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

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1. SUBMISSION DETAILS

_publ_contact_author_name # Name of author for correspondence
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Communication Ref.: B111343G

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3. TITLE AND AUTHOR LIST

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_publ_section_title_footnote
;
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;

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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_
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  _publ_author_address
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#=====

4. TEXT

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_publ_section_abstract

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;

Insert blank lines between paragraphs

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_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.

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

_publ_section_references

;

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

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Utrecht modified version October 1994.
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Edited by A.J.C Wilson, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

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University, The Netherlands.

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

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# 6. CRYSTAL DATA

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_symmetry_space_group_name_H-M  'P 21 21 21'

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_symmetry_equiv_pos_as_xyz
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
_cell_measurement_theta_min   16.42
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_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_F_000            864
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# 7. EXPERIMENTAL DATA

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;

_diffn_ambient_temperature      180(2)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK\alpha

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_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\alpha radiation,
\w/2\q scan, \D\w = (1.00 + 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_%           'no decay, variation 1.1'

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_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
_reflns_number_total             4401
_reflns_number_gt                4018
_reflns_threshold_expression      >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, 1997)'
_computing_structure_solution

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;
DIRDIF-99 (Beurskens et al., 1999)
;
_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

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_refine_special_details
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Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type                full
_refine_ls_weighting_scheme
'calc w=1/[\s2(Fo2)+(0.0434P)2+0.3772P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary          Patterson
_atom_sites_solution_secondary        direct
_atom_sites_solution_hydrogens        difmap
_refine_ls_hydrogen_treatment         refall
_refine_ls_extinction_method          none
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'Flack H.D. (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack        0.5
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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
_refine_diff_density_min              -0.311
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9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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 _atom_site_U_iso_or_equiv

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_23
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 _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	C11	2.3045(7)	.	.	yes
Ti	C12	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

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_

_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

C11	Ti	C12	100.90(2)	.	.	.	yes
C11	Ti	N1	104.92(6)	.	.	.	yes
C11	Ti	C1	95.80(7)	.	.	.	yes
C11	Ti	C2	130.01(7)	.	.	.	yes
C11	Ti	C3	143.81(7)	.	.	.	yes
C11	Ti	C4	111.84(7)	.	.	.	yes
C11	Ti	C5	86.72(7)	.	.	.	yes
C12	Ti	N1	105.55(6)	.	.	.	yes
C12	Ti	C1	144.09(7)	.	.	.	yes
C12	Ti	C2	124.35(7)	.	.	.	yes
C12	Ti	C3	91.49(6)	.	.	.	yes
C12	Ti	C4	86.71(7)	.	.	.	yes
C12	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

_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

C11	Ti	N1	C6	-139.0(3)	.	.	.	.	no
C12	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
C11	Ti	C1	C2	169.65(13)	.	.	.	.	no
C11	Ti	C1	C5	-75.86(15)	.	.	.	.	no
C12	Ti	C1	C2	-72.69(19)	.	.	.	.	no
C12	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
C11	Ti	C2	C1	-13.50(17)	.	.	.	.	no
C11	Ti	C2	C3	-129.70(14)	.	.	.	.	no
C12	Ti	C2	C1	137.29(14)	.	.	.	.	no
C12	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
Cl11	Ti	C3	C2	86.44(18)	.	.	.	.	no
Cl11	Ti	C3	C4	-28.8(2)	.	.	.	.	no
Cl12	Ti	C3	C2	-162.71(13)	.	.	.	.	no
Cl12	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
Cl11	Ti	C4	C3	162.13(13)	.	.	.	.	no
Cl11	Ti	C4	C5	45.03(16)	.	.	.	.	no
Cl12	Ti	C4	C3	-97.44(15)	.	.	.	.	no
Cl12	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
Cl11	Ti	C5	C1	104.91(15)	.	.	.	.	no
Cl11	Ti	C5	C4	-138.88(15)	.	.	.	.	no
Cl12	Ti	C5	C1	-154.60(13)	.	.	.	.	no
Cl12	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
Cl11	Ti	C3	H3	-155(2)	.	.	.	.	no
Cl12	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
Cl11	Ti	C4	H4	-78(2)	.	.	.	.	no
Cl12	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
Cl11	Ti	C5	H5	-20(2)	.	.	.	.	no

C12	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
C11	Ti	C2	H2	104.7(17)	.	.	.	.	no
C12	Ti	C2	H2	-104.5(17)	.	.	.	.	no
C11	Ti	C1	H1	49(2)	.	.	.	.	no
C12	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

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_

_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

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
C12	C13	3.612(3)	.	.	no
C12	C7	3.494(2)	.	4_545	no
C12	C18	3.583(3)	.	2_565	no
C12	C14	3.364(2)	.	.	no
C11	H10	3.14(3)	.	4_545	no
C11	H12	3.03(3)	.	2_564	no
C11	H16	3.05(3)	.	.	no
C12	H18	2.87(4)	.	2_565	no
C12	H14	3.00(3)	.	.	no
C12	H5	3.02(3)	.	4_645	no
C12	H7'	2.76(3)	.	4_545	no
C12	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	C12	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	C12	3.612(3)	.	.	no
C14	N1	3.077(3)	.	.	no
C14	Ti	3.699(2)	.	.	no
C14	C12	3.364(2)	.	.	no
C16	N1	3.016(3)	.	.	no
C16	Ti	3.954(3)	.	.	no
C18	C12	3.583(3)	.	2_564	no

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	C12	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'	C12	2.76(3)	.	4_555	no
H8	C10	2.90(3)	.	.	no
H8	H10	2.39(4)	.	.	no
H8	C12	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	C11	3.14(3)	.	4_555	no
H11	C17	3.07(4)	.	4_555	no
H11	C18	2.99(4)	.	4_555	no
H12	C11	3.03(3)	.	2_565	no
H14	Ti	3.45(3)	.	.	no
H14	C12	3.00(3)	.	.	no
H14	N1	2.72(3)	.	.	no
H14	C6	2.87(3)	.	.	no
H16	Ti	3.13(3)	.	.	no
H16	C11	3.05(3)	.	.	no
H16	N1	2.49(3)	.	.	no
H16	C6	2.82(3)	.	.	no
H18	C12	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

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

loop_

_geom_hbond_atom_site_label_D

_geom_hbond_atom_site_label_H

_geom_hbond_atom_site_label_A

_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'	C12	0.97(3)	2.76(3)	3.494(2)	133(2)	4_555	yes
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C16	H16	N1	0.93(3)	2.49(3)	3.016(3)	116(2)	.	yes
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#==End of Crystallographic Information File