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Highly efficient hydrosilylation of alkenes by organoyttrium catalysts with sterically demanding amidinate and guanidinate ligands

Ge, Shaozhong; Meetsma, Auke; Hessen, Bart

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;
?
;

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name   of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address         # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Organometallics'
# Publication choose FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
_publ_requested_category              ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                 # Include date of submission
;
  Date of submission :  2007-12-19  15:20:02

  Consider this CIF submission for deposition of the first
  X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : q1321)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_to_coeditor            ?

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_journal_date_from_coeditor      ?
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_journal_date_printers_final     ?
_journal_date_proofs_out         ?
_journal_date_proofs_in         ?

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_journal_coeditor_code           ?
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_journal_techeditor_code         ?
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_journal_page_last              ?

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3. TITLE AND AUTHOR LIST

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_publ_section_title
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;
_publ_section_title_footnote
;
;

```

The loop structure below should contain the names and addresses of all
authors, in the required order of publication. Repeat as necessary.

```

loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
; # author related footnote
;
; # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote
;
;

```

Crystal Structure Center, Chemical Physics,
Zernike Institute for Advanced Materials,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen, The Netherlands.

;

#=====

4. TEXT

_publ_section_synopsis

;

;

_publ_section_abstract

;

;

Insert blank lines between paragraphs

_publ_section_comment

;

;

_publ_section_exptl_prep

;

;

_publ_section_exptl_refinement

;

The hydrogen atoms were generated by geometrical considerations,
constrained to idealized geometries, and allowed to ride on the
carrier atom with an isotropic displacement parameter related to the
equivalent displacement parameter of their carrier atoms,
with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

The methyl-groups were refined as rigid groups, which were allowed
to rotate freely.

Assigned values of bond distances: tertiary C-H = 1.00 \%,
secondary C-H₂ = 0.99 \%, methyl C-H₃ = 0.98 \%,
aromatic C-H = 0.95 \%.

C-H distances were in the range of 0.95 -- 1.00(3) \%.

;

_publ_section_related_literature

;

;

Insert blank lines between references

_publ_section_references

;

Allen, F.H. (2000). Acta Cryst. B58, 380-388.

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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. Perspective PLUTO drawings of the molecule illustrating the configuration and the adopted numbering scheme.

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

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

;

_publ_section_acknowledgements

;

;

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C39 H70 N3 O Si2 Y'

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)₃, (C6 N6 Cr 3-)₂, 2(H2 O)'

_chemical_formula_structural ?

```

_chemical_formula_sum
'C39 H70 N3 O Si2 Y'
_chemical_formula_iupac
?
_chemical_formula_weight
742.08
_chemical_compound_source
'see text'

```

```

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
Y Y -2.7962 3.5667
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Si Si 0.0817 0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.0060
'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'
H H 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

```

#=====

```

``` # 6. CRYSTAL DATA ```

```

_symmetry_cell_setting
orthorhombic
_symmetry_space_group_name_Hall
'P 2ac 2ab'
_symmetry_space_group_name_H-M
'P 21 21 21'
_symmetry_Int_Tables_number
19

```

```

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,-y,1/2+z
3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z

```

```

_cell_length_a
12.9822(8)
_cell_length_b
17.6370(11)
_cell_length_c
18.8875(12)
_cell_angle_alpha
90
_cell_angle_beta
90
_cell_angle_gamma
90
_cell_volume
4324.6(5)
_cell_formula_units_Z
4

```

```

_cell_measurement_temperature
100(1)
_cell_measurement_reflns_used
9028
_cell_measurement_theta_min
2.55
_cell_measurement_theta_max
25.66
_cell_special_details

```

```

;
```

The final unit cell was obtained from the xyz centroids of 9028 reflections after integration using the SAINTPLUS software package (Bruker, 2000).

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      'block'
_exptl_crystal_colour          'colorless'
_exptl_crystal_size_max        0.52
_exptl_crystal_size_mid        0.46
_exptl_crystal_size_min        0.42
_exptl_crystal_size_rad        ?
_exptl_crystal_density_meas    ?
_exptl_crystal_density_diffn   1.140
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           1600
_exptl_absorpt_coefficient_mu   1.434
_exptl_absorpt_correction_type  'multi-scan'
_exptl_absorpt_process_details '(SADABS, (Bruker, 2006))'
_exptl_absorpt_correction_T_min 0.4644
_exptl_absorpt_correction_T_max 0.5476
```

#=====

7. EXPERIMENTAL DATA

```
_exptl_special_details
;
;
_diffn_ambient_temperature      100(1)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           'MoK\alpha'
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2006)).
;
_diffn_detector_area_resol_mean  66.06

_diffn_standards_number          0
_diffn_standards_interval_count  .
_diffn_standards_interval_time   .
_diffn_standards_decay_%         0

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?
```

number of measured reflections (redundant set)

```

_diffrn_reflms_number          34204
_diffrn_reflms_av_R_equivalents 0.0520
_diffrn_reflms_av_sigmaI/netI  0.0535
_diffrn_reflms_limit_h_min     -16
_diffrn_reflms_limit_h_max      16
_diffrn_reflms_limit_k_min     -20
_diffrn_reflms_limit_k_max      22
_diffrn_reflms_limit_l_min     -23
_diffrn_reflms_limit_l_max      22
_diffrn_reflms_theta_min       2.67
_diffrn_reflms_theta_max       26.37
_diffrn_measured_fraction_theta_max 0.998
_diffrn_reflms_theta_full      25.00
_diffrn_measured_fraction_theta_full 0.998

_diffrn_reflms_reduction_process
;
  Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to  $F_o^2$ 
  using SAINT-Plus & SADABS (Bruker, 2006).
;

# number of unique reflections
_reflms_number_total          8832
_reflms_number_gt             7374
_reflms_threshold_expression  I>2\sigma(I)

_computing_data_collection     'SMART (Bruker, 2006)'
_computing_cell_refinement     'SAINT-Plus (Bruker, 2006)'
_computing_data_reduction      'SAINT-Plus'
_computing_structure_solution
;
  DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
  PLATON (Spek, 2003)
  PLUTO (Meetsma, 2007)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 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
   $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is
  not relevant to the choice of reflections for refinement. R-factors based
  on  $F^2$  are statistically about twice as large as those based on F, and R-
  factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full

```



```

_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0468P)^2^+0.8703P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary    heavy
_atom_sites_solution_secondary  direct
_atom_sites_solution_hydrogens  geom
_refine_ls_hydrogen_treatment   constr
_refine_ls_extinction_method    none
_refine_ls_extinction_coef      ?
_refine_ls_abs_structure_details

```

```

;
  The absolute structure of the molecule actually chosen was
  determined by Flack's x-refinement.

```

(Flack & Bernardinelli, 1999, 2000)

```

;
_chemical_absolute_configuration  ad
_refine_ls_abs_structure_Flack    0.039(4)
_refine_ls_number_reflns         8832
_refine_ls_number_parameters     431
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0570
_refine_ls_R_factor_gt           0.0399
_refine_ls_wR_factor_ref         0.0906
_refine_ls_wR_factor_gt         0.0837
_refine_ls_goodness_of_fit_ref   1.023
_refine_ls_restrained_S_all     1.023
_refine_ls_shift/su_max          0.001
_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         0.619
_refine_diff_density_min        -0.418
_refine_diff_density_rms        0.063

_vrn_publ_code_void_volume       35.4
_vrn_publ_code_frame_time_sec    5.0
_vrn_publ_code_meas_time_hour    5.4

```

#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Y Y Uani 0.38700(2) 0.50855(1) 0.03285(2) 1.000 0.0191(1) . .
Si1 Si Uani 0.12559(5) 0.50930(5) -0.04072(4) 1.000 0.0239(3) . .
Si2 Si Uani 0.42713(7) 0.68977(5) 0.14185(5) 1.000 0.0296(3) . .
O O Uani 0.35889(18) 0.44369(12) 0.14061(13) 1.000 0.0369(8) . .
N1 N Uani 0.54079(17) 0.44035(13) 0.01939(13) 1.000 0.0196(8) . .
N2 N Uani 0.50510(18) 0.53433(13) -0.05742(13) 1.000 0.0194(8) . .
N3 N Uani 0.67026(18) 0.47590(14) -0.06530(14) 1.000 0.0238(8) . .

```

C1	C	Uani	0.6020(2)	0.38978(16)	0.06063(16)	1.000	0.0208(9)	. . .
C2	C	Uani	0.5850(2)	0.31088(17)	0.05188(17)	1.000	0.0269(10)	. . .
C3	C	Uani	0.6400(3)	0.26084(18)	0.0951(2)	1.000	0.0356(11)	. . .
C4	C	Uani	0.7079(3)	0.2863(2)	0.1450(2)	1.000	0.0388(11)	. . .
C5	C	Uani	0.7228(3)	0.3634(2)	0.1540(2)	1.000	0.0357(11)	. . .
C6	C	Uani	0.6692(2)	0.41646(18)	0.11333(18)	1.000	0.0279(10)	. . .
C7	C	Uani	0.5085(3)	0.28205(19)	-0.00225(19)	1.000	0.0350(11)	. . .
C8	C	Uani	0.4059(3)	0.26166(19)	0.0322(2)	1.000	0.0434(11)	. . .
C9	C	Uani	0.5497(3)	0.2147(2)	-0.0452(2)	1.000	0.0540(16)	. . .
C10	C	Uani	0.6827(2)	0.5005(2)	0.12786(18)	1.000	0.0355(11)	. . .
C11	C	Uani	0.7820(3)	0.5321(2)	0.0970(2)	1.000	0.0513(17)	. . .
C12	C	Uani	0.6801(3)	0.5197(2)	0.2068(2)	1.000	0.0463(14)	. . .
C13	C	Uani	0.5749(2)	0.48210(15)	-0.03518(16)	1.000	0.0187(8)	. . .
C14	C	Uani	0.7338(3)	0.40758(19)	-0.0617(2)	1.000	0.0363(11)	. . .
C15	C	Uani	0.7210(2)	0.54229(19)	-0.09721(19)	1.000	0.0293(11)	. . .
C16	C	Uani	0.5051(2)	0.56002(17)	-0.12920(17)	1.000	0.0223(10)	. . .
C17	C	Uani	0.5065(2)	0.63880(19)	-0.14328(19)	1.000	0.0295(10)	. . .
C18	C	Uani	0.5106(3)	0.6636(2)	-0.2129(2)	1.000	0.0390(11)	. . .
C19	C	Uani	0.5115(3)	0.6125(3)	-0.2687(2)	1.000	0.0470(14)	. . .
C20	C	Uani	0.5039(3)	0.5359(2)	-0.25510(19)	1.000	0.0390(13)	. . .
C21	C	Uani	0.4994(2)	0.50809(19)	-0.18609(16)	1.000	0.0275(10)	. . .
C22	C	Uani	0.5044(3)	0.69755(18)	-0.0844(2)	1.000	0.0327(11)	. . .
C23	C	Uani	0.6010(3)	0.74827(19)	-0.0852(2)	1.000	0.0442(13)	. . .
C24	C	Uani	0.4078(3)	0.7477(2)	-0.0896(2)	1.000	0.0473(14)	. . .
C25	C	Uani	0.4854(3)	0.4231(2)	-0.17616(19)	1.000	0.0387(12)	. . .
C26	C	Uani	0.3818(3)	0.3974(3)	-0.2078(2)	1.000	0.0600(16)	. . .
C27	C	Uani	0.5742(3)	0.3771(2)	-0.2093(2)	1.000	0.0527(16)	. . .
C28	C	Uani	0.2415(2)	0.45217(18)	-0.0238(2)	1.000	0.0318(10)	. . .
C29	C	Uani	0.0587(3)	0.5327(2)	0.0440(2)	1.000	0.0410(11)	. . .
C30	C	Uani	0.1657(3)	0.5995(2)	-0.0851(2)	1.000	0.0580(17)	. . .
C31	C	Uani	0.0265(3)	0.4658(2)	-0.1006(2)	1.000	0.0403(11)	. . .
C32	C	Uani	0.3500(2)	0.63201(17)	0.08081(18)	1.000	0.0273(10)	. . .
C33	C	Uani	0.3804(3)	0.79014(18)	0.1547(2)	1.000	0.0433(11)	. . .
C34	C	Uani	0.4277(3)	0.6431(2)	0.2313(2)	1.000	0.0443(12)	. . .
C35	C	Uani	0.5645(3)	0.69829(19)	0.1110(2)	1.000	0.0374(11)	. . .
C36	C	Uani	0.4220(3)	0.4060(3)	0.1927(2)	1.000	0.0550(16)	. . .
C37	C	Uani	0.3609(4)	0.3448(3)	0.2217(3)	1.000	0.074(2)	. . .
C38	C	Uani	0.2557(5)	0.3664(6)	0.2082(4)	1.000	0.187(5)	. . .
C39	C	Uani	0.2589(4)	0.4407(4)	0.1702(3)	1.000	0.111(3)	. . .
H3	H	Uiso	0.62998	0.20782	0.08953	1.000	0.0425	. . .
H4	H	Uiso	0.74482	0.25122	0.17354	1.000	0.0468	. . .
H5	H	Uiso	0.77047	0.38061	0.18854	1.000	0.0427	. . .
H7	H	Uiso	0.49513	0.32433	-0.03630	1.000	0.0419	. . .
H8	H	Uiso	0.41639	0.22061	0.06643	1.000	0.0648	. . .
H8'	H	Uiso	0.35717	0.24506	-0.00429	1.000	0.0648	. . .
H8''	H	Uiso	0.37806	0.30621	0.05665	1.000	0.0648	. . .
H9	H	Uiso	0.61381	0.22936	-0.06888	1.000	0.0810	. . .
H9'	H	Uiso	0.49853	0.19982	-0.08069	1.000	0.0810	. . .
H9''	H	Uiso	0.56302	0.17194	-0.01333	1.000	0.0810	. . .
H10	H	Uiso	0.62403	0.52773	0.10477	1.000	0.0424	. . .
H11	H	Uiso	0.78425	0.58703	0.10437	1.000	0.0769	. . .
H11'	H	Uiso	0.78464	0.52108	0.04617	1.000	0.0769	. . .
H11''	H	Uiso	0.84101	0.50837	0.12058	1.000	0.0769	. . .
H12	H	Uiso	0.61705	0.49915	0.22796	1.000	0.0694	. . .
H12'	H	Uiso	0.68140	0.57485	0.21292	1.000	0.0694	. . .
H12''	H	Uiso	0.74025	0.49731	0.23023	1.000	0.0694	. . .
H14	H	Uiso	0.77966	0.41069	-0.02063	1.000	0.0544	. . .
H14'	H	Uiso	0.77503	0.40330	-0.10502	1.000	0.0544	. . .
H14''	H	Uiso	0.68930	0.36296	-0.05718	1.000	0.0544	. . .
H15	H	Uiso	0.71502	0.53959	-0.14888	1.000	0.0439	. . .
H15'	H	Uiso	0.79398	0.54271	-0.08387	1.000	0.0439	. . .

H15" H Uiso 0.68788 0.58873 -0.08013 1.000 0.0439 . .
 H18 H Uiso 0.51284 0.71639 -0.22257 1.000 0.0469 . .
 H19 H Uiso 0.51734 0.63021 -0.31600 1.000 0.0563 . .
 H20 H Uiso 0.50175 0.50128 -0.29362 1.000 0.0468 . .
 H22 H Uiso 0.50226 0.67017 -0.03809 1.000 0.0390 . .
 H23 H Uiso 0.66251 0.71682 -0.07851 1.000 0.0664 . .
 H23' H Uiso 0.59649 0.78556 -0.04688 1.000 0.0664 . .
 H23" H Uiso 0.60559 0.77467 -0.13076 1.000 0.0664 . .
 H24 H Uiso 0.41158 0.77881 -0.13257 1.000 0.0708 . .
 H24' H Uiso 0.40384 0.78081 -0.04803 1.000 0.0708 . .
 H24" H Uiso 0.34628 0.71556 -0.09164 1.000 0.0708 . .
 H25 H Uiso 0.48417 0.41237 -0.12419 1.000 0.0464 . .
 H26 H Uiso 0.32579 0.42702 -0.18672 1.000 0.0900 . .
 H26' H Uiso 0.37115 0.34345 -0.19753 1.000 0.0900 . .
 H26" H Uiso 0.38254 0.40520 -0.25912 1.000 0.0900 . .
 H27 H Uiso 0.57066 0.38088 -0.26099 1.000 0.0785 . .
 H27' H Uiso 0.56802 0.32382 -0.19514 1.000 0.0785 . .
 H27" H Uiso 0.64026 0.39730 -0.19276 1.000 0.0785 . .
 H28 H Uiso 0.26516 0.43198 -0.06995 1.000 0.0383 . .
 H28' H Uiso 0.22028 0.40811 0.00519 1.000 0.0383 . .
 H29 H Uiso 0.03675 0.48578 0.06733 1.000 0.0618 . .
 H29' H Uiso -0.00170 0.56429 0.03408 1.000 0.0618 . .
 H29" H Uiso 0.10598 0.56038 0.07516 1.000 0.0618 . .
 H30 H Uiso 0.20108 0.63215 -0.05085 1.000 0.0870 . .
 H30' H Uiso 0.10471 0.62577 -0.10335 1.000 0.0870 . .
 H30" H Uiso 0.21246 0.58790 -0.12441 1.000 0.0870 . .
 H31 H Uiso 0.06011 0.44689 -0.14361 1.000 0.0603 . .
 H31' H Uiso -0.02486 0.50416 -0.11346 1.000 0.0603 . .
 H31" H Uiso -0.00747 0.42371 -0.07614 1.000 0.0603 . .
 H32 H Uiso 0.33840 0.66482 0.03904 1.000 0.0326 . .
 H32' H Uiso 0.28209 0.62670 0.10410 1.000 0.0326 . .
 H33 H Uiso 0.38101 0.81672 0.10909 1.000 0.0649 . .
 H33' H Uiso 0.42575 0.81646 0.18805 1.000 0.0649 . .
 H33" H Uiso 0.31002 0.78937 0.17349 1.000 0.0649 . .
 H34 H Uiso 0.35731 0.64126 0.24986 1.000 0.0662 . .
 H34' H Uiso 0.47137 0.67235 0.26363 1.000 0.0662 . .
 H34" H Uiso 0.45483 0.59149 0.22691 1.000 0.0662 . .
 H35 H Uiso 0.59003 0.64825 0.09683 1.000 0.0558 . .
 H35' H Uiso 0.60711 0.71816 0.14956 1.000 0.0558 . .
 H35" H Uiso 0.56777 0.73291 0.07045 1.000 0.0558 . .
 H36 H Uiso 0.44195 0.44192 0.23060 1.000 0.0658 . .
 H36' H Uiso 0.48533 0.38586 0.17046 1.000 0.0658 . .
 H37 H Uiso 0.37747 0.29626 0.19792 1.000 0.0887 . .
 H37' H Uiso 0.37340 0.33923 0.27311 1.000 0.0887 . .
 H38 H Uiso 0.21741 0.37152 0.25329 1.000 0.2240 . .
 H38' H Uiso 0.22098 0.32767 0.17870 1.000 0.2240 . .
 H39 H Uiso 0.20569 0.44271 0.13271 1.000 0.1333 . .
 H39' H Uiso 0.24775 0.48325 0.20347 1.000 0.1333 . .

loop_

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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

Y 0.0175(1) 0.0179(1) 0.0218(1) 0.0007(1) 0.0014(1) 0.0007(1)
 Si1 0.0219(4) 0.0230(4) 0.0269(5) -0.0001(4) -0.0016(3) 0.0015(3)
 Si2 0.0334(5) 0.0209(5) 0.0346(6) -0.0049(4) -0.0049(4) 0.0041(4)
 O 0.0437(15) 0.0307(13) 0.0362(15) 0.0123(11) 0.0169(12) 0.0071(10)

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N1 0.0212(12) 0.0171(12) 0.0206(16) 0.0036(11) 0.0014(11) 0.0006(9)
N2 0.0214(12) 0.0158(13) 0.0210(14) 0.0032(10) 0.0016(10) -0.0018(10)
N3 0.0221(13) 0.0233(15) 0.0261(14) 0.0049(11) 0.0042(11) 0.0009(10)
C1 0.0176(14) 0.0210(15) 0.0238(16) 0.0070(12) 0.0039(12) 0.0058(12)
C2 0.0287(16) 0.0249(17) 0.027(2) 0.0019(14) 0.0062(13) 0.0041(12)
C3 0.040(2) 0.0208(17) 0.046(2) 0.0099(16) 0.0105(17) 0.0111(14)
C4 0.0304(18) 0.038(2) 0.048(2) 0.0189(19) -0.0022(18) 0.0120(16)
C5 0.0250(17) 0.044(2) 0.038(2) 0.0140(18) -0.0099(16) -0.0002(15)
C6 0.0204(16) 0.0304(18) 0.033(2) 0.0101(15) -0.0017(14) 0.0015(13)
C7 0.055(2) 0.0209(17) 0.029(2) -0.0003(15) -0.0008(17) 0.0028(15)
C8 0.046(2) 0.0331(18) 0.051(2) -0.005(2) -0.012(2) -0.0020(15)
C9 0.084(3) 0.033(2) 0.045(3) -0.0113(19) 0.006(2) 0.003(2)
C10 0.0300(16) 0.0294(19) 0.047(2) 0.0061(18) -0.0156(14) -0.0060(16)
C11 0.061(3) 0.050(3) 0.043(3) 0.009(2) -0.011(2) -0.031(2)
C12 0.041(2) 0.041(2) 0.057(3) -0.004(2) -0.0020(18) -0.0067(17)
C13 0.0216(12) 0.0149(14) 0.0195(15) -0.0029(14) 0.0009(13) -0.0016(10)
C14 0.0320(18) 0.032(2) 0.045(2) -0.0009(17) 0.0166(16) 0.0102(15)
C15 0.0230(16) 0.0319(19) 0.033(2) 0.0065(16) 0.0030(15) -0.0030(14)
C16 0.0165(14) 0.0254(17) 0.0250(19) 0.0043(14) -0.0004(13) -0.0028(12)
C17 0.0193(15) 0.0352(19) 0.034(2) 0.0129(17) -0.0004(15) -0.0015(14)
C18 0.0311(19) 0.043(2) 0.043(2) 0.023(2) -0.0004(17) -0.0013(16)
C19 0.034(2) 0.076(3) 0.031(2) 0.024(2) -0.0033(17) -0.009(2)
C20 0.0320(18) 0.060(3) 0.025(2) 0.0039(18) -0.0016(15) -0.0117(17)
C21 0.0236(14) 0.0352(19) 0.0237(17) 0.0056(16) -0.0027(12) -0.0113(15)
C22 0.0320(18) 0.0221(18) 0.044(2) 0.0121(16) 0.0042(16) 0.0001(14)
C23 0.041(2) 0.0265(18) 0.065(3) 0.0026(18) 0.011(2) -0.0077(16)
C24 0.043(2) 0.035(2) 0.064(3) 0.0209(19) 0.014(2) 0.0090(17)
C25 0.054(2) 0.040(2) 0.022(2) -0.0059(16) 0.0082(17) -0.0200(18)
C26 0.072(3) 0.078(3) 0.030(2) -0.006(2) 0.001(2) -0.051(3)
C27 0.082(3) 0.036(2) 0.040(3) -0.0108(19) 0.014(2) -0.019(2)
C28 0.0239(16) 0.0246(17) 0.047(2) -0.0085(17) 0.0006(16) -0.0019(12)
C29 0.0299(17) 0.050(2) 0.043(2) -0.0119(19) 0.0067(17) 0.0065(15)
C30 0.057(3) 0.050(3) 0.067(3) 0.023(2) -0.016(2) -0.014(2)
C31 0.0309(18) 0.046(2) 0.044(2) -0.0094(18) -0.0133(17) 0.0050(16)
C32 0.0262(16) 0.0246(17) 0.031(2) -0.0011(15) 0.0023(14) 0.0008(13)
C33 0.050(2) 0.0270(18) 0.053(2) -0.0095(17) -0.013(2) 0.0095(18)
C34 0.052(2) 0.041(2) 0.040(2) -0.0063(19) 0.0012(19) 0.0113(18)
C35 0.041(2) 0.0231(18) 0.048(2) -0.0006(17) -0.0067(17) -0.0019(15)
C36 0.034(2) 0.103(4) 0.028(2) 0.015(2) 0.0034(17) -0.008(2)
C37 0.124(5) 0.057(3) 0.042(3) 0.024(2) -0.011(3) -0.001(3)
C38 0.071(4) 0.344(14) 0.145(7) 0.174(9) -0.022(5) -0.070(6)
C39 0.049(3) 0.211(7) 0.073(4) 0.079(4) 0.034(3) 0.055(4)

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10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's 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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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

Y	O	2.363 (2)	.	.	yes
Y	N1	2.345 (2)	.	.	yes
Y	N2	2.338 (2)	.	.	yes
Y	C13	2.796 (3)	.	.	yes
Y	C28	2.388 (3)	.	.	yes
Y	C32	2.407 (3)	.	.	yes
Si1	C28	1.839 (3)	.	.	yes
Si1	C29	1.867 (4)	.	.	yes
Si1	C30	1.872 (4)	.	.	yes
Si1	C31	1.877 (4)	.	.	yes
Si2	C32	1.836 (3)	.	.	yes
Si2	C33	1.887 (3)	.	.	yes
Si2	C34	1.879 (4)	.	.	yes
Si2	C35	1.882 (4)	.	.	yes
O	C36	1.443 (5)	.	.	yes
O	C39	1.414 (6)	.	.	yes
N1	C1	1.426 (4)	.	.	yes
N1	C13	1.342 (4)	.	.	yes
N2	C13	1.359 (4)	.	.	yes
N2	C16	1.430 (4)	.	.	yes
N3	C13	1.367 (4)	.	.	yes
N3	C14	1.462 (4)	.	.	yes
N3	C15	1.473 (4)	.	.	yes
C1	C2	1.419 (4)	.	.	no
C1	C6	1.405 (4)	.	.	no
C2	C3	1.398 (5)	.	.	no
C2	C7	1.513 (5)	.	.	no
C3	C4	1.366 (5)	.	.	no
C4	C5	1.384 (5)	.	.	no
C5	C6	1.396 (5)	.	.	no
C6	C10	1.518 (5)	.	.	no
C7	C8	1.525 (5)	.	.	no
C7	C9	1.535 (5)	.	.	no
C10	C11	1.521 (5)	.	.	no
C10	C12	1.529 (5)	.	.	no
C16	C17	1.415 (5)	.	.	no
C16	C21	1.414 (4)	.	.	no
C17	C18	1.387 (5)	.	.	no
C17	C22	1.520 (5)	.	.	no
C18	C19	1.387 (6)	.	.	no
C19	C20	1.379 (6)	.	.	no
C20	C21	1.394 (5)	.	.	no
C21	C25	1.522 (5)	.	.	no
C22	C23	1.541 (5)	.	.	no
C22	C24	1.538 (5)	.	.	no
C25	C26	1.540 (6)	.	.	no
C25	C27	1.542 (5)	.	.	no
C36	C37	1.447 (7)	.	.	no
C37	C38	1.441 (9)	.	.	no
C38	C39	1.495 (12)	.	.	no
C3	H3	0.9500	.	.	no
C4	H4	0.9500	.	.	no
C5	H5	0.9500	.	.	no
C7	H7	1.0000	.	.	no
C8	H8	0.9800	.	.	no
C8	H8'	0.9800	.	.	no
C8	H8''	0.9800	.	.	no
C9	H9	0.9800	.	.	no
C9	H9'	0.9800	.	.	no

C9	H9"	0.9800	.	.	no
C10	H10	1.0000	.	.	no
C11	H11	0.9800	.	.	no
C11	H11'	0.9800	.	.	no
C11	H11"	0.9800	.	.	no
C12	H12	0.9800	.	.	no
C12	H12'	0.9800	.	.	no
C12	H12"	0.9800	.	.	no
C14	H14	0.9800	.	.	no
C14	H14'	0.9800	.	.	no
C14	H14"	0.9800	.	.	no
C15	H15	0.9800	.	.	no
C15	H15'	0.9800	.	.	no
C15	H15"	0.9800	.	.	no
C18	H18	0.9500	.	.	no
C19	H19	0.9500	.	.	no
C20	H20	0.9500	.	.	no
C22	H22	1.0000	.	.	no
C23	H23	0.9800	.	.	no
C23	H23'	0.9800	.	.	no
C23	H23"	0.9800	.	.	no
C24	H24	0.9800	.	.	no
C24	H24'	0.9800	.	.	no
C24	H24"	0.9800	.	.	no
C25	H25	1.0000	.	.	no
C26	H26	0.9800	.	.	no
C26	H26'	0.9800	.	.	no
C26	H26"	0.9800	.	.	no
C27	H27	0.9800	.	.	no
C27	H27'	0.9800	.	.	no
C27	H27"	0.9800	.	.	no
C28	H28	0.9900	.	.	no
C28	H28'	0.9900	.	.	no
C29	H29	0.9800	.	.	no
C29	H29'	0.9800	.	.	no
C29	H29"	0.9800	.	.	no
C30	H30	0.9800	.	.	no
C30	H30'	0.9800	.	.	no
C30	H30"	0.9800	.	.	no
C31	H31	0.9800	.	.	no
C31	H31'	0.9800	.	.	no
C31	H31"	0.9800	.	.	no
C32	H32	0.9900	.	.	no
C32	H32'	0.9900	.	.	no
C33	H33	0.9800	.	.	no
C33	H33'	0.9800	.	.	no
C33	H33"	0.9800	.	.	no
C34	H34	0.9800	.	.	no
C34	H34'	0.9800	.	.	no
C34	H34"	0.9800	.	.	no
C35	H35	0.9800	.	.	no
C35	H35'	0.9800	.	.	no
C35	H35"	0.9800	.	.	no
C36	H36	0.9900	.	.	no
C36	H36'	0.9900	.	.	no
C37	H37	0.9900	.	.	no
C37	H37'	0.9900	.	.	no
C38	H38	0.9900	.	.	no
C38	H38'	0.9900	.	.	no
C39	H39	0.9900	.	.	no
C39	H39'	0.9900	.	.	no

loop_							
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O	Y	N1	88.66(8)	.	.	.	yes
O	Y	N2	145.45(8)	.	.	.	yes
O	Y	C13	116.73(8)	.	.	.	yes
O	Y	C28	93.57(10)	.	.	.	yes
O	Y	C32	94.76(10)	.	.	.	yes
N1	Y	N2	57.47(8)	.	.	.	yes
N1	Y	C13	28.57(8)	.	.	.	yes
N1	Y	C28	114.29(9)	.	.	.	yes
N1	Y	C32	132.45(9)	.	.	.	yes
N2	Y	C13	28.97(8)	.	.	.	yes
N2	Y	C28	105.84(10)	.	.	.	yes
N2	Y	C32	103.26(9)	.	.	.	yes
C13	Y	C28	114.50(10)	.	.	.	yes
C13	Y	C32	119.87(9)	.	.	.	yes
C28	Y	C32	112.80(10)	.	.	.	yes
C28	Si1	C29	110.66(17)	.	.	.	yes
C28	Si1	C30	108.41(16)	.	.	.	yes
C28	Si1	C31	116.21(16)	.	.	.	yes
C29	Si1	C30	108.99(16)	.	.	.	yes
C29	Si1	C31	106.74(17)	.	.	.	yes
C30	Si1	C31	105.56(17)	.	.	.	yes
C32	Si2	C33	115.22(15)	.	.	.	yes
C32	Si2	C34	108.89(16)	.	.	.	yes
C32	Si2	C35	111.51(15)	.	.	.	yes
C33	Si2	C34	107.25(17)	.	.	.	yes
C33	Si2	C35	105.64(16)	.	.	.	yes
C34	Si2	C35	108.03(17)	.	.	.	yes
Y	O	C36	136.3(2)	.	.	.	yes
Y	O	C39	120.0(3)	.	.	.	yes
C36	O	C39	103.6(3)	.	.	.	yes
Y	N1	C1	137.40(19)	.	.	.	yes
Y	N1	C13	94.75(16)	.	.	.	yes
C1	N1	C13	125.4(2)	.	.	.	yes
Y	N2	C13	94.59(17)	.	.	.	yes
Y	N2	C16	138.89(18)	.	.	.	yes
C13	N2	C16	120.5(2)	.	.	.	yes
C13	N3	C14	123.9(3)	.	.	.	yes
C13	N3	C15	120.8(2)	.	.	.	yes
C14	N3	C15	115.0(2)	.	.	.	yes
N1	C1	C2	117.6(2)	.	.	.	yes
N1	C1	C6	121.6(3)	.	.	.	yes
C2	C1	C6	120.5(3)	.	.	.	no
C1	C2	C3	118.1(3)	.	.	.	no
C1	C2	C7	120.7(3)	.	.	.	no
C3	C2	C7	121.2(3)	.	.	.	no
C2	C3	C4	121.7(3)	.	.	.	no
C3	C4	C5	119.9(3)	.	.	.	no
C4	C5	C6	121.4(3)	.	.	.	no
C1	C6	C5	118.3(3)	.	.	.	no
C1	C6	C10	121.8(3)	.	.	.	no
C5	C6	C10	119.8(3)	.	.	.	no

C2	C7	C8	111.4 (3)	.	.	.	no
C2	C7	C9	112.9 (3)	.	.	.	no
C8	C7	C9	110.3 (3)	.	.	.	no
C6	C10	C11	112.7 (3)	.	.	.	no
C6	C10	C12	113.0 (3)	.	.	.	no
C11	C10	C12	108.1 (3)	.	.	.	no
Y	C13	N1	56.68 (14)	.	.	.	yes
Y	C13	N2	56.44 (14)	.	.	.	yes
Y	C13	N3	174.1 (2)	.	.	.	yes
N1	C13	N2	112.9 (2)	.	.	.	yes
N1	C13	N3	125.1 (2)	.	.	.	yes
N2	C13	N3	122.0 (3)	.	.	.	yes
N2	C16	C17	119.3 (3)	.	.	.	yes
N2	C16	C21	121.0 (3)	.	.	.	yes
C17	C16	C21	119.6 (3)	.	.	.	no
C16	C17	C18	119.2 (3)	.	.	.	no
C16	C17	C22	122.1 (3)	.	.	.	no
C18	C17	C22	118.6 (3)	.	.	.	no
C17	C18	C19	121.1 (3)	.	.	.	no
C18	C19	C20	119.6 (4)	.	.	.	no
C19	C20	C21	121.5 (3)	.	.	.	no
C16	C21	C20	118.7 (3)	.	.	.	no
C16	C21	C25	123.4 (3)	.	.	.	no
C20	C21	C25	117.8 (3)	.	.	.	no
C17	C22	C23	112.0 (3)	.	.	.	no
C17	C22	C24	111.1 (3)	.	.	.	no
C23	C22	C24	109.2 (3)	.	.	.	no
C21	C25	C26	110.3 (3)	.	.	.	no
C21	C25	C27	112.3 (3)	.	.	.	no
C26	C25	C27	109.9 (3)	.	.	.	no
Y	C28	Si1	119.80 (16)	.	.	.	yes
Y	C32	Si2	129.02 (14)	.	.	.	yes
O	C36	C37	106.9 (3)	.	.	.	yes
C36	C37	C38	104.8 (5)	.	.	.	no
C37	C38	C39	106.9 (6)	.	.	.	no
O	C39	C38	104.4 (5)	.	.	.	yes
C2	C3	H3	119.00	.	.	.	no
C4	C3	H3	119.00	.	.	.	no
C3	C4	H4	120.00	.	.	.	no
C5	C4	H4	120.00	.	.	.	no
C4	C5	H5	119.00	.	.	.	no
C6	C5	H5	119.00	.	.	.	no
C2	C7	H7	107.00	.	.	.	no
C8	C7	H7	107.00	.	.	.	no
C9	C7	H7	107.00	.	.	.	no
C7	C8	H8	110.00	.	.	.	no
C7	C8	H8'	110.00	.	.	.	no
C7	C8	H8''	110.00	.	.	.	no
H8	C8	H8'	109.00	.	.	.	no
H8	C8	H8''	109.00	.	.	.	no
H8'	C8	H8''	109.00	.	.	.	no
C7	C9	H9	109.00	.	.	.	no
C7	C9	H9'	109.00	.	.	.	no
C7	C9	H9''	109.00	.	.	.	no
H9	C9	H9'	110.00	.	.	.	no
H9	C9	H9''	109.00	.	.	.	no
H9'	C9	H9''	109.00	.	.	.	no
C6	C10	H10	108.00	.	.	.	no
C11	C10	H10	108.00	.	.	.	no
C12	C10	H10	108.00	.	.	.	no
C10	C11	H11	109.00	.	.	.	no

C10	C11	H11'	109.00	.	.	.	no
C10	C11	H11"	109.00	.	.	.	no
H11	C11	H11'	110.00	.	.	.	no
H11	C11	H11"	110.00	.	.	.	no
H11'	C11	H11"	109.00	.	.	.	no
C10	C12	H12	110.00	.	.	.	no
C10	C12	H12'	110.00	.	.	.	no
C10	C12	H12"	109.00	.	.	.	no
H12	C12	H12'	109.00	.	.	.	no
H12	C12	H12"	109.00	.	.	.	no
H12'	C12	H12"	109.00	.	.	.	no
N3	C14	H14	109.00	.	.	.	no
N3	C14	H14'	109.00	.	.	.	no
N3	C14	H14"	109.00	.	.	.	no
H14	C14	H14'	109.00	.	.	.	no
H14	C14	H14"	110.00	.	.	.	no
H14'	C14	H14"	109.00	.	.	.	no
N3	C15	H15	109.00	.	.	.	no
N3	C15	H15'	109.00	.	.	.	no
N3	C15	H15"	109.00	.	.	.	no
H15	C15	H15'	109.00	.	.	.	no
H15	C15	H15"	109.00	.	.	.	no
H15'	C15	H15"	109.00	.	.	.	no
C17	C18	H18	120.00	.	.	.	no
C19	C18	H18	119.00	.	.	.	no
C18	C19	H19	120.00	.	.	.	no
C20	C19	H19	120.00	.	.	.	no
C19	C20	H20	119.00	.	.	.	no
C21	C20	H20	119.00	.	.	.	no
C17	C22	H22	108.00	.	.	.	no
C23	C22	H22	108.00	.	.	.	no
C24	C22	H22	108.00	.	.	.	no
C22	C23	H23	109.00	.	.	.	no
C22	C23	H23'	110.00	.	.	.	no
C22	C23	H23"	110.00	.	.	.	no
H23	C23	H23'	109.00	.	.	.	no
H23	C23	H23"	109.00	.	.	.	no
H23'	C23	H23"	109.00	.	.	.	no
C22	C24	H24	109.00	.	.	.	no
C22	C24	H24'	110.00	.	.	.	no
C22	C24	H24"	110.00	.	.	.	no
H24	C24	H24'	109.00	.	.	.	no
H24	C24	H24"	109.00	.	.	.	no
H24'	C24	H24"	109.00	.	.	.	no
C21	C25	H25	108.00	.	.	.	no
C26	C25	H25	108.00	.	.	.	no
C27	C25	H25	108.00	.	.	.	no
C25	C26	H26	109.00	.	.	.	no
C25	C26	H26'	109.00	.	.	.	no
C25	C26	H26"	110.00	.	.	.	no
H26	C26	H26'	109.00	.	.	.	no
H26	C26	H26"	110.00	.	.	.	no
H26'	C26	H26"	109.00	.	.	.	no
C25	C27	H27	109.00	.	.	.	no
C25	C27	H27'	109.00	.	.	.	no
C25	C27	H27"	109.00	.	.	.	no
H27	C27	H27'	109.00	.	.	.	no
H27	C27	H27"	110.00	.	.	.	no
H27'	C27	H27"	109.00	.	.	.	no
Y	C28	H28	107.00	.	.	.	no
Y	C28	H28'	107.00	.	.	.	no

Si1	C28	H28	107.00	.	.	.	no
Si1	C28	H28'	107.00	.	.	.	no
H28	C28	H28'	107.00	.	.	.	no
Si1	C29	H29	110.00	.	.	.	no
Si1	C29	H29'	110.00	.	.	.	no
Si1	C29	H29"	109.00	.	.	.	no
H29	C29	H29'	109.00	.	.	.	no
H29	C29	H29"	109.00	.	.	.	no
H29'	C29	H29"	109.00	.	.	.	no
Si1	C30	H30	110.00	.	.	.	no
Si1	C30	H30'	110.00	.	.	.	no
Si1	C30	H30"	110.00	.	.	.	no
H30	C30	H30'	109.00	.	.	.	no
H30	C30	H30"	109.00	.	.	.	no
H30'	C30	H30"	109.00	.	.	.	no
Si1	C31	H31	109.00	.	.	.	no
Si1	C31	H31'	109.00	.	.	.	no
Si1	C31	H31"	110.00	.	.	.	no
H31	C31	H31'	109.00	.	.	.	no
H31	C31	H31"	109.00	.	.	.	no
H31'	C31	H31"	109.00	.	.	.	no
Y	C32	H32	105.00	.	.	.	no
Y	C32	H32'	105.00	.	.	.	no
Si2	C32	H32	105.00	.	.	.	no
Si2	C32	H32'	105.00	.	.	.	no
H32	C32	H32'	106.00	.	.	.	no
Si2	C33	H33	109.00	.	.	.	no
Si2	C33	H33'	110.00	.	.	.	no
Si2	C33	H33"	109.00	.	.	.	no
H33	C33	H33'	109.00	.	.	.	no
H33	C33	H33"	109.00	.	.	.	no
H33'	C33	H33"	110.00	.	.	.	no
Si2	C34	H34	109.00	.	.	.	no
Si2	C34	H34'	109.00	.	.	.	no
Si2	C34	H34"	109.00	.	.	.	no
H34	C34	H34'	110.00	.	.	.	no
H34	C34	H34"	110.00	.	.	.	no
H34'	C34	H34"	110.00	.	.	.	no
Si2	C35	H35	109.00	.	.	.	no
Si2	C35	H35'	109.00	.	.	.	no
Si2	C35	H35"	109.00	.	.	.	no
H35	C35	H35'	110.00	.	.	.	no
H35	C35	H35"	109.00	.	.	.	no
H35'	C35	H35"	109.00	.	.	.	no
O	C36	H36	110.00	.	.	.	no
O	C36	H36'	110.00	.	.	.	no
C37	C36	H36	110.00	.	.	.	no
C37	C36	H36'	110.00	.	.	.	no
H36	C36	H36'	109.00	.	.	.	no
C36	C37	H37	111.00	.	.	.	no
C36	C37	H37'	111.00	.	.	.	no
C38	C37	H37	111.00	.	.	.	no
C38	C37	H37'	111.00	.	.	.	no
H37	C37	H37'	109.00	.	.	.	no
C37	C38	H38	110.00	.	.	.	no
C37	C38	H38'	110.00	.	.	.	no
C39	C38	H38	110.00	.	.	.	no
C39	C38	H38'	110.00	.	.	.	no
H38	C38	H38'	109.00	.	.	.	no
O	C39	H39	111.00	.	.	.	no
O	C39	H39'	111.00	.	.	.	no

C38	C39	H39	111.00	.	.	.	no
C38	C39	H39'	111.00	.	.	.	no
H39	C39	H39'	109.00	.	.	.	no

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N1	Y	O	C36	24.4 (3)	.	.	.	.	no
N1	Y	O	C39	-160.7 (3)	.	.	.	.	no
N2	Y	O	C36	13.7 (4)	.	.	.	.	no
N2	Y	O	C39	-171.4 (3)	.	.	.	.	no
C13	Y	O	C36	18.9 (4)	.	.	.	.	no
C13	Y	O	C39	-166.2 (3)	.	.	.	.	no
C28	Y	O	C36	138.7 (3)	.	.	.	.	no
C28	Y	O	C39	-46.4 (3)	.	.	.	.	no
C32	Y	O	C36	-108.1 (3)	.	.	.	.	no
C32	Y	O	C39	66.8 (3)	.	.	.	.	no
O	Y	N1	C1	-8.1 (3)	.	.	.	.	no
O	Y	N1	C13	-169.65 (17)	.	.	.	.	no
N2	Y	N1	C1	164.7 (3)	.	.	.	.	no
N2	Y	N1	C13	3.18 (15)	.	.	.	.	no
C13	Y	N1	C1	161.5 (4)	.	.	.	.	no
C28	Y	N1	C1	-101.4 (3)	.	.	.	.	no
C28	Y	N1	C13	97.04 (18)	.	.	.	.	no
C32	Y	N1	C1	87.1 (3)	.	.	.	.	no
C32	Y	N1	C13	-74.4 (2)	.	.	.	.	no
O	Y	N2	C13	9.6 (2)	.	.	.	.	no
O	Y	N2	C16	159.7 (2)	.	.	.	.	no
N1	Y	N2	C13	-3.14 (15)	.	.	.	.	no
N1	Y	N2	C16	147.0 (3)	.	.	.	.	no
C13	Y	N2	C16	150.1 (4)	.	.	.	.	no
C28	Y	N2	C13	-112.17 (17)	.	.	.	.	no
C28	Y	N2	C16	38.0 (3)	.	.	.	.	no
C32	Y	N2	C13	129.09 (17)	.	.	.	.	no
C32	Y	N2	C16	-80.8 (3)	.	.	.	.	no
O	Y	C13	N1	11.60 (19)	.	.	.	.	no
O	Y	C13	N2	-173.94 (15)	.	.	.	.	no
N1	Y	C13	N2	174.5 (3)	.	.	.	.	no
N2	Y	C13	N1	-174.5 (3)	.	.	.	.	no
C28	Y	C13	N1	-96.22 (18)	.	.	.	.	no
C28	Y	C13	N2	78.24 (18)	.	.	.	.	no
C32	Y	C13	N1	124.94 (17)	.	.	.	.	no
C32	Y	C13	N2	-60.59 (19)	.	.	.	.	no
O	Y	C28	Si1	107.31 (19)	.	.	.	.	no
N1	Y	C28	Si1	-162.56 (16)	.	.	.	.	no
N2	Y	C28	Si1	-101.59 (19)	.	.	.	.	no
C13	Y	C28	Si1	-131.12 (17)	.	.	.	.	no
C32	Y	C28	Si1	10.6 (2)	.	.	.	.	no
O	Y	C32	Si2	71.9 (2)	.	.	.	.	no
N1	Y	C32	Si2	-20.6 (3)	.	.	.	.	no
N2	Y	C32	Si2	-78.4 (2)	.	.	.	.	no
C13	Y	C32	Si2	-52.7 (2)	.	.	.	.	no
C28	Y	C32	Si2	167.81 (19)	.	.	.	.	no

C29	Si1	C28	Y	-69.6 (2)	.	.	.	.	no
C30	Si1	C28	Y	49.9 (2)	.	.	.	.	no
C31	Si1	C28	Y	168.52 (17)	.	.	.	.	no
C33	Si2	C32	Y	170.42 (18)	.	.	.	.	no
C34	Si2	C32	Y	-69.1 (2)	.	.	.	.	no
C35	Si2	C32	Y	50.0 (2)	.	.	.	.	no
Y	O	C36	C37	-148.2 (3)	.	.	.	.	no
C39	O	C36	C37	36.4 (5)	.	.	.	.	no
Y	O	C39	C38	148.9 (4)	.	.	.	.	no
C36	O	C39	C38	-34.7 (5)	.	.	.	.	no
Y	N1	C1	C2	94.1 (3)	.	.	.	.	no
Y	N1	C1	C6	-79.5 (3)	.	.	.	.	no
C13	N1	C1	C2	-108.7 (3)	.	.	.	.	no
C13	N1	C1	C6	77.7 (4)	.	.	.	.	no
Y	N1	C13	N2	-5.0 (2)	.	.	.	.	no
Y	N1	C13	N3	173.2 (3)	.	.	.	.	no
C1	N1	C13	Y	-164.8 (3)	.	.	.	.	no
C1	N1	C13	N2	-169.8 (3)	.	.	.	.	no
C1	N1	C13	N3	8.5 (4)	.	.	.	.	no
Y	N2	C13	N1	5.0 (2)	.	.	.	.	no
Y	N2	C13	N3	-173.3 (2)	.	.	.	.	no
C16	N2	C13	Y	-157.7 (3)	.	.	.	.	no
C16	N2	C13	N1	-152.6 (2)	.	.	.	.	no
C16	N2	C13	N3	29.1 (4)	.	.	.	.	no
Y	N2	C16	C17	86.8 (3)	.	.	.	.	no
Y	N2	C16	C21	-90.6 (3)	.	.	.	.	no
C13	N2	C16	C17	-128.4 (3)	.	.	.	.	no
C13	N2	C16	C21	54.3 (4)	.	.	.	.	no
C14	N3	C13	N1	23.6 (5)	.	.	.	.	no
C14	N3	C13	N2	-158.3 (3)	.	.	.	.	no
C15	N3	C13	N1	-149.3 (3)	.	.	.	.	no
C15	N3	C13	N2	28.8 (4)	.	.	.	.	no
N1	C1	C2	C3	-176.2 (3)	.	.	.	.	no
N1	C1	C2	C7	3.2 (4)	.	.	.	.	no
C6	C1	C2	C3	-2.5 (4)	.	.	.	.	no
C6	C1	C2	C7	176.8 (3)	.	.	.	.	no
N1	C1	C6	C5	176.8 (3)	.	.	.	.	no
N1	C1	C6	C10	-1.8 (4)	.	.	.	.	no
C2	C1	C6	C5	3.5 (4)	.	.	.	.	no
C2	C1	C6	C10	-175.1 (3)	.	.	.	.	no
C1	C2	C3	C4	0.5 (5)	.	.	.	.	no
C7	C2	C3	C4	-178.8 (3)	.	.	.	.	no
C1	C2	C7	C8	-99.5 (3)	.	.	.	.	no
C1	C2	C7	C9	135.8 (3)	.	.	.	.	no
C3	C2	C7	C8	79.9 (4)	.	.	.	.	no
C3	C2	C7	C9	-44.9 (4)	.	.	.	.	no
C2	C3	C4	C5	0.5 (6)	.	.	.	.	no
C3	C4	C5	C6	0.4 (6)	.	.	.	.	no
C4	C5	C6	C1	-2.4 (5)	.	.	.	.	no
C4	C5	C6	C10	176.2 (3)	.	.	.	.	no
C1	C6	C10	C11	-102.8 (3)	.	.	.	.	no
C1	C6	C10	C12	134.2 (3)	.	.	.	.	no
C5	C6	C10	C11	78.6 (4)	.	.	.	.	no
C5	C6	C10	C12	-44.4 (4)	.	.	.	.	no
N2	C16	C17	C18	177.5 (3)	.	.	.	.	no
N2	C16	C17	C22	-2.1 (4)	.	.	.	.	no
C21	C16	C17	C18	-5.1 (4)	.	.	.	.	no
C21	C16	C17	C22	175.3 (3)	.	.	.	.	no
N2	C16	C21	C20	-177.4 (3)	.	.	.	.	no
N2	C16	C21	C25	4.4 (4)	.	.	.	.	no
C17	C16	C21	C20	5.3 (4)	.	.	.	.	no

C17	C16	C21	C25	-172.9 (3)	.	.	.	.	no
C16	C17	C18	C19	1.2 (5)	.	.	.	.	no
C22	C17	C18	C19	-179.3 (3)	.	.	.	.	no
C16	C17	C22	C23	119.2 (3)	.	.	.	.	no
C16	C17	C22	C24	-118.3 (3)	.	.	.	.	no
C18	C17	C22	C23	-60.3 (4)	.	.	.	.	no
C18	C17	C22	C24	62.1 (4)	.	.	.	.	no
C17	C18	C19	C20	2.7 (6)	.	.	.	.	no
C18	C19	C20	C21	-2.6 (6)	.	.	.	.	no
C19	C20	C21	C16	-1.4 (5)	.	.	.	.	no
C19	C20	C21	C25	176.9 (3)	.	.	.	.	no
C16	C21	C25	C26	115.8 (3)	.	.	.	.	no
C16	C21	C25	C27	-121.3 (3)	.	.	.	.	no
C20	C21	C25	C26	-62.4 (4)	.	.	.	.	no
C20	C21	C25	C27	60.5 (4)	.	.	.	.	no
O	C36	C37	C38	-22.4 (6)	.	.	.	.	no
C36	C37	C38	C39	0.6 (7)	.	.	.	.	no
C37	C38	C39	O	21.5 (7)	.	.	.	.	no

loop_

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Y	C7	4.346 (3)	.	.	.	no
Y	C8	4.361 (3)	.	.	.	no
Y	C10	4.240 (3)	.	.	.	no
Y	C22	4.282 (3)	.	.	.	no
Y	C25	4.414 (4)	.	.	.	no
Y	H7	3.7700	.	.	.	no
Y	H8"	3.6000	.	.	.	no
Y	H10	3.3800	.	.	.	no
Y	H22	3.4900	.	.	.	no
Y	H25	3.6400	.	.	.	no
Y	H29"	3.8400	.	.	.	no
Y	H30	3.6200	.	.	.	no
Y	H35	3.8100	.	.	.	no
Si1	H9"	3.4500	.	3_455	.	no
O	H8"	2.9100	.	.	.	no
N1	N2	2.251 (3)	.	.	.	no
N1	N3	2.404 (3)	.	.	.	no
N2	N1	2.251 (3)	.	.	.	no
N2	N3	2.384 (3)	.	.	.	no
N3	N2	2.384 (3)	.	.	.	no
N3	C25	3.318 (4)	.	.	.	no
N3	N1	2.404 (3)	.	.	.	no
N3	C21	3.232 (4)	.	.	.	no
N1	H10	2.4800	.	.	.	no
N1	H7	2.3800	.	.	.	no
N1	H25	2.8500	.	.	.	no
N1	H14"	2.7700	.	.	.	no
N2	H22	2.4200	.	.	.	no
N2	H25	2.5100	.	.	.	no
N2	H15"	2.6000	.	.	.	no
N3	H11'	2.7000	.	.	.	no
N3	H25	2.8900	.	.	.	no
N3	H27"	2.8100	.	.	.	no
C1	C14	2.892 (5)	.	.	.	no
C1	C36	3.430 (5)	.	.	.	no

C2	C14	3.353 (5)	.	.	no
C6	C14	3.414 (5)	.	.	no
C6	C36	3.547 (5)	.	.	no
C7	Y	4.346 (3)	.	.	no
C8	Y	4.361 (3)	.	.	no
C10	C13	3.398 (4)	.	.	no
C10	Y	4.240 (3)	.	.	no
C13	C10	3.398 (4)	.	.	no
C13	C16	2.421 (4)	.	.	no
C13	C25	3.086 (5)	.	.	no
C13	C1	2.460 (4)	.	.	no
C14	C2	3.353 (5)	.	.	no
C14	C1	2.892 (5)	.	.	no
C14	C6	3.414 (5)	.	.	no
C14	C27	3.515 (5)	.	.	no
C15	C17	3.378 (4)	.	.	no
C15	C21	3.385 (4)	.	.	no
C15	C16	2.884 (4)	.	.	no
C16	C15	2.884 (4)	.	.	no
C17	C15	3.378 (4)	.	.	no
C19	C38	3.516 (8)	.	2_564	no
C21	C15	3.385 (4)	.	.	no
C21	N3	3.232 (4)	.	.	no
C22	Y	4.282 (3)	.	.	no
C25	C13	3.086 (5)	.	.	no
C25	N3	3.318 (4)	.	.	no
C25	Y	4.414 (4)	.	.	no
C27	C14	3.515 (5)	.	.	no
C36	C1	3.430 (5)	.	.	no
C36	C6	3.547 (5)	.	.	no
C38	C19	3.516 (8)	.	2_565	no
C1	H14	2.7900	.	.	no
C1	H14"	2.5400	.	.	no
C1	H36'	2.5700	.	.	no
C2	H14"	2.6300	.	.	no
C2	H36'	2.9100	.	.	no
C3	H8	3.0400	.	.	no
C3	H9"	2.7700	.	.	no
C5	H12	3.0900	.	.	no
C5	H12"	2.7800	.	.	no
C5	H11"	3.0500	.	.	no
C6	H14	2.9100	.	.	no
C6	H36'	2.6700	.	.	no
C7	H14"	2.9400	.	.	no
C9	H3	2.7500	.	.	no
C10	H35	2.9300	.	.	no
C11	H14	3.0900	.	.	no
C12	H5	2.7400	.	.	no
C13	H25	2.3900	.	.	no
C13	H7	2.9700	.	.	no
C13	H10	2.8400	.	.	no
C14	H27"	2.7600	.	.	no
C14	H11'	2.9300	.	.	no
C15	H11'	2.8600	.	.	no
C16	H15"	2.6000	.	.	no
C16	H15	2.7700	.	.	no
C17	H15"	2.7800	.	.	no
C18	H24	2.8400	.	.	no
C18	H38	3.0900	.	2_564	no
C18	H23"	2.7900	.	.	no
C19	H5	2.9500	.	2_664	no

C19	H38	3.0100	.	2_564	no
C20	H27	2.8700	.	.	no
C20	H26"	2.7900	.	.	no
C21	H15	2.9400	.	.	no
C22	H15"	3.0600	.	.	no
C23	H35"	2.9800	.	.	no
C23	H15"	3.0300	.	.	no
C23	H18	2.8900	.	.	no
C24	H32	2.9800	.	.	no
C24	H18	2.9100	.	.	no
C26	H28	3.0700	.	.	no
C26	H20	2.9000	.	.	no
C27	H20	2.8700	.	.	no
C28	H39	3.0000	.	.	no
C29	H39	2.9900	.	.	no
C30	H37'	2.9300	.	2_564	no
C32	H22	3.0700	.	.	no
C34	H31	2.8500	.	2_565	no
C35	H22	2.9700	.	.	no
C36	H12	3.0900	.	.	no
H3	C9	2.7500	.	.	no
H3	H9"	2.2200	.	.	no
H4	H26'	2.3800	.	3_555	no
H5	C12	2.7400	.	.	no
H5	H12"	2.2400	.	.	no
H5	C19	2.9500	.	2_665	no
H7	Y	3.7700	.	.	no
H7	N1	2.3800	.	.	no
H7	C13	2.9700	.	.	no
H7	H25	2.2800	.	.	no
H8	C3	3.0400	.	.	no
H8	H9"	2.5700	.	.	no
H8'	H9'	2.4700	.	.	no
H8"	Y	3.6000	.	.	no
H8"	O	2.9100	.	.	no
H9	H14"	2.5600	.	.	no
H9'	H8'	2.4700	.	.	no
H9'	H19	2.3100	.	4_644	no
H9"	C3	2.7700	.	.	no
H9"	H3	2.2200	.	.	no
H9"	H8	2.5700	.	.	no
H9"	Si1	3.4500	.	3_555	no
H9"	H28'	2.4900	.	3_555	no
H9"	H31"	2.5600	.	3_555	no
H10	Y	3.3800	.	.	no
H10	N1	2.4800	.	.	no
H10	C13	2.8400	.	.	no
H10	H35	2.1800	.	.	no
H11	H12'	2.4600	.	.	no
H11'	N3	2.7000	.	.	no
H11'	C14	2.9300	.	.	no
H11'	C15	2.8600	.	.	no
H11'	H14	2.3200	.	.	no
H11'	H15'	2.4900	.	.	no
H11"	C5	3.0500	.	.	no
H11"	H12"	2.4600	.	.	no
H12	C5	3.0900	.	.	no
H12	C36	3.0900	.	.	no
H12	H36	2.4900	.	.	no
H12'	H11	2.4600	.	.	no
H12"	C5	2.7800	.	.	no

H12"	H5	2.2400	.	.	no
H12"	H11"	2.4600	.	.	no
H12"	H15	2.4400	.	2_665	no
H14	C1	2.7900	.	.	no
H14	C6	2.9100	.	.	no
H14	C11	3.0900	.	.	no
H14	H11'	2.3200	.	.	no
H14'	H15'	2.5000	.	.	no
H14'	H27"	2.4100	.	.	no
H14"	N1	2.7700	.	.	no
H14"	C1	2.5400	.	.	no
H14"	C2	2.6300	.	.	no
H14"	C7	2.9400	.	.	no
H14"	H9	2.5600	.	.	no
H15	C16	2.7700	.	.	no
H15	C21	2.9400	.	.	no
H15	H12"	2.4400	.	2_664	no
H15'	H11'	2.4900	.	.	no
H15'	H14'	2.5000	.	.	no
H15'	H31'	2.5100	.	1_655	no
H15"	N2	2.6000	.	.	no
H15"	C16	2.6000	.	.	no
H15"	C17	2.7800	.	.	no
H15"	C22	3.0600	.	.	no
H15"	C23	3.0300	.	.	no
H15"	H23	2.2800	.	.	no
H18	C23	2.8900	.	.	no
H18	C24	2.9100	.	.	no
H18	H23"	2.3500	.	.	no
H18	H24	2.4100	.	.	no
H19	H9'	2.3100	.	4_654	no
H20	C26	2.9000	.	.	no
H20	C27	2.8700	.	.	no
H20	H26"	2.3900	.	.	no
H20	H27	2.3900	.	.	no
H22	Y	3.4900	.	.	no
H22	N2	2.4200	.	.	no
H22	C32	3.0700	.	.	no
H22	C35	2.9700	.	.	no
H22	H32	2.5800	.	.	no
H22	H35"	2.4800	.	.	no
H23	H15"	2.2800	.	.	no
H23'	H24'	2.5000	.	.	no
H23'	H35"	2.4300	.	.	no
H23"	C18	2.7900	.	.	no
H23"	H18	2.3500	.	.	no
H23"	H24	2.5200	.	.	no
H24	C18	2.8400	.	.	no
H24	H18	2.4100	.	.	no
H24	H23"	2.5200	.	.	no
H24'	H23'	2.5000	.	.	no
H24"	H30	2.5100	.	.	no
H25	Y	3.6400	.	.	no
H25	N1	2.8500	.	.	no
H25	N2	2.5100	.	.	no
H25	N3	2.8900	.	.	no
H25	C13	2.3900	.	.	no
H25	H7	2.2800	.	.	no
H26	H28	2.3400	.	.	no
H26'	H27'	2.5800	.	.	no
H26'	H4	2.3800	.	3_455	no

H26"	C20	2.7900	.	.	no
H26"	H20	2.3900	.	.	no
H26"	H27	2.4800	.	.	no
H27	C20	2.8700	.	.	no
H27	H20	2.3900	.	.	no
H27	H26"	2.4800	.	.	no
H27'	H26'	2.5800	.	.	no
H27"	N3	2.8100	.	.	no
H27"	C14	2.7600	.	.	no
H27"	H14'	2.4100	.	.	no
H28	C26	3.0700	.	.	no
H28	H26	2.3400	.	.	no
H28'	H39	2.4900	.	.	no
H28'	H9"	2.4900	.	3_455	no
H29"	Y	3.8400	.	.	no
H30	Y	3.6200	.	.	no
H30	H24"	2.5100	.	.	no
H30	H32	2.5300	.	.	no
H30'	H37'	2.4300	.	2_564	no
H30"	H37'	2.5800	.	2_564	no
H30"	H38	2.5800	.	2_564	no
H31	C34	2.8500	.	2_564	no
H31	H34"	2.5400	.	2_564	no
H31'	H15'	2.5100	.	1_455	no
H31"	H9"	2.5600	.	3_455	no
H32	C24	2.9800	.	.	no
H32	H22	2.5800	.	.	no
H32	H30	2.5300	.	.	no
H34"	H31	2.5400	.	2_565	no
H35	Y	3.8100	.	.	no
H35	C10	2.9300	.	.	no
H35	H10	2.1800	.	.	no
H35'	H37'	2.6000	.	4_655	no
H35"	C23	2.9800	.	.	no
H35"	H22	2.4800	.	.	no
H35"	H23'	2.4300	.	.	no
H36	H12	2.4900	.	.	no
H36'	C1	2.5700	.	.	no
H36'	C2	2.9100	.	.	no
H36'	C6	2.6700	.	.	no
H37'	C30	2.9300	.	2_565	no
H37'	H30'	2.4300	.	2_565	no
H37'	H30"	2.5800	.	2_565	no
H37'	H35'	2.6000	.	4_645	no
H38	C18	3.0900	.	2_565	no
H38	C19	3.0100	.	2_565	no
H38	H30"	2.5800	.	2_565	no
H39	C28	3.0000	.	.	no
H39	C29	2.9900	.	.	no
H39	H28'	2.4900	.	.	no

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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

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#
#D   H   A   D - H   H...A   D...A   D - H...A   symm(A)
#
C7      H7      N1      1.0000      2.3800      2.853(4)      108.00      .   yes
C10     H10     N1      1.0000      2.4800      2.952(4)      108.00      .   yes
C22     H22     N2      1.0000      2.4200      2.924(4)      110.00      .   yes
C25     H25     N2      1.0000      2.5100      2.991(4)      109.00      .   yes

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#===END of Crystallographic Information File

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