8)   0.0007(8)  -0.0032(8)
C7      0.0180(10) 0.0263(12) 0.0327(11)  0.0036(10)  -0.0010(8)   0.0030(9)
C8      0.0229(12) 0.0318(13) 0.0334(12)  0.0022(10)  0.0026(10)   0.0066(9)
C9      0.0238(10) 0.0295(12) 0.0249(11)   0.0017(9)   0.0031(9)  -0.0011(9)
C10     0.0368(14) 0.0359(14) 0.0328(13) -0.0045(11)  0.0032(11)  0.0046(11)
C11     0.0539(18) 0.0554(19) 0.0343(15) -0.0120(14)  0.0049(13)  0.0047(15)
C12     0.0463(16)   0.070(2) 0.0251(13) -0.0013(15) -0.0004(12)  0.0033(16)
C13     0.0316(13) 0.0535(17) 0.0309(13)  0.0094(12)  0.0028(10)  0.0051(13)
C14     0.0276(12) 0.0317(13) 0.0280(12)  0.0037(10)   0.0039(9) -0.0012(10)
C15     0.0274(11) 0.0220(11) 0.0265(11)   0.0021(9)  -0.0030(9)   0.0007(9)
C16     0.0257(12) 0.0560(18) 0.0312(13)  0.0009(13) -0.0041(10) -0.0067(12)
C17     0.0301(13)   0.082(2) 0.0312(14)  0.0065(15)  0.0030(11) -0.0013(16)
C18     0.0437(16)   0.089(3) 0.0223(13)  0.0014(14) -0.0008(11)  0.0036(17)
C19     0.0391(14)   0.080(2) 0.0297(13) -0.0043(14) -0.0093(11) -0.0096(16)
C20     0.0262(12) 0.0513(16) 0.0295(12)  0.0031(12)  -0.0066(9) -0.0062(11)

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

# 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
Ti      Cl1       2.3045(7)                    .       .                   yes
Ti      Cl2       2.2902(7)                    .       .                   yes
Ti      N1       1.7918(17)                    .       .                   yes
Ti      C1         2.331(2)                    .       .                   yes
Ti      C2         2.346(2)                    .       .                   yes
Ti      C3         2.360(2)                    .       .                   yes
Ti      C4         2.383(3)                    .       .                   yes
Ti      C5         2.374(2)                    .       .                   yes
N1      C6         1.305(3)                    .       .                   yes
N2      C6         1.359(3)                    .       .                   yes
N2      C7         1.465(3)                    .       .                   yes
N2      C15        1.421(3)                    .       .                   yes
N3      C6         1.362(3)                    .       .                   yes
N3      C8         1.467(4)                    .       .                   yes
N3      C9         1.413(3)                    .       .                   yes
C1      C2         1.403(4)                    .       .                   no
C1      C5         1.420(4)                    .       .                   no
C2      C3         1.402(4)                    .       .                   no
C3      C4         1.407(4)                    .       .                   no
C4      C5         1.387(4)                    .       .                   no
C7      C8         1.517(4)                    .       .                   no
```

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C9      C10        1.399(4)                    .      .                 no
C9      C14        1.388(3)                    .      .                 no
C10     C11        1.388(4)                    .      .                 no
C11     C12        1.377(5)                    .      .                 no
C12     C13        1.380(5)                    .      .                 no
C13     C14        1.393(4)                    .      .                 no
C15     C16        1.387(4)                    .      .                 no
C15     C20        1.391(3)                    .      .                 no
C16     C17        1.383(4)                    .      .                 no
C17     C18        1.373(4)                    .      .                 no
C18     C19        1.369(4)                    .      .                 no
C19     C20        1.386(4)                    .      .                 no
C1      H1          0.92(3)                    .      .                 no
C2      H2          0.97(3)                    .      .                 no
C3      H3          0.89(3)                    .      .                 no
C4      H4          0.84(3)                    .      .                 no
C5      H5          0.90(3)                    .      .                 no
C7      H7          1.01(2)                    .      .                 no
C7      H7'         0.97(3)                    .      .                 no
C8      H8          0.92(3)                    .      .                 no
C8      H8'         0.88(3)                    .      .                 no
C10     H10         0.95(3)                    .      .                 no
C11     H11         1.05(4)                    .      .                 no
C12     H12         0.91(3)                    .      .                 no
C13     H13         1.00(4)                    .      .                 no
C14     H14         0.90(3)                    .      .                 no
C16     H16         0.93(3)                    .      .                 no
C17     H17         0.91(3)                    .      .                 no
C18     H18         0.93(4)                    .      .                 no
C19     H19         0.98(3)                    .      .                 no
C20     H20         0.95(3)                    .      .                 no

loop_
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_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
Cl1     Ti      Cl2       100.90(2)             .      .      .          yes
Cl1     Ti      N1        104.92(6)             .      .      .          yes
Cl1     Ti      C1         95.80(7)             .      .      .          yes
Cl1     Ti      C2        130.01(7)             .      .      .          yes
Cl1     Ti      C3        143.81(7)             .      .      .          yes
Cl1     Ti      C4        111.84(7)             .      .      .          yes
Cl1     Ti      C5         86.72(7)             .      .      .          yes
Cl2     Ti      N1        105.55(6)             .      .      .          yes
Cl2     Ti      C1        144.09(7)             .      .      .          yes
Cl2     Ti      C2        124.35(7)             .      .      .          yes
Cl2     Ti      C3         91.49(6)             .      .      .          yes
Cl2     Ti      C4         86.71(7)             .      .      .          yes
Cl2     Ti      C5        114.28(6)             .      .      .          yes
N1      Ti      C1        100.43(9)             .      .      .          yes
N1      Ti      C2         83.99(8)             .      .      .          yes
N1      Ti      C3        104.19(9)             .      .      .          yes
N1      Ti      C4        138.18(9)             .      .      .          yes
N1      Ti      C5        135.50(8)             .      .      .          yes
C1      Ti      C2         34.92(9)             .      .      .          yes
C1      Ti      C3         57.95(9)             .      .      .          yes
C1      Ti      C4        57.50(10)             .      .      .          yes
C1      Ti      C5         35.11(9)             .      .      .          yes
C2      Ti      C3         34.66(9)             .      .      .          yes
```

C2	Ti	C4	57.31(9)	.	.	.	yes
C2	Ti	C5	57.70(7)	.	.	.	yes
C3	Ti	C4	34.51(10)	.	.	.	yes
C3	Ti	C5	57.32(9)	.	.	.	yes
C4	Ti	C5	33.91(10)	.	.	.	yes
Ti	N1	C6	152.92(16)	.	.	.	yes
C6	N2	C7	110.88(18)	.	.	.	yes
C6	N2	C15	127.48(18)	.	.	.	yes
C7	N2	C15	120.81(18)	.	.	.	yes
C6	N3	C8	111.14(18)	.	.	.	yes
C6	N3	C9	126.06(18)	.	.	.	yes
C8	N3	C9	122.59(19)	.	.	.	yes
Ti	C1	C2	73.13(13)	.	.	.	yes
Ti	C1	C5	74.12(12)	.	.	.	yes
C2	C1	C5	107.6(2)	.	.	.	no
Ti	C2	C1	71.95(12)	.	.	.	yes
Ti	C2	C3	73.23(12)	.	.	.	yes
C1	C2	C3	108.2(2)	.	.	.	no
Ti	C3	C2	72.11(14)	.	.	.	yes
Ti	C3	C4	73.63(16)	.	.	.	yes
C2	C3	C4	107.7(2)	.	.	.	no
Ti	C4	C3	71.86(15)	.	.	.	yes
Ti	C4	C5	72.70(15)	.	.	.	yes
C3	C4	C5	108.7(2)	.	.	.	no
Ti	C5	C1	70.77(12)	.	.	.	yes
Ti	C5	C4	73.39(15)	.	.	.	yes
C1	C5	C4	107.8(2)	.	.	.	no
N1	C6	N2	126.74(19)	.	.	.	yes
N1	C6	N3	124.65(19)	.	.	.	yes
N2	C6	N3	108.60(17)	.	.	.	yes
N2	C7	C8	102.72(18)	.	.	.	yes
N3	C8	C7	102.5(2)	.	.	.	yes
N3	C9	C10	119.1(2)	.	.	.	yes
N3	C9	C14	120.6(2)	.	.	.	yes
C10	C9	C14	120.3(2)	.	.	.	no
C9	C10	C11	118.9(3)	.	.	.	no
C10	C11	C12	120.9(3)	.	.	.	no
C11	C12	C13	120.2(3)	.	.	.	no
C12	C13	C14	120.0(3)	.	.	.	no
C9	C14	C13	119.7(3)	.	.	.	no
N2	C15	C16	122.1(2)	.	.	.	yes
N2	C15	C20	118.33(19)	.	.	.	yes
C16	C15	C20	119.5(2)	.	.	.	no
C15	C16	C17	119.7(3)	.	.	.	no
C16	C17	C18	120.8(3)	.	.	.	no
C17	C18	C19	119.6(3)	.	.	.	no
C18	C19	C20	120.9(3)	.	.	.	no
C15	C20	C19	119.5(2)	.	.	.	no
Ti	C1	H1	117.8(19)	.	.	.	no
C2	C1	H1	124.6(19)	.	.	.	no
C5	C1	H1	127.8(19)	.	.	.	no
Ti	C2	H2	118.7(18)	.	.	.	no
C1	C2	H2	122.9(15)	.	.	.	no
C3	C2	H2	128.8(15)	.	.	.	no
Ti	C3	H3	120(2)	.	.	.	no
C2	C3	H3	123.3(19)	.	.	.	no
C4	C3	H3	129.0(19)	.	.	.	no
Ti	C4	H4	116(2)	.	.	.	no
C3	C4	H4	124(2)	.	.	.	no
C5	C4	H4	127(2)	.	.	.	no
Ti	C5	H5	117(2)	.	.	.	no
C1	C5	H5	129.4(19)	.	.	.	no
C4	C5	H5	122.6(19)	.	.	.	no
N2	C7	H7	109.6(12)	.	.	.	no

```
N2      C7      H7'       110.8(17)              .       .       .          no
C8      C7      H7        112.1(13)              .       .       .          no
C8      C7      H7'       110.1(17)              .       .       .          no
H7      C7      H7'          111(2)              .       .       .          no
N3      C8      H8        108.8(19)              .       .       .          no
N3      C8      H8'       108.8(19)              .       .       .          no
C7      C8      H8        112.9(18)              .       .       .          no
C7      C8      H8'       114.0(19)              .       .       .          no
H8      C8      H8'          109(3)              .       .       .          no
C9      C10     H10       118.8(17)              .       .       .          no
C11     C10     H10       122.3(17)              .       .       .          no
C10     C11     H11          115(2)              .       .       .          no
C12     C11     H11          124(2)              .       .       .          no
C11     C12     H12          127(2)              .       .       .          no
C13     C12     H12          113(2)              .       .       .          no
C12     C13     H13          121(2)              .       .       .          no
C14     C13     H13          119(2)              .       .       .          no
C9      C14     H14       117.5(18)              .       .       .          no
C13     C14     H14       122.8(18)              .       .       .          no
C15     C16     H16       119.9(18)              .       .       .          no
C17     C16     H16       120.3(18)              .       .       .          no
C16     C17     H17       116.3(17)              .       .       .          no
C18     C17     H17       122.9(17)              .       .       .          no
C17     C18     H18          116(2)              .       .       .          no
C19     C18     H18          124(2)              .       .       .          no
C18     C19     H19       122.3(18)              .       .       .          no
C20     C19     H19       116.8(18)              .       .       .          no
C15     C20     H20       121.0(18)              .       .       .          no
C19     C20     H20       119.2(18)              .       .       .          no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
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_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
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Cl1     Ti      N1      C6        -139.0(3)     .       .       .       .   no
Cl2     Ti      N1      C6         114.9(3)     .       .       .       .   no
C1      Ti      N1      C6         -40.0(4)     .       .       .       .   no
C2      Ti      N1      C6          -9.1(3)     .       .       .       .   no
C3      Ti      N1      C6          19.3(4)     .       .       .       .   no
C4      Ti      N1      C6          12.1(4)     .       .       .       .   no
C5      Ti      N1      C6         -38.2(4)     .       .       .       .   no
Cl1     Ti      C1      C2       169.65(13)     .       .       .       .   no
Cl1     Ti      C1      C5       -75.86(15)     .       .       .       .   no
Cl2     Ti      C1      C2       -72.69(19)     .       .       .       .   no
Cl2     Ti      C1      C5          41.8(2)     .       .       .       .   no
N1      Ti      C1      C2        63.27(15)     .       .       .       .   no
N1      Ti      C1      C5       177.77(15)     .       .       .       .   no
C2      Ti      C1      C5         114.5(2)     .       .       .       .   no
C3      Ti      C1      C2       -37.02(14)     .       .       .       .   no
C3      Ti      C1      C5        77.47(17)     .       .       .       .   no
C4      Ti      C1      C2       -78.10(16)     .       .       .       .   no
C4      Ti      C1      C5        36.40(16)     .       .       .       .   no
C5      Ti      C1      C2        -114.5(2)     .       .       .       .   no
Cl1     Ti      C2      C1       -13.50(17)     .       .       .       .   no
Cl1     Ti      C2      C3      -129.70(14)     .       .       .       .   no
Cl2     Ti      C2      C1       137.29(14)     .       .       .       .   no
Cl2     Ti      C2      C3        21.09(16)     .       .       .       .   no
```

N1	Ti	C2	C1	-117.96(16)	.	.	.	.	no
N1	Ti	C2	C3	125.84(15)	.	.	.	.	no
C1	Ti	C2	C3	-116.2(2)	.	.	.	.	no
C3	Ti	C2	C1	116.2(2)	.	.	.	.	no
C4	Ti	C2	C1	78.70(16)	.	.	.	.	no
C4	Ti	C2	C3	-37.50(15)	.	.	.	.	no
C5	Ti	C2	C1	38.25(15)	.	.	.	.	no
C5	Ti	C2	C3	-77.95(16)	.	.	.	.	no
Cl1	Ti	C3	C2	86.44(18)	.	.	.	.	no
Cl1	Ti	C3	C4	-28.8(2)	.	.	.	.	no
Cl2	Ti	C3	C2	-162.71(13)	.	.	.	.	no
Cl2	Ti	C3	C4	82.00(15)	.	.	.	.	no
N1	Ti	C3	C2	-56.26(15)	.	.	.	.	no
N1	Ti	C3	C4	-171.55(16)	.	.	.	.	no
C1	Ti	C3	C2	37.30(14)	.	.	.	.	no
C1	Ti	C3	C4	-77.99(17)	.	.	.	.	no
C2	Ti	C3	C4	-115.3(2)	.	.	.	.	no
C4	Ti	C3	C2	115.3(2)	.	.	.	.	no
C5	Ti	C3	C2	79.13(14)	.	.	.	.	no
C5	Ti	C3	C4	-36.16(15)	.	.	.	.	no
Cl1	Ti	C4	C3	162.13(13)	.	.	.	.	no
Cl1	Ti	C4	C5	45.03(16)	.	.	.	.	no
Cl2	Ti	C4	C3	-97.44(15)	.	.	.	.	no
Cl2	Ti	C4	C5	145.46(14)	.	.	.	.	no
N1	Ti	C4	C3	12.3(2)	.	.	.	.	no
N1	Ti	C4	C5	-104.76(17)	.	.	.	.	no
C1	Ti	C4	C3	79.39(17)	.	.	.	.	no
C1	Ti	C4	C5	-37.72(14)	.	.	.	.	no
C2	Ti	C4	C3	37.67(15)	.	.	.	.	no
C2	Ti	C4	C5	-79.44(16)	.	.	.	.	no
C3	Ti	C4	C5	-117.1(2)	.	.	.	.	no
C5	Ti	C4	C3	117.1(2)	.	.	.	.	no
Cl1	Ti	C5	C1	104.91(15)	.	.	.	.	no
Cl1	Ti	C5	C4	-138.88(15)	.	.	.	.	no
Cl2	Ti	C5	C1	-154.60(13)	.	.	.	.	no
Cl2	Ti	C5	C4	-38.39(16)	.	.	.	.	no
N1	Ti	C5	C1	-3.1(2)	.	.	.	.	no
N1	Ti	C5	C4	113.08(17)	.	.	.	.	no
C1	Ti	C5	C4	116.2(2)	.	.	.	.	no
C2	Ti	C5	C1	-38.04(15)	.	.	.	.	no
C2	Ti	C5	C4	78.17(17)	.	.	.	.	no
C3	Ti	C5	C1	-79.40(16)	.	.	.	.	no
C3	Ti	C5	C4	36.81(16)	.	.	.	.	no
C4	Ti	C5	C1	-116.2(2)	.	.	.	.	no
N1	Ti	C2	H2	0.3(17)	.	.	.	.	no
C1	Ti	C2	H2	118.2(17)	.	.	.	.	no
C3	Ti	C2	H2	-125.6(17)	.	.	.	.	no
C4	Ti	C2	H2	-163.1(17)	.	.	.	.	no
C5	Ti	C2	H2	156.5(17)	.	.	.	.	no
Cl1	Ti	C3	H3	-155(2)	.	.	.	.	no
Cl2	Ti	C3	H3	-44(2)	.	.	.	.	no
N1	Ti	C3	H3	62(2)	.	.	.	.	no
C1	Ti	C3	H3	156(2)	.	.	.	.	no
C2	Ti	C3	H3	119(2)	.	.	.	.	no
C4	Ti	C3	H3	-126(2)	.	.	.	.	no
C5	Ti	C3	H3	-162(2)	.	.	.	.	no
Cl1	Ti	C4	H4	-78(2)	.	.	.	.	no
Cl2	Ti	C4	H4	22(2)	.	.	.	.	no
N1	Ti	C4	H4	132(2)	.	.	.	.	no
C1	Ti	C4	H4	-161(2)	.	.	.	.	no
C2	Ti	C4	H4	158(2)	.	.	.	.	no
C3	Ti	C4	H4	120(2)	.	.	.	.	no
C5	Ti	C4	H4	-123(2)	.	.	.	.	no
Cl1	Ti	C5	H5	-20(2)	.	.	.	.	no

Cl2	Ti	C5	H5	80(2)	.	.	.	.	no
N1	Ti	C5	H5	-128(2)	.	.	.	.	no
C1	Ti	C5	H5	-125(2)	.	.	.	.	no
C2	Ti	C5	H5	-163(2)	.	.	.	.	no
C3	Ti	C5	H5	155(2)	.	.	.	.	no
C4	Ti	C5	H5	119(2)	.	.	.	.	no
C2	Ti	C1	H1	-121(2)	.	.	.	.	no
C3	Ti	C1	H1	-158(2)	.	.	.	.	no
C4	Ti	C1	H1	161(2)	.	.	.	.	no
C5	Ti	C1	H1	125(2)	.	.	.	.	no
Cl1	Ti	C2	H2	104.7(17)	.	.	.	.	no
Cl2	Ti	C2	H2	-104.5(17)	.	.	.	.	no
Cl1	Ti	C1	H1	49(2)	.	.	.	.	no
Cl2	Ti	C1	H1	167(2)	.	.	.	.	no
N1	Ti	C1	H1	-57(2)	.	.	.	.	no
Ti	N1	C6	N2	120.0(3)	.	.	.	.	no
Ti	N1	C6	N3	-60.9(4)	.	.	.	.	no
C7	N2	C6	N3	-9.3(2)	.	.	.	.	no
C6	N2	C7	C8	18.5(2)	.	.	.	.	no
C15	N2	C6	N1	0.4(4)	.	.	.	.	no
C15	N2	C6	N3	-178.8(2)	.	.	.	.	no
C7	N2	C6	N1	169.9(2)	.	.	.	.	no
C7	N2	C15	C16	159.4(2)	.	.	.	.	no
C7	N2	C15	C20	-18.7(3)	.	.	.	.	no
C15	N2	C7	C8	-171.2(2)	.	.	.	.	no
C6	N2	C15	C16	-32.1(3)	.	.	.	.	no
C6	N2	C15	C20	149.8(2)	.	.	.	.	no
C8	N3	C6	N1	176.2(2)	.	.	.	.	no
C8	N3	C6	N2	-4.6(3)	.	.	.	.	no
C9	N3	C6	N1	1.4(3)	.	.	.	.	no
C6	N3	C9	C10	131.1(2)	.	.	.	.	no
C6	N3	C9	C14	-50.4(3)	.	.	.	.	no
C8	N3	C9	C10	-43.1(3)	.	.	.	.	no
C8	N3	C9	C14	135.4(2)	.	.	.	.	no
C9	N3	C6	N2	-179.4(2)	.	.	.	.	no
C6	N3	C8	C7	15.6(3)	.	.	.	.	no
C9	N3	C8	C7	-169.35(19)	.	.	.	.	no
C5	C1	C2	C3	-1.9(2)	.	.	.	.	no
Ti	C1	C5	C4	-64.55(18)	.	.	.	.	no
C2	C1	C5	Ti	66.00(15)	.	.	.	.	no
C2	C1	C5	C4	1.5(3)	.	.	.	.	no
Ti	C1	C2	C3	64.74(15)	.	.	.	.	no
C5	C1	C2	Ti	-66.67(15)	.	.	.	.	no
Ti	C2	C3	C4	65.57(18)	.	.	.	.	no
C1	C2	C3	C4	1.7(3)	.	.	.	.	no
C1	C2	C3	Ti	-63.91(15)	.	.	.	.	no
C2	C3	C4	Ti	-64.56(16)	.	.	.	.	no
C2	C3	C4	C5	-0.8(3)	.	.	.	.	no
Ti	C3	C4	C5	63.81(19)	.	.	.	.	no
C3	C4	C5	C1	-0.4(3)	.	.	.	.	no
Ti	C4	C5	C1	62.83(16)	.	.	.	.	no
C3	C4	C5	Ti	-63.27(19)	.	.	.	.	no
N2	C7	C8	N3	-19.5(2)	.	.	.	.	no
N3	C9	C10	C11	178.6(2)	.	.	.	.	no
C14	C9	C10	C11	0.1(4)	.	.	.	.	no
N3	C9	C14	C13	-179.8(2)	.	.	.	.	no
C10	C9	C14	C13	-1.3(4)	.	.	.	.	no
C9	C10	C11	C12	1.2(4)	.	.	.	.	no
C10	C11	C12	C13	-1.2(5)	.	.	.	.	no
C11	C12	C13	C14	-0.1(5)	.	.	.	.	no
C12	C13	C14	C9	1.3(4)	.	.	.	.	no
N2	C15	C16	C17	-178.5(3)	.	.	.	.	no
C20	C15	C16	C17	-0.4(4)	.	.	.	.	no
N2	C15	C20	C19	178.7(3)	.	.	.	.	no

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C16     C15     C20     C19          0.5(4)     .       .       .       .   no
C15     C16     C17     C18          0.1(5)     .       .       .       .   no
C16     C17     C18     C19          0.1(6)     .       .       .       .   no
C17     C18     C19     C20          0.0(6)     .       .       .       .   no
C18     C19     C20     C15         -0.3(5)     .       .       .       .   no

loop_
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_geom_contact_site_symmetry_1
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Ti      C9          3.873(2)                    .       .                   no
Ti      C14         3.699(2)                    .       .                   no
Ti      C16         3.954(3)                    .       .                   no
Ti      H14          3.45(3)                    .       .                   no
Ti      H16          3.13(3)                    .       .                   no
Cl2     C13         3.612(3)                    .       .                   no
Cl2     C7          3.494(2)                    .     4_545                 no
Cl2     C18         3.583(3)                    .     2_565                 no
Cl2     C14         3.364(2)                    .       .                   no
Cl1     H10          3.14(3)                    .     4_545                 no
Cl1     H12          3.03(3)                    .     2_564                 no
Cl1     H16          3.05(3)                    .       .                   no
Cl2     H18          2.87(4)                    .     2_565                 no
Cl2     H14          3.00(3)                    .       .                   no
Cl2     H5           3.02(3)                    .     4_645                 no
Cl2     H7'          2.76(3)                    .     4_545                 no
Cl2     H8           3.04(3)                    .     4_545                 no
N1      C14         3.077(3)                    .       .                   no
N1      C16         3.016(3)                    .       .                   no
N2      C2          3.195(3)                    .     4_545                 no
N3      C1          3.317(3)                    .     4_545                 no
N1      H16          2.49(3)                    .       .                   no
N1      H14          2.72(3)                    .       .                   no
N1      H2           2.81(3)                    .     4_545                 no
N3      H2           2.93(3)                    .       .                   no
C1      N3          3.317(3)                    .     4_555                 no
C1      C6          3.525(3)                    .     4_555                 no
C1      C7          3.458(3)                    .     4_555                 no
C1      C8          3.509(4)                    .     4_555                 no
C2      C6          3.133(3)                    .     4_555                 no
C2      C9          3.520(3)                    .       .                   no
C2      N2          3.195(3)                    .     4_555                 no
C2      C7          3.447(3)                    .     4_555                 no
C3      C20         3.471(4)                    .     4_555                 no
C3      C9          3.548(3)                    .       .                   no
C6      C1          3.525(3)                    .     4_545                 no
C6      C2          3.133(3)                    .     4_545                 no
C7      C1          3.458(3)                    .     4_545                 no
C7      Cl2         3.494(2)                    .     4_555                 no
C7      C2          3.447(3)                    .     4_545                 no
C8      C1          3.509(4)                    .     4_545                 no
C9      C2          3.520(3)                    .       .                   no
C9      C3          3.548(3)                    .       .                   no
C9      Ti          3.873(2)                    .       .                   no
C13     Cl2         3.612(3)                    .       .                   no
C14     N1          3.077(3)                    .       .                   no
C14     Ti          3.699(2)                    .       .                   no
C14     Cl2         3.364(2)                    .       .                   no
C16     N1          3.016(3)                    .       .                   no
C16     Ti          3.954(3)                    .       .                   no
C18     Cl2         3.583(3)                    .     2_564                 no
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C20	C3	3.471(4)	.	4_545	no
C1	H7	2.85(2)	.	4_555	no
C2	H7	2.90(2)	.	4_555	no
C3	H7	2.95(2)	.	4_555	no
C4	H7	2.89(2)	.	4_555	no
C5	H7	2.82(2)	.	4_555	no
C6	H14	2.87(3)	.	.	no
C6	H16	2.82(3)	.	.	no
C6	H2	2.79(3)	.	4_545	no
C6	H2	2.79(3)	.	.	no
C7	H20	2.52(3)	.	.	no
C7	H5	3.01(3)	.	1_455	no
C8	H10	2.78(3)	.	.	no
C9	H19	2.99(3)	.	2_465	no
C10	H8'	3.08(3)	.	.	no
C10	H8	2.90(3)	.	.	no
C13	H19	2.88(3)	.	2_465	no
C14	H1	3.04(3)	.	4_545	no
C14	H19	2.74(3)	.	2_465	no
C17	H11	3.07(4)	.	4_545	no
C18	H11	2.99(4)	.	4_545	no
C20	H7	2.82(2)	.	.	no
C20	H7'	2.86(3)	.	.	no
H1	C14	3.04(3)	.	4_555	no
H2	N3	2.93(3)	.	.	no
H2	C6	2.79(3)	.	.	no
H2	N1	2.81(3)	.	4_555	no
H2	C6	2.79(3)	.	4_555	no
H5	C7	3.01(3)	.	1_655	no
H5	H7'	2.39(4)	.	1_655	no
H5	Cl2	3.02(3)	.	4_655	no
H7	C20	2.82(2)	.	.	no
H7	H20	2.27(4)	.	.	no
H7	C1	2.85(2)	.	4_545	no
H7	C2	2.90(2)	.	4_545	no
H7	C3	2.95(2)	.	4_545	no
H7	C4	2.89(2)	.	4_545	no
H7	C5	2.82(2)	.	4_545	no
H7'	C20	2.86(3)	.	.	no
H7'	H5	2.39(4)	.	1_455	no
H7'	H20	2.45(4)	.	.	no
H7'	Cl2	2.76(3)	.	4_555	no
H8	C10	2.90(3)	.	.	no
H8	H10	2.39(4)	.	.	no
H8	Cl2	3.04(3)	.	4_555	no
H8'	C10	3.08(3)	.	.	no
H10	C8	2.78(3)	.	.	no
H10	H8	2.39(4)	.	.	no
H10	Cl1	3.14(3)	.	4_555	no
H11	C17	3.07(4)	.	4_555	no
H11	C18	2.99(4)	.	4_555	no
H12	Cl1	3.03(3)	.	2_565	no
H14	Ti	3.45(3)	.	.	no
H14	Cl2	3.00(3)	.	.	no
H14	N1	2.72(3)	.	.	no
H14	C6	2.87(3)	.	.	no
H16	Ti	3.13(3)	.	.	no
H16	Cl1	3.05(3)	.	.	no
H16	N1	2.49(3)	.	.	no
H16	C6	2.82(3)	.	.	no
H18	Cl2	2.87(4)	.	2_564	no
H19	C9	2.99(3)	.	2_464	no
H19	C13	2.88(3)	.	2_464	no
H19	C14	2.74(3)	.	2_464	no

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H20     C7          2.52(3)                     .       .                   no
H20     H7          2.27(4)                     .       .                   no
H20     H7'         2.45(4)                     .       .                   no

loop_
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_geom_hbond_atom_site_label_H
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_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C7      H7'     Cl2        0.97(3)    2.76(3)   3.494(2)     133(2)   4_555 yes
C16     H16     N1         0.93(3)    2.49(3)   3.016(3)     116(2)     .   yes

#===End of Crystallographic Information File
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