

University of Groningen

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

Ge, Shaozhong; Meetsma, Auke; Hessen, Bart

Published in:
Organometallics

DOI:
[10.1021/om800032g](https://doi.org/10.1021/om800032g)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2008

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Ge, S., Meetsma, A., & Hessen, B. (2008). Highly efficient hydrosilylation of alkenes by organoyttrium catalysts with sterically demanding amidinate and guanidinate ligands. *Organometallics*, 27(13), 3131-3135. <https://doi.org/10.1021/om800032g>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

CIF-file generated for C39H70N3OSi2Y P212121 q1321

data_DATNAM

0. AUDIT DETAILS

_audit_creation_date '2007-10-09 15:03:02'

_audit_creation_method

;

PLATON <TABLE ACC> option (version :: 250307)

SHELXL97-2 & Manual Editing

;

_audit_update_record

;

?

;

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 choice 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)

;

2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic ?

_journal_date_to_coeditor ?

```

_journal_date_from_coeditor      ?
_journal_date_accepted           ?

_journal_date_printers_first     ?
_journal_date_printers_final     ?
_journal_date_proofs_out         ?
_journal_date_proofs_in         ?

_journal_coeditor_name           ?
_journal_coeditor_code           ?
_journal_coeditor_notes         ;
;

_journal_techeditor_code         ?
_journal_techeditor_notes       ;
;

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

_journal_suppl_publ_number      ?
_journal_suppl_publ_pages       ?

```

```

#=====

```

```

# 3. TITLE AND AUTHOR LIST

```

```

_publ_section_title
;
;
_publ_section_title_footnote
;
;

```

```

# The loop structure below should contain the names and 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.

Beurskens, P.T., Beurskens, G., Gelder, R. de, Garcia-Granda, S., Gould, R.O., Israel, R. & Smits, J.M.M. (1999).

The DIRDIF99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

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

Bruker, (2006). SMART (Version 5.632), SAINT-Plus (Version 6.45) and

SADABS (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Flack, H.D. & Bernardinelli, G. (1999). Acta Cryst. A55, 908-915.

Flack, H.D. & Bernardinelli, G. (2000). J. Appl. Cryst. 33, 1143-1148.

Hahn, T. (1983). Ed. International Tables for Crystallography, Volume A, Space-group symmetry, Kluwer Academic Publishers, Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2007). Extended version of the program PLUTO. University of Groningen, The Netherlands. (unpublished).

Sheldrick, G.M. (1997). SHELXL-97. Program for Crystal Structure Refinement. University of Göttingen, Germany.

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

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

Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.

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)

```

_diffirn_reflms_number          34204
_diffirn_reflms_av_R_equivalents 0.0520
_diffirn_reflms_av_sigmaI/netI  0.0535
_diffirn_reflms_limit_h_min     -16
_diffirn_reflms_limit_h_max     16
_diffirn_reflms_limit_k_min     -20
_diffirn_reflms_limit_k_max     22
_diffirn_reflms_limit_l_min     -23
_diffirn_reflms_limit_l_max     22
_diffirn_reflms_theta_min       2.67
_diffirn_reflms_theta_max       26.37
_diffirn_measured_fraction_theta_max 0.998
_diffirn_reflms_theta_full      25.00
_diffirn_measured_fraction_theta_full 0.998

```

```
_diffirn_reflms_reduction_process
```

```

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

```

```

# number of unique reflections
_reflms_number_total          8832
_reflms_number_gt             7374
_reflms_threshold_expression  I>2\|s(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_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

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)

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)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

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

;

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_
_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
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 |

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

| | | | | | | | | | |
|-----|---|-----|-----|--------------|---|---|---|---|----|
| 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_

_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

| | | | | | | | | |
|-----|------|-----------|---|-------|---|---|---|----|
| 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 |

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      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

```

#===END of Crystallographic Information File